SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-470	2. Software Title and Version: TPA 5.0s	3. Project No: 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): reader.f

The TPA automatically generates a tpameans.out file that contains the mean values of each parameter distribution in a format suitable for submission as a valid input file for TPA. It is desired that two additional files be generated in the same manner such that one contains the minimum values and one the maximum values of each parameter distribution. The file names should be tpamin.out and tpamax.out.

5. Change Requested by: R. Janetzke Date: 4-15-2004	6. Change Authorized by (*Software Developer*): R. Janetzke Date: 4-15-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Modify the subroutine **writemeanvalues** in *reader.f* so that, in addition to *tpameans.out*, files *tpamin.out* and *tpamax.out* are created. Wherever mean values are written to *tpameans.out*, write out the minimum values to *tpamin.out* and the maximum values to *tpamax.out*. See Attachment A.

8. Implemented by: C. Scherer	Date: 5-7-2004

9. Description of Acceptance Tests:

The software was tested as presented in Attachment B.
All tests passed.

10. Tested by: Zbigniew Wojcik	Date: June 24, 2004

ATTACHMENT A

In the subroutine **writemeanvalues** in the file *reader.f*, the code was modified as follows:

```
.
.
.
c css - SCR470:  4-19-2004; add files with minimum and
c                           maximum values
      integer imaxunit
      integer iminunit
.
.
.
      inquire( file='tpameans.out', EXIST=lexist)
      if ( lexist) istatus = zportsh( 'rm tpameans.out')
      inquire( file='tpamax.out', EXIST=lexist)
      if ( lexist) istatus = zportsh( 'rm tpamax.out')
      inquire( file='tpamin.out', EXIST=lexist)
      if ( lexist) istatus = zportsh( 'rm tpamin.out')
      iunitout = igetunitnumber('exec    ')
      open( unit=iunitout, file='tpameans.out', status='NEW' )
      imaxunit = igetunitnumber('exec    ')
      open( unit=imaxunit, file='tpamax.out', status='NEW' )
      iminunit = igetunitnumber('exec    ')
      open( unit=iminunit, file='tpamin.out', status='NEW' )
      read( iunit, fmt='(a30)' ) pdftype
      write( iunitout, fmt='(a30)' ) pdftype
      write( imaxunit, fmt='(a30)' ) pdftype
      write( iminunit, fmt='(a30)' ) pdftype

      read( iunit, fmt='(a80)' ) title1
      write( iunitout, fmt='(a80)' ) title1
      write( imaxunit, fmt='(a80)' ) title1
      write( iminunit, fmt='(a80)' ) title1

      read( iunit, fmt='(a80)' ) title2
      write( iunitout, fmt='(a80)' ) title2
      write( imaxunit, fmt='(a80)' ) title2
      write( iminunit, fmt='(a80)' ) title2

      write( iunitout, fmt='(a)' ) '** ** '
      write( iunitout, fmt='(a)' )
     & '** ** This file was automatically generated by the TPA code '
      write( iunitout, fmt='(a)' )
     & '** ** and contains the mean values of the sampled parameters '
      write( iunitout, fmt='(a)' )
     & '** ** submitted for the run on '// datetim // '.'
      write( iunitout, fmt='(a)' ) '** ** '
      write( iunitout, fmt='(a)' ) '** ** '

      write( imaxunit, fmt='(a)' ) '** ** '
      write( imaxunit, fmt='(a)' )
     & '** ** This file was automatically generated by the TPA code '
      write( imaxunit, fmt='(a)' ) '** ** and contains the maximum ' //
```

```
     &                              'values of the sampled parameters '
      write( imaxunit, fmt='(a)' )
     & '** ** submitted for the run on '// datetim // '.'
      write( imaxunit, fmt='(a)' ) '** ** '
      write( imaxunit, fmt='(a)' ) '** ** '

      write( iminunit, fmt='(a)' ) '** ** '
      write( iminunit, fmt='(a)' )
     & '** ** This file was automatically generated by the TPA code '
      write( iminunit, fmt='(a)' ) '** ** and contains the minimum ' //
     &                              'values of the sampled parameters '
      write( iminunit, fmt='(a)' )
     & '** ** submitted for the run on '// datetim // '.'
      write( iminunit, fmt='(a)' ) '** ** '
      write( iminunit, fmt='(a)' ) '** ** '
.
.
.
      if( pdftype .eq. 'uniform' ) then
.
.
.
         write( iunitout, * ) xmean
         write( imaxunit, '(a)' ) 'constant'
         write( iminunit, '(a)' ) 'constant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
         write( imaxunit, * ) xmax
         write( iminunit, * ) xmin
      elseif( pdftype .eq. 'iuniform' ) then
.
.
.
         write( iunitout, * ) ixmean
         write( imaxunit, '(a)' ) 'iconstant'
         write( iminunit, '(a)' ) 'iconstant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
         write( imaxunit, * ) ixmax
         write( iminunit, * ) ixmin
      elseif( pdftype .eq. 'loguniform' ) then
.
.
.
         write( iunitout, * ) xmean
         write( imaxunit, '(a)' ) 'constant'
         write( iminunit, '(a)' ) 'constant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
         write( imaxunit, * ) xmax
         write( iminunit, * ) xmin
      elseif( pdftype .eq. 'normal' ) then
.
.
.
         write( iunitout, * ) xmean
         write( imaxunit, '(a)' ) 'constant'
         write( iminunit, '(a)' ) 'constant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
```

```
      write( imaxunit, * ) xmax
      write( iminunit, * ) xmin
   elseif( pdftype .eq. 'lognormal' ) then
.
.
.
      write( iunitout, * ) xmean
      write( imaxunit, '(a)' ) 'constant'
      write( iminunit, '(a)' ) 'constant'
      write( imaxunit, '(a)' ) line(1:itrimlen)
      write( iminunit, '(a)' ) line(1:itrimlen)
      write( imaxunit, * ) xmax
      write( iminunit, * ) xmin
   elseif( pdftype .eq. 'triangular' ) then
.
.
.
      write( iunitout, * ) xmean
      write( imaxunit, '(a)' ) 'constant'
      write( iminunit, '(a)' ) 'constant'
      write( imaxunit, '(a)' ) line(1:itrimlen)
      write( iminunit, '(a)' ) line(1:itrimlen)
      write( imaxunit, * ) xmax
      write( iminunit, * ) xmin
   elseif( pdftype .eq. 'logtriangular' ) then
.
.
.
      write( iunitout, * ) xmean
      write( imaxunit, '(a)' ) 'constant'
      write( iminunit, '(a)' ) 'constant'
      write( imaxunit, '(a)' ) line(1:itrimlen)
      write( iminunit, '(a)' ) line(1:itrimlen)
      write( imaxunit, * ) xmax
      write( iminunit, * ) xmin
   elseif( pdftype .eq. 'beta' ) then
.
.
.
      write( iunitout, * ) xmean
      write( imaxunit, '(a)' ) 'constant'
      write( iminunit, '(a)' ) 'constant'
      write( imaxunit, '(a)' ) line(1:itrimlen)
      write( iminunit, '(a)' ) line(1:itrimlen)
      write( imaxunit, * ) xmax
      write( iminunit, * ) xmin
   elseif( pdftype .eq. 'logbeta' ) then
.
.
.
      write( iunitout, * ) xmean
      write( imaxunit, '(a)' ) 'constant'
      write( iminunit, '(a)' ) 'constant'
      write( imaxunit, '(a)' ) line(1:itrimlen)
      write( iminunit, '(a)' ) line(1:itrimlen)
      write( imaxunit, * ) xmax
      write( iminunit, * ) xmin
   elseif( pdftype .eq. 'exponential' ) then
.
.
```

```
.
         write( iunitout, * ) xmean
         write( imaxunit, '(a)' ) 'constant'
         write( iminunit, '(a)' ) 'constant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
         write( imaxunit, * ) -dlog(0.0001d0)/xlambda
         write( iminunit, * ) -dlog(0.9999d0)/xlambda
      elseif( pdftype .eq. 'finiteexponential' ) then
.
.
.
         write( iunitout, * ) xmean
         write( imaxunit, '(a)' ) 'constant'
         write( iminunit, '(a)' ) 'constant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
         write( imaxunit, * ) xmax
         write( iminunit, * ) xmin
      elseif( pdftype .eq. 'userdiscreteempirical' ) then
.
.
.
         write( iunitout, * ) xmean
         write( imaxunit, '(a)' ) 'constant'
         write( iminunit, '(a)' ) 'constant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
         write( imaxunit, * ) udist(nudist)
         write( iminunit, * ) udist(1)
      elseif( pdftype .eq. 'usersupplieddiscrete' ) then
.
.
.
         write( iunitout, * ) xmean
         write( imaxunit, '(a)' ) 'constant'
         write( iminunit, '(a)' ) 'constant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
         write( imaxunit, * ) udist(nudist)
         write( iminunit, * ) udist(1)
      elseif( pdftype .eq. 'usersuppliedpwisecdf' ) then
.
.
.
         write( iunitout, * ) xmean
         write( imaxunit, '(a)' ) 'constant'
         write( iminunit, '(a)' ) 'constant'
         write( imaxunit, '(a)' ) line(1:itrimlen)
         write( iminunit, '(a)' ) line(1:itrimlen)
         write( imaxunit, * ) udist(nudist)
         write( iminunit, * ) udist(1)
      elseif( pdftype .eq. 'correlateinputs' ) then
         write( iunitout, '(a)' ) '** correlateinputs'
         write( imaxunit, '(a)' ) '** correlateinputs'
         write( iminunit, '(a)' ) '** correlateinputs'
         read(  iunit,    '(a80)' ) line
         itrimlen = trimlen(line)
         write( iunitout, '(a)' ) '** '//line(1:itrimlen)
         write( imaxunit, '(a)' ) '** '//line(1:itrimlen)
```

```
      write( iminunit, '(a)' ) '** '//line(1:itrimlen)
      read(  iunit,    '(a80)' ) line
      itrimlen = trimlen(line)
      write( iunitout, '(a)' ) '** '//line(1:itrimlen)
      write( imaxunit, '(a)' ) '** '//line(1:itrimlen)
      write( iminunit, '(a)' ) '** '//line(1:itrimlen)
      read(  iunit,    '(a80)' ) line
      itrimlen = trimlen(line)
      write( iunitout, '(a)' ) '** '//line(1:itrimlen)
      write( imaxunit, '(a)' ) '** '//line(1:itrimlen)
      write( iminunit, '(a)' ) '** '//line(1:itrimlen)
   elseif( pdftype .eq. 'iflag' ) then
      itrimlen = trimlen(line)
      write( iunitout, '(a)' ) line(1:itrimlen)
      write( imaxunit, '(a)' ) line(1:itrimlen)
      write( iminunit, '(a)' ) line(1:itrimlen)
      read(  iunit,    '(a80)' ) line
      itrimlen = trimlen(line)
      write( iunitout, '(a)' ) line(1:itrimlen)
      write( imaxunit, '(a)' ) line(1:itrimlen)
      write( iminunit, '(a)' ) line(1:itrimlen)
      if (line(1:34) .eq. 'LatinHypercubeSampling(yes=1,no=0)') then
         read(  iunit,    * ) iflag
         iflag = 0
         write( iunitout, * ) iflag
         write( imaxunit, * ) iflag
         write( iminunit, * ) iflag
      endif
   elseif( pdftype(1:9) .eq. 'endoffile' ) then
      write( iunitout, '(a)' ) 'endoffile'
      write( imaxunit, '(a)' ) 'endoffile'
      write( iminunit, '(a)' ) 'endoffile'
.
.
.
      if (lkeep) then
         close( iunitout )
         close( imaxunit )
         close( iminunit )
      else
         close( iunitout, STATUS='DELETE' )
         close( imaxunit, STATUS='DELETE' )
         close( iminunit, STATUS='DELETE' )
      endif
      return
   else
     itrimlen = trimlen(line)
     write( iunitout, '(a)' ) line(1:itrimlen)
     write( imaxunit, '(a)' ) line(1:itrimlen)
     write( iminunit, '(a)' ) line(1:itrimlen)
.
.
.
```

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-488	2. Software Title and Version: TPA 5.0x	3. Project No: 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): climato2.dat, nfenv.f, uzflow.f, tpanames.dbs, tpa.inp.
The basis for climato2.dat cannot be supported.
The relative humidity for the pre-closure period is based on repository temperature rather than ground surface temperature.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
R. Fedors Date: 7-20-2004	R. Janetzke Date: 7-21-2004 R. Janetzke

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):
Because the DOE estimates for precipitation with climate change are dramatically greater than those used by the NRC, the climato2.dat file was modified. The DOE analyses (CRWMS M&O, 2000; USGS, 2000) since NRC (1997) was completed suggest the modern climate will persist for 600 years, followed by 1400 years of monsoonal climate with 303 mm/yr precipitation. The remaining years to the performance period of 10,000 years are described as glacial transition with an mean case of 323 mm/yr precipitation. Values used DOE precipitation estimates are based on repository averages from USGS (2000). The climato2.dat file was modified with a smoothly increasing fraction such that the first 10,000 years of the file were similar to fractions used by DOE. After full glacial begins at approximately 40,000 years, the remaining years to 100,000 are left unchanged in the climato2.dat file. Thus, maintaining the NRC (1997) conclusion that 60-80% of the 100,000 year cycle will be glacial climate.

An equation was added to nfenv.f to calculate the relative humidity for the pre-closure period using the ground surface temperature.

8. Implemented by:	Date:
R. Janetzke R. Janetzke	8-21-04

9. Description of Acceptance Tests:
The software was tested in accordance with the Test Plan for TPA SCR #488 (see tp_scr488.wpd). The software, test directories, and test results are contained on a CD labeled "TPA SCR #488 - Test Directories (Code Development)." All tests passed.

10. Tested by:	Date:
C. Scherer Carol S. Scherer	9-13-04

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description** **1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton** **1. site references (journals, sci. notebooks, publishings)** **2. is uncertainty covered by the distribution / range ?** **3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
Add	uzflow nfenv	GroundSurfaceTe mperature[C]	Temperature of the ground surface to be used as the temperature for ventilated air up to the time of backfill, and also as the initial climate temperature.	constant	17.38 C		
Add	uzflow	CurrentAnnualPre cipitation[mm/yr]	Current climate annual precipitation for initial climate conditions.	constant	162.8		

09/17/4

Test Plan/Report for TPA SCR #488

Test Plan Name: New Climato2.dat and Relative Humidity Calculation Based on Ground Surface Temperature

Tested By: Carol S. Scherer

Date: September 16, 2004

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0x
(4.2 solapps compiler)

Test Version: TPA 5.0y
(4.2 solapps compiler)

Testing Setup:

Directories/paths used for testing:
$HOME = /home/cscherer
Path for run directory:***$HOME/scr488***

Environment variables:

TPA_TEST = $HOME ***/scr488***
TPA_DATA = $HOME ***/scr488***

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 488 - Test Directories*" (attached).

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***scr488*** and ***tpa50x***.

2. In the directory ***scr488***, create the following subdirectories: ***slt1***, ***slt2***, ***slt3***, ***slt4***, ***slt5***, and ***slt6***.

3. Copy **TPA** version 5.0x to the ***tpa50x*** directory. Compile *tpa.e* using *Makefile4.2*. Save a copy of the executable as *tpa_x.e*. Save a copy of the original *tpa.inp* as *tpa_orig.inp*. Run *tpa.e*. Copy *tpameans.out* to *tpa_x.inp*. Set OutputMode to 1 in *tpa_x.inp*. Copy *tpa_x.e* and *tpa_x.inp* to the run directory. Copy *burnup.dat* to run/***data*** as *burnup_x.dat*. Copy *climato2.dat* to the run/***data*** directory as *climato2_x.dat*.

4. Copy **TPA** version 5.0y to the run directory. Compile *tpa.e* using *Makefile4.2*. Save a copy of the executable as *tpa_y.e*. Save a copy of the original *tpa.inp* as *tpa_orig.inp*. Run *tpa.e*. Copy *tpameans.out* to *tpa_y.inp*. Set OutputMode to 1 in *tpa_y.inp*. Copy the latest version of *burnup.dat* (see *scr_518.wpd*) to the run***/data*** directory as *burnup-scr518.dat*. Save a copy of *climato2.dat* as *climato2_y.dat* in the run***/data*** directory.

Functional Level Tests:

1. Name: Compare Modified *climato2.dat* to Previous Version of *climato2.dat*.

   Path for archives of results: ***$HOME /scr488/flt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: none.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to show that specified modifications were carried out to the data file.
   - assumptions: none.
   - constraints: none.
   - output files to compare or examine: none
   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>***/data***
     2. compare *climato2_y*.dat with *climato2_x.dat*.
   - pass/fail criteria: the test passes if:
     1. The modified *climato2_y.dat* file contains the changes described in *scr_488.wpd*.

Results of running test:

PASSED.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

NOTE: Changes had to be made to TPA5.0y versions *nuclides.dat* and *burnup.dat* (change year from 2033 to 2008), as well as *tpa.inp* (change CalendarYearOfEmplacement[A.D.] from 2034 to 2033) before test results looked like expected results from a basecase run. More changes were made to *burnup.dat* (see SCR # 518) around the same time as testing was done for SCR # 488. Since the *burnup.dat* changes affected the validity of the output for the SCR # 488 tests, the modified *burnup.dat* was used for these tests.

1. Name: Compare Modified Code To Previous Version Of The Code.

   Paths for archives of results: ***$HOME /scr488/slt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use *tpa_x.inp* and tpa_y.inp

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to show that the modified **TPA** code generates different results and the results differ in the way expected

   - assumptions: all setup instructions have been carried out.

   - constraints: the file *tpa_meanscase_y.out* does not exist in the run directory and *tpa_meanscase.out* does not exist in **$HOME/*tpa50x***.

- output files to compare or examine: *ebsfail.ech & infilper.res* in the run directory and in **$HOME/*tpa50x***.

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. run *tpa.e* using command "***tpa.e > tpa_meanscase_y.out***"
  4. —> change directory to **$HOME/*tpa50x***
  5. copy *tpa_x.e* to *tpa.e*
  6. run *tpa.e* using command "***tpa.e > tpa_meanscase_x.out***"
  7. compare the files *ebsfail.ech* and *infilper.res* from each run (see spreadsheets *ebsfail_ech.xls* and *infilper_res.xls*) for a single subarea (subarea 7 was used for this test report)

- pass/fail criteria: the test passes if:

  1. The modified code runs successfully to completion.

  2. *infilper_res.xls*: Infiltration is higher for TPA5.0y. Reflux and divert start out lower for TPA5.0y than TPA5.0x, then go higher (around 1900 years for subarea 7).

  3. *ebsfail_ech.xls*: Relhumwp, tempwp, and temprep are all higher for TPA5.0y, especially relhumwp in the preclosure period (0 - 50 years).

Results of running test:

PASSED.

2. Name: Run TPA5.0y Using *climato2.dat* from TPA5.0x.

Paths for archives of results: ***$HOME /scr488/slt2***

Special input files or modifications to input files required: *use climato2_x.dat*

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp*

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code and data file do not cause unintended side effects

- assumptions: all setup instructions have been carried out.

- constraints: the file *tpa_50y-clim2x.out* does not exist in the run directory.

- output files to compare or examine: *ebsfail.ech & infilper.res*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. run *tpa.e* using command "***tpa.e > tpa_50y-clim2x.out***"
  4. compare ebsfail.ech and infilper.res files from this run and the TPA5.0y run in slt1 (see spreadsheets ebsfail_ech.xls and infilper_res.xls).

- pass/fail criteria: the test passes if:

  1. The modified code runs successfully to completion.

  2. *infilper_res.xls*: Results are the same for this run as for the TPA5.0x run from slt1.

  3. *ebsfail_ech.xls*: Results are the same for this run as for the TPA5.0x run from slt1 for tempwp, temprep, and postclosure relhumwp. However, for preclosure relhumwp, the results for this run are the same as for the TPA5.0y from slt1.

Results of running test:

PASSED.

3. Name: Vary Ground Surface Temperature from 17.38 to 10.0, 15.0, and 20.0.

Paths for archives of results: ***$HOME /scr488/slt3***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp* and change GroundSurfaceTemperature to 10.0 for run A, 15.0 for run B, and 20.0 for run C.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that modifying the ground surface temperature affects temperature and humidity in a predictable way. (**CAVEAT**: The results from this test have limited implications. For a change in ground surface temperature to be valid, the data files resulting from ITYM should also be regenerated using the current temperature.)

- assumptions: all setup instructions have been carried out.

- constraints: the files *tpa_GST10.out*, *tpa_GST10.out*, and *tpa_GST10.out* do not exist in the run directory.

- output files to compare or examine: *ebsfail.ech*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. use tpa.inp for run A and run *tpa.e* using command "***tpa.e > tpa_GST10.out***"
  4. use tpa.inp for run B and run *tpa.e* using command "***tpa.e > tpa_GST15.out***"
  5. use tpa.inp for run C and run *tpa.e* using command "***tpa.e > tpa_GST20.out***"
  6. compare *ebsfail.ech* from all three runs and TPA5.0y run in slt1 (see spreadsheet *ebsfail_ech.xls*).

- pass/fail criteria: the test passes if:

  1. The modified code runs successfully to completion.

  2. *ebsfail_ech.xls*: There are no differences among the runs for tempwp and temprep and postclosure relhumwp. Preclosure relhumwp is highest when ground surface temperature is 20.0, next highest when ground surface temperature is 17.38 (basecase),

third highest when ground surface temperature is 15.0, and lowest when ground surface temperature is 10.0.

Results of running test:

PASSED.

4. Name: Vary CurrentAnnualPrecipitation[mm/yr] from 162.8 to 100.0 and 200.0.

Paths for archives of results: ***$HOME /scr488/slt4***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp* and change CurrentAnnualPrecipitation[mm/yr] to 100.0 for run A and to 200.0 for run B.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that modifying the current annual precipitation affects temperature and humidity in a predictable way.

- assumptions: all setup instructions have been carried out

- constraints: the files *tpa_CAP100.out* and *tpa_CAP100.out* do not exist in the run directory.

- output files to compare or examine: *ebsfail.ech*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. use *tpa.inp* for run A and run *tpa.e* using command "***tpa.e > tpa_CAP100.out***"
  4. use *tpa.inp* for run B and run *tpa.e* using command "***tpa.e > tpa_CAP200.out***"

5. compare *ebsfail.ech* from both runs and from TPA5.0y in slt1 (see spreadsheet *ebsfail_ech.xls*).

- pass/fail criteria: the test passes if:

1. The modified code runs successfully to completion.

2. *ebsfail.ech*: There are no differences in tempwp, temprep, and relhumwp.

Results of running test:

PASSED.

5. Name: Vary FactorForVentilationHeatlosses[] from 0.7 to 0.86.

Paths for archives of results: ***$HOME /scr488/slt5***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp* and change FactorForVentilationHeatlosses[] to 0.86.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modifying the factor for ventilation heat loss affects temperature and humidity in a predictable way.

- assumptions: all setup instructions have been carried out

- constraints: the files *tpa_Vent-86.out* does not exist in the run directory.

- output files to compare or examine: *ebsfail.ech*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>

2. copy *tpa_y.e* to *tpa.e*
3. run *tpa.e* using command "***tpa.e > tpa_Vent-86.out***"
4. compare files *ebsfail.ech* from this run and from TPA5.0y run in slt1 (see spreadsheet *ebsfail_ech.xls*).

- pass/fail criteria: the test passes if:

1. The modified code runs successfully to completion.

2. *ebsfail.ech*: Tempwp and temprep are lower when ventilation is increased while relhumwp is higher.

Results of running test:

PASSED.

6. Name: Vary CalendarYearOfEmplacement[A.D.] to year 2034 from 2033.

Paths for archives of results: ***$HOME /scr488/slt6***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp* and change CalendarYearOfEmplacement[A.D.] to 2034.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that modifying year of emplacement affects the results of TPA in a predictable way.

- assumptions: all setup instructions have been carried out

- constraints: the files *tpa_Emplace2034.out* does not exist in the run directory.

- output files to compare or examine: *ebsfail.ech*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. run *tpa.e* using command "***tpa.e > tpa_Emplace2034.out***"
  4. compare *ebsfail.ech* files from this run and the TPA5.0y run in slt1 (see spreadsheet *ebsfail_ech.xls*).

- pass/fail criteria: the test passes if:

  1. The modified code runs successfully to completion.

  2. *ebsfail.ech*: Tempwp and temprep is slightly lower when year of emplacement increases by one year. Relhumwp is slightly higher at first then becomes slighter lower (after 1250 years for subarea 7).

Results of running test:

PASSED.

NOTES:

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-489	**2. Software Title and Version:** TPA 5.0v	**3. Project No:** 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): uzft.f, szft.f, actinide_kdrd.out
It is desirable to enable the TPA code to produce an intermediate output file (actinide_kdrd.out) that contains the Kd, Rd, surface area, effective porosity, and matrix porosity values used for each radionuclide, layer, zone (unsaturated/saturated), realization combinations for a given run.

5. Change Requested by: P. Bertetti Date: 7-8-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: R. Janetzke

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): Fracture and matrix coefficients Kds and Rds are computed for the elements Am, Np, Pu, Th and U by subroutines uzsf() and szft() by calls to calc_dk() and calc_rd(). Rds only for all nuclides are collected from tpa.inp in szft() by call to prenefmksa(). The collection of these coefficients was done at proper places of the code modeling the flow of the nuclides through the rock layers.
See Attachment A for details.

8. Implemented by: Zbigniew Wojcik	**Date:** July 30, 2004

9. Description of Acceptance Tests:
See Attachment B

10. Tested by:	**Date:** Apr. 13, 2006

CNWRA Form TOP-5 (05/2000)

Attachment A.

The distribution (or partition) coefficient kd is a ratio (fraction) of a contaminant concentration in soil to that in water. The retardation coefficient rd is the ratio of the velocity of water to that of a contaminant. The array kds(i) is computed by subroutine calc_kd() for each rock layer separately, where i is the contaminant Am, Np, Pn, Th, U. Subroutine calc_rd takes kds(i) and computes the array of retardation coefficients rds(i).
Rds are also read from TPA.INP file for the saturated layer and should be the same as Rdd computed by CALC_RD().
The specific surface area ssArea parameter is computed for each rock layer and also needs to be collected with all kds(i) and rds(i).
Run directory: /home/zwojcik/rd/run
Affected modules: uzft.f, szft.f, exec.f, actinide_kdrd.out

1. Made modifications in the uzft.f and in szft.f to save RealizationNumber, Subarea ID and saturated / unsaturated zone, then Layer of Rock and SpecificSurfaceArea, then header listing columns: Nuclide, matrix_KD, matrix_RD, fracture_KD, fracture_RD.
2. Modified uzft() to save the parameters in the new file actinide_kdrd.out: a. Declared the names of the rock layers specific to unsaturated zone; b. Designed with details and implemented the transfer of the new file actinide_kdrd.out for the append operations between calls of subsequent realizations; c) Designed, implemented and tested the mechanism of temporal saving parameters of matrix kds() from the call to calc_kd() (computing the matrix Kd equations) to save them in file actinide_kdrd.out together with the fracture Kd computed later. The loop through rock layers was over the matrix and fracture Kd an Rd computations; d) Done the same for the Rd parameters, however, added new call to calc_rd() in uzft() to get all matrix Rd; e) Followed the required format for the new output file actinide_kdrd.out.
3. Tested the modifications made to uzft(): compared the matrix Rds computed in uzft() as a result of the modification with matrix Rds computed in prenefmksa(). Made the comparison at the corresponding layer rocks and elements. The calc_kd() computes Kds for the nuclides in the sequence: Am, Np, Pu, Th, U. The prenefmksa() extracts these matrix Kds, associates them with the elements Am, Np, Pu, Th, U and then computes matrix Rds.
The Rds computed in prenefmksa() are associated with the right elements Am, Np, Pu, Th, U as in uzft() and are of the same values.
4. Made another, parallel test of correctness of passing matrix Kds from uzft() to prenefmksa() to compute RDs. Took advantage of the call (in uzft.f) to sub setconsmv() saving results of the first call to calc_kd as matrix kd. The values of matrix kd are saved in datc() by layer rock (see common / mvb4 /, include 'mve.i'). The indexes to Kds corresponding to Am, Np, Pu, Th, U extracted by invquery() were the same both in uzft() and in prenefmksa(). So, the indexes to Kds (and Rds) whose values were saved in file actinide_kdrd.out were associated with the right elements Am, Np, Pu, Th, U and with their right values of Kds and Rds existing in prenefmksa().
6. Tested if the values under fields Nuclide, matrixRD, matrixKD, fractureKD, fractureRD computed in uzft.f were written correctly to the file actinide_kdrd.out by comparing the values printed to the screen during execution with the contents of the file actinide_kdrd.out. They were the same.
7. Modified szft.f to save the RD parameters computed by calc_kd() and calc_rd()) into the new file actinide_kdrd.out: a. Declared the names of the rock layers specific to saturated zone; b. Implemented the transfer of the new file actinide_kdrd.out for the append operations between calls of subsequent realizations; c) Designed, implemented and tested the mechanism of transfer of parameters kds() from the call to calc_kd() computing the matrix KD equations to save these matrix parameters in new file actinide_kdrd.out after calling calc_kd() to compute the fracture KD equations. The differences with uzft were: (i) the loop through rock layers was only over the matrix KR an RD computations; (ii) the call to make matrix RDs() parameters were not made from another module; (iii) the fracture parameters were only for the layer 2 of rock, so the matrix parameters had to be transferred to the file actinide_kdrd.out for the layer 2 of rock only.

8. Modified szft.f to save the RD parameters taken from TPA.inp file (not computed by calc_kd() and calc_rd()) into the new file actinide_kdrd.out. Utilized two loop structures over which all the elements and the rock layers are scanned. Identified and saved temporarily the required RDs inside the body of the loop structures. Resolved the differences between the number and names of the nuclides handled when computing Rds by using calc_RD() and when reading RD coefficients from tpa.inp: only 5 nuclides are processed by using calc_kd() and calc_rd(): Am, Np, Pu, Th, U, whereas

all nuclides are processed when reading Rds from tpa.inp.
9. Tested. Compared the matrix Rds for the elements Am, Np, Pu, Th, U computed by calc_rd() in szft() with those collected from tpa.inp for two layers: STFF and SAV. They were the same.
The value of fracture RD computed by calc_rd() was always equal to 1. This is because the value frac_forcefac is always equal to 0, because that frac_forcefac = valuesp(ifforcefac), and that
ifforcefac = ispquery(UZFractureForceFactorForKdToRd).
UZFractureForceFactorForKdToRd = 0 in tpa.inp. So, the values of RDs were as expected.
The outputs of Kds computed by calc_rd() are for only the first area of the first realization, because of the condition in the code:

```
 IF (ir .ne. ir_now) THEN
    Making actinide_kdrd.out
   END IF
```

where ir is the current realization number. This condition is true only for the first area of the first realization, and this explains, why.

Delivarables:
The version of the TPA code providing Kds and Rds for both the unsaturated and saturated zones is in the subdirectory kdrd_all. The new versions of uzft.f, szft.f and exec.f. are necessary can to provide the Kds and Rds for both the unsaturated and saturated zones.

10. To the general requirements to provide the Rds in both unsaturated and saturated zones, Paul requested in addition also the code outputting only the Rds and Kds in the saturated zone. Made updates on the copy of the TPA code described above: commented-out all write statements resulting Kds and Rds from the unsaturated zone, and modified the szft.f to output only the KDs and RDS for the first area only on each realization.

Delivarables:
The version of the TPA code providing Kds and Rds for the saturated zone only is in the subdirectory kdrd.
The initial version of uzft.f can be used to provide the Kds and Rds for the saturated zone only, together with new szft.f and exec.f.

ATTACHMENT B

Test Plan for TPA SCR489

Tested By: Michael Muller Date: Aug 20, 2004
Host Machine: spock Host OS: Solaris
Baseline Version: TPA 5.0v Test Version: TPA 5.0v with SCR mods.

Process Level (PL) Tests

PL-1. Name: scr489_proclevl1
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/scr489_proclelv1
Environment variables: TPA_DATA=. TPA_TEST=.
Special input files or modifications to input files required: none
Special diagnostic code modifications required: none
Program modes to be used (append flags, scenario/model switches,etc.):
NumberOfRealizations: 1
Utility scripts needed to perform the test: none
Utility codes needed in the analysis of the test data: none
Test description:
objective: Compare values in nefiisz.inp to values in file actinide_kdrd.out
assumptions: Numbers will be identical.
constraints: none.
output files to compare/examine: nefii.inp and actinide_kdrd.out
procedure to be used:
Run tpa50v+scr489.
Code for scr489 is in exec.f, uzft.f, and szft.f. Check output from szft.f.
Compare nefiisz.inp and numbers in actinide_kdrd.out
Pass/fail criteria: Success is if numbers in nefiisz.inp and actinide_kdrd.out are the same (for the same nuclides).
Overall test status: FAIL Retested in SCR 523 RJ. 4-13-06

Comments: appears that code saves values for tuff in aluvium variable and vice versa. Also, from output, looks like incorrect index is used to save values for U,Am,Np,Pu, etc.
Suggest av() be changed to alv() for recognition and consistancy.
Also, when looking through code, noted that file actinide_kdrd.out is opened and closed every time it is written to. This is inefficient and it appears that opening/closing it once is possible.
Also noted that tpa version number was hard-coded in write of header of file. This would require editing for each new version.

SL-1. syslevl1
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/scr489_syslevl1

Environment variables: TPA_DATA=. TPA_TEST=.
Program modes to be used (append flags, scenario/model switches,etc.):
NumberOfRealizations: 403
MaximumTime[yr]: 2.5e4
VolcanismDisruptiveScenarioFlag(yes=1,no=0): 1
DirectReleaseOnlyFlag(yes=1,no=0): 1
Test description:
procedure to be used:
Run TPA50v+scr489 for 25Kyears and 403 realizations.
Set: VolcanismDisruptiveScenarioFlag(yes=1,no=0) = 1 and
DirectReleaseOnlyFlag(yes=1,no=0) = 1
objective: To run a long run with many years and realizations and directrelease and volcanism ON.
The values picked are mostly arbitrary (ie. 50yrs and 500 realizations could be used just as well but would take longer to run).
assumptions: 25K years is a sufficiently long time and 403 realizations is sufficiently long.
Pass/fail criteria: Success is when program runs to completion and 'success' line is printed.
Overall test status: PASS

SL-2. syslevl2
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/scr489_syslevl2
Environment variables: TPA_DATA=. TPA_TEST=.
Program modes to be used (append flags, scenario/model switches,etc.):
NumberOfRealizations: 100
MaximumTime[yr]: 5.0e4
Test description:
procedure to be used:
Run TPA50v+scr489 for 50Kyears and 100 realizations.
objective: To run a long run with many years and realizations.
The values picked are mostly arbitrary (ie. 25yrs and 500 realizations could be used just as well but would take longer to run).
assumptions: 50K years is a sufficiently long time and 100 realizations is sufficiently long.
pass/fail criteria: Success is when program runs to completion and 'success' line is printed.
Overall test status: PASS

File actinide_kdrd.out
SpecificSurfaceArea, KD & RD coefficients
TPA 5.0x, Job started: Wed Aug 04 15:32:28 2004

Realization = 1 Subarea = 1 UNSATURATED ZONE

Layer=TSw_ ssAreaMatrix=2.9268E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.6832E+04	4.8405E+08	9.1675E+00	1.0000E+00
Np	4.0790E-03	7.4584E+01	1.3936E-06	1.0000E+00
Pu	1.5389E+00	2.7762E+04	5.2578E-04	1.0000E+00
Th	9.1979E+01	1.6593E+06	3.1426E-02	1.0000E+00
U	8.9352E-02	1.6129E+03	3.0529E-05	1.0000E+00

Layer=CHnv ssAreaMatrix=8.7611E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	8.0317E+04	3.6854E+08	9.1675E+00	1.0000E+00
Np	1.2210E-02	5.7025E+01	1.3936E-06	1.0000E+00
Pu	4.6064E+00	2.1137E+04	5.2578E-04	1.0000E+00
Th	2.7533E+02	1.2633E+06	3.1426E-02	1.0000E+00
U	2.6746E-01	1.2283E+03	3.0529E-05	1.0000E+00

Layer=CHnz ssAreaMatrix=8.0000E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	7.3340E+04	3.7404E+08	9.1675E+00	1.0000E+00
Np	1.1149E-02	5.7861E+01	1.3936E-06	1.0000E+00
Pu	4.2063E+00	2.1453E+04	5.2578E-04	1.0000E+00
Th	2.5141E+02	1.2822E+06	3.1426E-02	1.0000E+00
U	2.4423E-01	1.2466E+03	3.0529E-05	1.0000E+00

Layer=PPw_ ssAreaMatrix=6.6142E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	6.0636E+04	3.9604E+08	9.1675E+00	1.0000E+00
Np	9.2178E-03	6.1205E+01	1.3936E-06	1.0000E+00
Pu	3.4776E+00	2.2715E+04	5.2578E-04	1.0000E+00
Th	2.0786E+02	1.3576E+06	3.1426E-02	1.0000E+00
U	2.0192E-01	1.3198E+03	3.0529E-05	1.0000E+00

Layer=UCF_ ssAreaMatrix=6.9421E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	6.3642E+04	3.9604E+08	9.1675E+00	1.0000E+00
Np	9.6749E-03	6.1205E+01	1.3936E-06	1.0000E+00
Pu	3.6501E+00	2.2715E+04	5.2578E-04	1.0000E+00
Th	2.1816E+02	1.3576E+06	3.1426E-02	1.0000E+00
U	2.1194E-01	1.3198E+03	3.0529E-05	1.0000E+00

Layer=BFw_ ssAreaMatrix=2.8016E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.5683E+04	4.8405E+08	9.1675E+00	1.0000E+00
Np	3.9044E-03	7.4584E+01	1.3936E-06	1.0000E+00
Pu	1.4730E+00	2.7762E+04	5.2578E-04	1.0000E+00
Th	8.8042E+01	1.6593E+06	3.1426E-02	1.0000E+00
U	8.5528E-02	1.6129E+03	3.0529E-05	1.0000E+00

Layer=UFZ_ ssAreaMatrix=2.7376E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.5097E+04	4.8405E+08	9.1675E+00	1.0000E+00
Np	3.8153E-03	7.4584E+01	1.3936E-06	1.0000E+00
Pu	1.4394E+00	2.7762E+04	5.2578E-04	1.0000E+00
Th	8.6033E+01	1.6593E+06	3.1426E-02	1.0000E+00
U	8.3577E-02	1.6129E+03	3.0529E-05	1.0000E+00

Realization = 1 Subarea = 1 SATURATED ZONE

Layer=SAV ssAreaMatrix= 2.6169E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.3990E+04	4.9077E+08	0.0000E+00	0.0000E+00
Np	3.6470E-03	7.5607E+01	0.0000E+00	0.0000E+00
Pu	1.3759E+00	2.8148E+04	0.0000E+00	0.0000E+00
Th	8.2239E+01	1.6824E+06	0.0000E+00	0.0000E+00
U	7.9890E-02	1.6353E+03	0.0000E+00	0.0000E+00

Layer=STFF ssAreaMatrix= 4.8574E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.4530E+04	4.4004E+08	9.1675E+00	1.0000E+00
Np	6.7695E-03	6.7895E+01	1.3936E-06	1.0000E+00
Pu	2.5539E+00	2.5239E+04	5.2578E-04	1.0000E+00
Th	1.5265E+02	1.5085E+06	3.1426E-02	1.0000E+00
U	1.4829E-01	1.4664E+03	3.0529E-05	1.0000E+00

Realization = 1 Subarea = 1 SATURATED ZONE

Layer=SAV.

Nuclide	MobileRd
U	0.1635E+04
Am	0.4908E+09
Np	0.7561E+02
Pu	0.2815E+05
Th	0.1682E+07

Layer=STFF.

Nuclide	ImmobileRd
U	0.1466E+04
Am	0.4400E+09
Np	0.6789E+02
Pu	0.2524E+05
Th	0.1508E+07

Realization = 2 Subarea = 1 UNSATURATED ZONE

Layer=TSw_ ssAreaMatrix=2.9268E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.6358E+04	2.9510E+08	5.5889E+00	1.0000E+00
Np	5.9040E-03	1.0751E+02	2.0172E-06	1.0000E+00
Pu	1.2993E+00	2.3440E+04	4.4392E-04	1.0000E+00
Th	8.1654E+01	1.4730E+06	2.7898E-02	1.0000E+00
U	4.6442E-03	8.4781E+01	1.5868E-06	1.0000E+00

Layer=CHnv ssAreaMatrix=8.7611E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.8965E+04	2.2468E+08	5.5889E+00	1.0000E+00
Np	1.7673E-02	8.2092E+01	2.0172E-06	1.0000E+00
Pu	3.8892E+00	1.7847E+04	4.4392E-04	1.0000E+00
Th	2.4442E+02	1.1215E+06	2.7898E-02	1.0000E+00
U	1.3902E-02	6.4788E+01	1.5868E-06	1.0000E+00

Layer=CHnz ssAreaMatrix=8.0000E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.4712E+04	2.2803E+08	5.5889E+00	1.0000E+00
Np	1.6138E-02	8.3302E+01	2.0172E-06	1.0000E+00
Pu	3.5514E+00	1.8113E+04	4.4392E-04	1.0000E+00
Th	2.2319E+02	1.1383E+06	2.7898E-02	1.0000E+00
U	1.2694E-02	6.5740E+01	1.5868E-06	1.0000E+00

Layer=PPw_ ssAreaMatrix=6.6142E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	3.6966E+04	2.4144E+08	5.5889E+00	1.0000E+00
Np	1.3342E-02	8.8144E+01	2.0172E-06	1.0000E+00
Pu	2.9362E+00	1.9178E+04	4.4392E-04	1.0000E+00
Th	1.8452E+02	1.2052E+06	2.7898E-02	1.0000E+00
U	1.0495E-02	6.9548E+01	1.5868E-06	1.0000E+00

Layer=UCF_ ssAreaMatrix=6.9421E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	3.8799E+04	2.4144E+08	5.5889E+00	1.0000E+00
Np	1.4004E-02	8.8144E+01	2.0172E-06	1.0000E+00
Pu	3.0818E+00	1.9178E+04	4.4392E-04	1.0000E+00
Th	1.9367E+02	1.2052E+06	2.7898E-02	1.0000E+00
U	1.1016E-02	6.9548E+01	1.5868E-06	1.0000E+00

Layer=BFw_ ssAreaMatrix=2.8016E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5658E+04	2.9510E+08	5.5889E+00	1.0000E+00
Np	5.6513E-03	1.0751E+02	2.0172E-06	1.0000E+00
Pu	1.2437E+00	2.3440E+04	4.4392E-04	1.0000E+00
Th	7.8159E+01	1.4730E+06	2.7898E-02	1.0000E+00
U	4.4454E-03	8.4781E+01	1.5868E-06	1.0000E+00

Layer=UFZ_ ssAreaMatrix=2.7376E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5301E+04	2.9510E+08	5.5889E+00	1.0000E+00
Np	5.5224E-03	1.0751E+02	2.0172E-06	1.0000E+00
Pu	1.2153E+00	2.3440E+04	4.4392E-04	1.0000E+00
Th	7.6376E+01	1.4730E+06	2.7898E-02	1.0000E+00
U	4.3440E-03	8.4781E+01	1.5868E-06	1.0000E+00

Realization = 2 Subarea = 1 SATURATED ZONE

Layer=SAV ssAreaMatrix= 3.2900E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.8387E+04	2.8991E+08	0.0000E+00	0.0000E+00
Np	6.6366E-03	1.0564E+02	0.0000E+00	0.0000E+00
Pu	1.4605E+00	2.3028E+04	0.0000E+00	0.0000E+00
Th	9.1785E+01	1.4472E+06	0.0000E+00	0.0000E+00
U	5.2204E-03	8.3309E+01	0.0000E+00	0.0000E+00

Layer=STFF ssAreaMatrix= 4.8586E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.7154E+04	2.6827E+08	5.5889E+00	1.0000E+00
Np	9.8008E-03	9.7826E+01	2.0172E-06	1.0000E+00
Pu	2.1568E+00	2.1309E+04	4.4392E-04	1.0000E+00
Th	1.3555E+02	1.3391E+06	2.7898E-02	1.0000E+00
U	7.7094E-03	7.7164E+01	1.5868E-06	1.0000E+00

Realization = 2 Subarea = 1 SATURATED ZONE

Layer=SAV.

Nuclide	MobileRd
U	0.8331E+02

Am	0.2899E+09
Np	0.1056E+03
Pu	0.2303E+05
Th	0.1447E+07

Layer=STFF.

Nuclide	ImmobileRd
U	0.7716E+02
Am	0.2683E+09
Np	0.9783E+02
Pu	0.2131E+05
Th	0.1339E+07

Realization = 3 Subarea = 1 UNSATURATED ZONE

Layer=TSw_ ssAreaMatrix=2.9268E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.6670E+04	3.0072E+08	5.6955E+00	1.0000E+00
Np	8.6410E-03	1.5688E+02	2.9523E-06	1.0000E+00
Pu	1.5366E+00	2.7721E+04	5.2500E-04	1.0000E+00
Th	5.9877E+01	1.0802E+06	2.0458E-02	1.0000E+00
U	2.0062E-04	4.6192E+00	6.8546E-08	1.0000E+00

Layer=CHnv ssAreaMatrix=8.7611E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.9899E+04	2.2896E+08	5.6955E+00	1.0000E+00
Np	2.5866E-02	1.1968E+02	2.9523E-06	1.0000E+00
Pu	4.5995E+00	2.1106E+04	5.2500E-04	1.0000E+00
Th	1.7923E+02	8.2241E+05	2.0458E-02	1.0000E+00
U	6.0054E-04	3.7556E+00	6.8546E-08	1.0000E+00

Layer=CHnz ssAreaMatrix=8.0000E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.5564E+04	2.3238E+08	5.6955E+00	1.0000E+00
Np	2.3619E-02	1.2146E+02	2.9523E-06	1.0000E+00
Pu	4.2000E+00	2.1421E+04	5.2500E-04	1.0000E+00
Th	1.6366E+02	8.3468E+05	2.0458E-02	1.0000E+00
U	5.4837E-04	3.7967E+00	6.8546E-08	1.0000E+00

Layer=PPw_ ssAreaMatrix=6.6142E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	3.7671E+04	2.4605E+08	5.6955E+00	1.0000E+00
Np	1.9527E-02	1.2854E+02	2.9523E-06	1.0000E+00
Pu	3.4724E+00	2.2681E+04	5.2500E-04	1.0000E+00
Th	1.3531E+02	8.8378E+05	2.0458E-02	1.0000E+00
U	4.5338E-04	3.9612E+00	6.8546E-08	1.0000E+00

Layer=UCF_ ssAreaMatrix=6.9421E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	3.9539E+04	2.4605E+08	5.6955E+00	1.0000E+00
Np	2.0496E-02	1.2854E+02	2.9523E-06	1.0000E+00
Pu	3.6446E+00	2.2681E+04	5.2500E-04	1.0000E+00
Th	1.4202E+02	8.8378E+05	2.0458E-02	1.0000E+00
U	4.7586E-04	3.9612E+00	6.8546E-08	1.0000E+00

Layer=BFw_ ssAreaMatrix=2.8016E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5956E+04	3.0072E+08	5.6955E+00	1.0000E+00
Np	8.2711E-03	1.5688E+02	2.9523E-06	1.0000E+00
Pu	1.4708E+00	2.7721E+04	5.2500E-04	1.0000E+00
Th	5.7314E+01	1.0802E+06	2.0458E-02	1.0000E+00
U	1.9204E-04	4.6192E+00	6.8546E-08	1.0000E+00

Layer=UFZ_ ssAreaMatrix=2.7376E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5592E+04	3.0072E+08	5.6955E+00	1.0000E+00
Np	8.0824E-03	1.5688E+02	2.9523E-06	1.0000E+00
Pu	1.4373E+00	2.7721E+04	5.2500E-04	1.0000E+00
Th	5.6006E+01	1.0802E+06	2.0458E-02	1.0000E+00
U	1.8766E-04	4.6192E+00	6.8546E-08	1.0000E+00

Realization = 3 Subarea = 1 SATURATED ZONE

Layer=SAV ssAreaMatrix= 2.7505E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5665E+04	3.0304E+08	0.0000E+00	0.0000E+00
Np	8.1203E-03	1.5809E+02	0.0000E+00	0.0000E+00
Pu	1.4440E+00	2.7935E+04	0.0000E+00	0.0000E+00
Th	5.6268E+01	1.0885E+06	0.0000E+00	0.0000E+00
U	1.8853E-04	4.6471E+00	0.0000E+00	0.0000E+00

Layer=STFF ssAreaMatrix= 4.8602E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.7681E+04	2.7338E+08	5.6955E+00	1.0000E+00
Np	1.4349E-02	1.4271E+02	2.9523E-06	1.0000E+00
Pu	2.5516E+00	2.5201E+04	5.2500E-04	1.0000E+00
Th	9.9430E+01	9.8198E+05	2.0458E-02	1.0000E+00
U	3.3315E-04	4.2902E+00	6.8546E-08	1.0000E+00

Realization = 3 Subarea = 1 SATURATED ZONE

Layer=SAV.

Nuclide	MobileRd
U	0.4647E+01
Am	0.3030E+09
Np	0.1581E+03
Pu	0.2793E+05
Th	0.1089E+07

Layer=STFF.

Nuclide	ImmobileRd
U	0.4290E+01
Am	0.2734E+09
Np	0.1427E+03
Pu	0.2520E+05
Th	0.9820E+06

Realization = 4 Subarea = 1 UNSATURATED ZONE

Layer=TSw_ ssAreaMatrix=2.9268E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	9.9600E+01	1.7968E+06	3.4030E-02	1.0000E+00
Np	1.9668E-04	4.5481E+00	6.7199E-08	1.0000E+00
Pu	9.3831E-02	1.6937E+03	3.2059E-05	1.0000E+00
Th	2.9939E+01	5.4010E+05	1.0229E-02	1.0000E+00
U	1.3479E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=CHnv ssAreaMatrix=8.7611E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.9814E+02	1.3680E+06	3.4030E-02	1.0000E+00
Np	5.8873E-04	3.7014E+00	6.7199E-08	1.0000E+00
Pu	2.8087E-01	1.2898E+03	3.2059E-05	1.0000E+00
Th	8.9618E+01	4.1121E+05	1.0229E-02	1.0000E+00
U	4.0348E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=CHnz ssAreaMatrix=8.0000E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.7224E+02	1.3884E+06	3.4030E-02	1.0000E+00
Np	5.3759E-04	3.7417E+00	6.7199E-08	1.0000E+00
Pu	2.5647E-01	1.3090E+03	3.2059E-05	1.0000E+00
Th	8.1833E+01	4.1735E+05	1.0229E-02	1.0000E+00
U	3.6843E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=PPw_ ssAreaMatrix=6.6142E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.2508E+02	1.4701E+06	3.4030E-02	1.0000E+00
Np	4.4447E-04	3.9030E+00	6.7199E-08	1.0000E+00
Pu	2.1204E-01	1.3860E+03	3.2059E-05	1.0000E+00
Th	6.7657E+01	4.4190E+05	1.0229E-02	1.0000E+00
U	3.0460E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=UCF_ ssAreaMatrix=6.9421E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.3624E+02	1.4701E+06	3.4030E-02	1.0000E+00
Np	4.6650E-04	3.9030E+00	6.7199E-08	1.0000E+00
Pu	2.2256E-01	1.3860E+03	3.2059E-05	1.0000E+00
Th	7.1012E+01	4.4190E+05	1.0229E-02	1.0000E+00
U	3.1971E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=BFw_ ssAreaMatrix=2.8016E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	9.5337E+01	1.7968E+06	3.4030E-02	1.0000E+00
Np	1.8826E-04	4.5481E+00	6.7199E-08	1.0000E+00
Pu	8.9815E-02	1.6937E+03	3.2059E-05	1.0000E+00
Th	2.8657E+01	5.4010E+05	1.0229E-02	1.0000E+00
U	1.2902E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=UFZ_ ssAreaMatrix=2.7376E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	9.3162E+01	1.7968E+06	3.4030E-02	1.0000E+00
Np	1.8397E-04	4.5481E+00	6.7199E-08	1.0000E+00
Pu	8.7766E-02	1.6937E+03	3.2059E-05	1.0000E+00
Th	2.8004E+01	5.4010E+05	1.0229E-02	1.0000E+00
U	1.2608E-08	1.0002E+00	4.6053E-12	1.0000E+00

Realization = 4 Subarea = 1 SATURATED ZONE

Layer=SAV ssAreaMatrix= 3.5900E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.2217E+02	1.7401E+06	0.0000E+00	0.0000E+00
Np	2.4124E-04	4.4362E+00	0.0000E+00	0.0000E+00
Pu	1.1509E-01	1.6403E+03	0.0000E+00	0.0000E+00
Th	3.6722E+01	5.2307E+05	0.0000E+00	0.0000E+00
U	1.6533E-08	1.0002E+00	0.0000E+00	0.0000E+00

Layer=STFF ssAreaMatrix= 4.8572E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.6529E+02	1.6334E+06	3.4030E-02	1.0000E+00

Np	3.2640E-04	4.2255E+00	6.7199E-08	1.0000E+00
Pu	1.5572E-01	1.5398E+03	3.2059E-05	1.0000E+00
Th	4.9685E+01	4.9100E+05	1.0229E-02	1.0000E+00
U	2.2369E-08	1.0002E+00	4.6053E-12	1.0000E+00

Realization = 4 Subarea = 1 SATURATED ZONE

Layer=SAV.

Nuclide	MobileRd
U	0.1000E+01
Am	0.1740E+07
Np	0.4436E+01
Pu	0.1640E+04
Th	0.5231E+06

Layer=STFF.

Nuclide	ImmobileRd
U	0.1000E+01
Am	0.1633E+07
Np	0.4226E+01
Pu	0.1540E+04
Th	0.4910E+06

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-490	**2. Software Title and Version:** TPA 5.0.0b	**3. Project No:** 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): *volcano.f, tpa.inp, tpanames.dbs* and *driftsa.i.*

See Attachment A for selected text from a series of e-mails from B. Hill for the description.

5. Change Requested by: B. Hill Date: 8-20-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 8-20-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

#1 - Parameter name change:
OLD= `'DiameterOfVolcanicCone[m]'`
NEW= `'DiameterOfVolcanicConduit[m]'`
New values used as described in Attachment A.
#2 - In order to keep the intent of the geometric model the suggested change was not made, but rather a fully disrupted drift (similar to dogleg) algorithm was added to the geometric model. This required a new subroutine called *getdrifts*(), located in *volcano.f.*
#3 - Two points were added to the *usersuppliedpwisecdf* distribution in Attachment A to replace the first point:
0.0 0.0
0.1 0.084
#4 - new values used as described in Attachment A.

8. Implemented by: R. Janetzke	**Date:** 9-25-2004

9. Description of Acceptance Tests:

See ATTACHMENTS B & C.

10. Tested by: R. Nes	**Date:** 03-25-2005

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
DELETE	Volcano	DiameterOfVolcanicCone[m]					
ADD	Volcano	DiameterOfVolcanicConduit[m]	Used for calculating the number of packages ejected for an extrusive event in the geometric model. (Applies to ash evolution mode = 0 only)	Uniform	28, 280	Reflect a more accurate designation of the conduit.	

MODIFY TO	Volcano	NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]	Used for calculating the number of packages failed for the intrusive event in the distribution model.	usersuppliedpwisecdf	19 0 0. 0.1 0.084 200 0.094 600 0.117 1000 0.141 1400 0.175 1800 0.213 2110 0.257 2111 0.475 2827 0.562 3147 0.588 3148 0.712 5000 0.781 6300 0.813 7800 0.843 9122 0.881 9123 0.967 9444 0.969 9445 1.000		
MODIFY TO	Ashplumo	VolcanicEventDuration[s]		loguniform	8.64e4 2.59e5		
MODIFY TO	Ashplumo	VolcanicEventPower[W]		loguniform	9.0e9 5.0e11		

ATTACHMENT A

1) Conduit diameters (DiameterOfVolcanicCone) should thus be 28-280 m to represent 1-10 WP ejected with these HLW loadings. Currently, we're using 24.6-77.9 which was based on the SR design.

2) Assuming a rigid dike geometry grossly underestimates the number of failed WP during an intrusive event. Thus, NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[] should always be sampled, regardless of VolcanoModel=1 or 2.

3)
usersuppliedpwisecdf
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]
18
0 0.084
200 0.094
600 0.117
1000 0.141
1400 0.175
1800 0.213
2110 0.257
2111 0.475
2827 0.562
3147 0.588
3148 0.712
5000 0.781
6300 0.813
7800 0.843
9122 0.881
9123 0.967
9444 0.969
9445 1.000

4)
loguniform
VolcanicEventDuration[s]
8.64e4, 2.59e5
**
loguniform
VolcanicEventPower[W]
9.0e9, 5.0e11

ATTACHMENT B

Test Plan for TPA SCR#490

Test Plan Name:

Tested By: Razvan Nes, Albert Lozano Date: 03-25-2005

Host Machine: Frisco, Spock Host OS: Windows 2000 Professional, Unix

Baseline Version: tpa500b Test Version: tpa500c

Process Level (PL) Tests

PL-1. Name: Parameter name change in tpa.inp
Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : N/A
Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:
Test description:
- objective: ensure that old parameter name was replaced with the new one
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: N/A
- step by step test procedure to be used:
  1-visually examine tpa.inp of tpa500b and tpa500c, and identify in each situation where the parameter of interest is located
  2-ensure that old name 'DiameterOf VocanicCone[m]' used in the input file of tpa500b was replaced in tpa500c with 'DiameterOfVolcanicConduit[m], and check also *volcano.f*.
- pass/fail criteria: pass if the replacement was made correctly(i.e. according to PA-SCR-490)

Test Results:
-See ATTACHMENT C;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

PL-2.: Name: Implementation of a fully disrupted drift algorithm, and adding a new subroutine, getdrifts(), in volcano.f
Path for run directory:

Path for archive of results:
Environment variables:
Special input files or modifications to input files required : N/A
Special diagnostic code modifications required : add 'Print ' instructions in volcano.f (see ATTACHMENT C)
Program modes to be used (append flags, scenario/model switches, etc.): set VolcanoModel flag to 1 (Geometric Model)
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:N/A
Test description:
- objective: ensure that old distribution parameters were replaced with the new ones.
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: N/A
- step by step test procedure to be used:
  1-open volcano.f and go where subroutine getdrifts(drxy1out, drxy2out, nWPindrift, maxnumdrifts, ndrifts) is called
  2-put Print statements in volcano.f module of tpa500c, so the code will print drxy1out, x1, y1, drxy2out, x2, y2, nWPindrift
  3-visually compare the data printed in tpa output file tparun.txt as the result of these statements with the ones in *drifts. dat*
- pass/fail criteria: pass, if the two sets of data are identical.

Test Results:
-See ATTACHMENT C;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL): **PASS**

PL-3. Name: New points added in NumberOfMagmaInducedMechanicalFailuresRemainingInDrift distribution of tpa.inp-Volcano

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : N/A
Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:
Test description:
- objective: ensure that old parameter name was replaced with the new one
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: N/A
- step by step test procedure to be used:
  1-visually examine tpa.inp of tpa500b and tpa500c, and identify in each situation where NumberOfMagmaInducedMechanicalFailuresRemainingInDrift

distribution is located
2-visually compare the two distributions and ensure that old distribution used by tpa500b was replaced in tpa500c with the new one, that includes the new points as per PA-SCR-490.
- pass/fail criteria: pass if the replacement was made correctly (i.e. as per PA-SCR-490).

Test Results: -See ATTACHMENT C;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL): **PASS**

PL-4. Name: New values for 'VolcanicEventDuration[s]' and VolcanicEventPower[W]' in tpa.inp-Volcano

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : N/A
Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:

Test description:
- objective: ensure that old distribution parameters were replaced with the new ones.
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: N/A
- step by step test procedure to be used:
  1-visually examine tpa.inp of tpa500b and tpa500c, and identify in each situation where 'VolcanicEventDuration[s]' and VolcanicEventPower[W]' distributions are located
  2-visually compare the two distributions and ensure that old distribution used by tpa500b was replaced in tpa500c with the new ones, that includes the new points as per PA-SCR-490.
- pass/fail criteria: pass if the replacement was made correctly (i.e. as per PA-SCR-490).

Test Results: -See ATTACHMENT C;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL): **PASS**

ATTACHMENT C

PL-1: Input files of tpa 5.0.0b and 5.0.0c, shown below, were visually compared:

-Version 5.0.0b:

```
uniform
DiameterOfVolcanicCone[m]
24.6, 77.9
```

-Version 5.0.0c:

```
uniform
DiameterOfVolcanicConduit[m]
28.0, 280.0
```

Conclusion: Proposed name change was correctly implemented in tpa 5.0.0c, in the input file and tpanames.dbs of the same code version.

Volcano.f file of tpa500c:

```
c rwj 8-22-04; SCR 490;
c       name = 'DiameterOfVolcanicCone[m]'
        name = 'DiameterOfVolcanicConduit[m]'
```

PL-2: Print statements placed in *volcano.f*, and compared tpa output file with *drifts.dat*.

-Print statements in *volcano.f*:

```
                cc rwj 9-25-04; SCR490
                call getdrifts(drxy1out, drxy2out, nWPindrift, maxnumdrifts,
&                       ndrifts)
 print *,"maxnumdrifts = ",maxnumdrifts
 print *,"ndrifts = ",ndrifts
   print *," drxy1out     x1                y1",
&  " drxy2out     x2                y2"," nWPindrift"
   do i=1,ndrifts
     print '(4(1x,1pe15.7),i6)',drxy1out(1,i),drxy1out(2,i),
&    drxy2out(1,i),drxy2out(2,i), nWPindrift(i)
 enddo
 print *," "
   ikey=30231
```

-Printed data in the output file:

drxy1out x1	y1	drxy2out x2	y2	nWPindrift
5.4856719E+05	4.0789380E+06	5.4751062E+05	4.0792695E+06	180
5.4856305E+05	4.0788544E+06	5.4750210E+05	4.0791873E+06	181
5.4855890E+05	4.0787708E+06	5.4749357E+05	4.0791051E+06	181
5.4855476E+05	4.0786872E+06	5.4748505E+05	4.0790228E+06	182

5.4855062E+05	4.0786037E+06	5.4747653E+05	4.0789406E+06	183
5.4854648E+05	4.0785201E+06	5.4746801E+05	4.0788584E+06	184
5.4854233E+05	4.0784365E+06	5.4745948E+05	4.0787762E+06	184
5.4853819E+05	4.0783529E+06	5.4745096E+05	4.0786940E+06	185
5.4853405E+05	4.0782693E+06	5.4744244E+05	4.0786118E+06	186
5.4852990E+05	4.0781857E+06	5.4743392E+05	4.0785295E+06	187
5.4852576E+05	4.0781021E+06	5.4742540E+05	4.0784473E+06	187
5.4852162E+05	4.0780185E+06	5.4741687E+05	4.0783651E+06	188
5.4851747E+05	4.0779349E+06	5.4740835E+05	4.0782829E+06	189
5.4851333E+05	4.0778513E+06	5.4739983E+05	4.0782006E+06	190
5.4850919E+05	4.0777677E+06	5.4739131E+05	4.0781184E+06	190
5.4850505E+05	4.0776841E+06	5.4738279E+05	4.0780362E+06	191
5.4850090E+05	4.0776005E+06	5.4737426E+05	4.0779540E+06	192
5.4849676E+05	4.0775170E+06	5.4737981E+05	4.0778674E+06	190
5.4849261E+05	4.0774334E+06	5.4739430E+05	4.0777779E+06	187
5.4848847E+05	4.0773498E+06	5.4740879E+05	4.0776885E+06	184
5.4848433E+05	4.0772662E+06	5.4742327E+05	4.0775990E+06	181
5.4848018E+05	4.0771826E+06	5.4743776E+05	4.0775096E+06	177
5.4847604E+05	4.0770990E+06	5.4745225E+05	4.0774202E+06	174
5.4847190E+05	4.0770154E+06	5.4746674E+05	4.0773307E+06	171
5.4846775E+05	4.0769318E+06	5.4748099E+05	4.0772414E+06	168
5.4846361E+05	4.0768482E+06	5.4749496E+05	4.0771521E+06	165
5.4845947E+05	4.0767646E+06	5.4750893E+05	4.0770628E+06	162
5.4845532E+05	4.0766810E+06	5.4752290E+05	4.0769735E+06	159
5.4842592E+05	4.0766054E+06	5.4753687E+05	4.0768843E+06	151
5.4839439E+05	4.0765304E+06	5.4755084E+05	4.0767950E+06	144
5.4836286E+05	4.0764554E+06	5.4756481E+05	4.0767057E+06	136
5.4833133E+05	4.0763804E+06	5.4757877E+05	4.0766165E+06	128
5.4829979E+05	4.0763054E+06	5.4759274E+05	4.0765272E+06	120
5.4826826E+05	4.0762304E+06	5.4760671E+05	4.0764379E+06	112
5.4823673E+05	4.0761554E+06	5.4762068E+05	4.0763486E+06	105
5.4820519E+05	4.0760804E+06	5.4763465E+05	4.0762594E+06	97
5.4817366E+05	4.0760054E+06	5.4764861E+05	4.0761701E+06	89
5.4857133E+05	4.0790216E+06	5.4752920E+05	4.0793486E+06	177
5.4857548E+05	4.0791052E+06	5.4755785E+05	4.0794245E+06	173
5.4857962E+05	4.0791888E+06	5.4758651E+05	4.0795004E+06	169
5.4858377E+05	4.0792724E+06	5.4761516E+05	4.0795763E+06	165
5.4858791E+05	4.0793560E+06	5.4764381E+05	4.0796522E+06	161
5.4859258E+05	4.0794394E+06	5.4765057E+05	4.0797350E+06	160
5.4859744E+05	4.0795228E+06	5.4765615E+05	4.0798181E+06	160
5.4860230E+05	4.0796062E+06	5.4766173E+05	4.0799012E+06	160
5.4860715E+05	4.0796895E+06	5.4766731E+05	4.0799844E+06	160
5.4861201E+05	4.0797729E+06	5.4767290E+05	4.0800675E+06	160
5.4861686E+05	4.0798563E+06	5.4767848E+05	4.0801507E+06	160
5.4862172E+05	4.0799396E+06	5.4768406E+05	4.0802338E+06	160
5.4862657E+05	4.0800230E+06	5.4768964E+05	4.0803169E+06	159
5.4863143E+05	4.0801064E+06	5.4769523E+05	4.0804001E+06	159
5.4863629E+05	4.0801897E+06	5.4770081E+05	4.0804832E+06	159
5.4864114E+05	4.0802731E+06	5.4770639E+05	4.0805664E+06	159
5.4864600E+05	4.0803565E+06	5.4771197E+05	4.0806495E+06	116

-Printed data in *drifts. dat* :

```
Emplacement Block
          1
**  Drift Endpoints
**   x1              y1              x2              y2          numWP
 5.48567190E+05 4.07893803E+06 5.47510619E+05 4.07926950E+06   180
```

5.48563047E+05	4.07885444E+06	5.47502097E+05	4.07918728E+06	181
5.48558904E+05	4.07877084E+06	5.47493574E+05	4.07910506E+06	181
5.48554761E+05	4.07868725E+06	5.47485052E+05	4.07902284E+06	182
5.48550618E+05	4.07860366E+06	5.47476530E+05	4.07894062E+06	183
5.48546476E+05	4.07852006E+06	5.47468007E+05	4.07885841E+06	184
5.48542333E+05	4.07843647E+06	5.47459485E+05	4.07877619E+06	184
5.48538190E+05	4.07835288E+06	5.47450963E+05	4.07869397E+06	185
5.48534047E+05	4.07826929E+06	5.47442441E+05	4.07861175E+06	186
5.48529904E+05	4.07818569E+06	5.47433918E+05	4.07852953E+06	187
5.48525761E+05	4.07810210E+06	5.47425396E+05	4.07844731E+06	187
5.48521618E+05	4.07801851E+06	5.47416874E+05	4.07836509E+06	188
5.48517475E+05	4.07793491E+06	5.47408352E+05	4.07828287E+06	189
5.48513332E+05	4.07785132E+06	5.47399829E+05	4.07820065E+06	190
5.48509189E+05	4.07776773E+06	5.47391307E+05	4.07811844E+06	190
5.48505046E+05	4.07768414E+06	5.47382785E+05	4.07803622E+06	191
5.48500902E+05	4.07760054E+06	5.47374262E+05	4.07795400E+06	192
5.48496758E+05	4.07751695E+06	5.47379807E+05	4.07786737E+06	190
5.48492614E+05	4.07743336E+06	5.47394296E+05	4.07777793E+06	187
5.48488470E+05	4.07734977E+06	5.47408785E+05	4.07768849E+06	184
5.48484326E+05	4.07726617E+06	5.47423274E+05	4.07759905E+06	181
5.48480182E+05	4.07718258E+06	5.47437762E+05	4.07750961E+06	177
5.48476039E+05	4.07709899E+06	5.47452251E+05	4.07742017E+06	174
5.48471896E+05	4.07701539E+06	5.47466740E+05	4.07733074E+06	171
5.48467752E+05	4.07693180E+06	5.47480994E+05	4.07724137E+06	168
5.48463609E+05	4.07684821E+06	5.47494963E+05	4.07715210E+06	165
5.48459466E+05	4.07676462E+06	5.47508931E+05	4.07706282E+06	162
5.48455323E+05	4.07668102E+06	5.47522900E+05	4.07697355E+06	159
5.48425924E+05	4.07660535E+06	5.47536868E+05	4.07688427E+06	151
5.48394392E+05	4.07653035E+06	5.47550836E+05	4.07679500E+06	144
5.48362859E+05	4.07645535E+06	5.47564805E+05	4.07670572E+06	136
5.48331326E+05	4.07638035E+06	5.47578773E+05	4.07661645E+06	128
5.48299793E+05	4.07630535E+06	5.47592742E+05	4.07652717E+06	120
5.48268261E+05	4.07623035E+06	5.47606710E+05	4.07643790E+06	112
5.48236728E+05	4.07615535E+06	5.47620679E+05	4.07634862E+06	105
5.48205195E+05	4.07608035E+06	5.47634647E+05	4.07625935E+06	97
5.48173663E+05	4.07600535E+06	5.47648615E+05	4.07617007E+06	89

**
Emplacement Block
2
** Drift Endpoints

** x1	y1	x2	y2	numWP
5.48571334E+05	4.07902162E+06	5.47529205E+05	4.07934856E+06	177
5.48575478E+05	4.07910521E+06	5.47557855E+05	4.07942447E+06	173
5.48579623E+05	4.07918881E+06	5.47586505E+05	4.07950037E+06	169
5.48583767E+05	4.07927240E+06	5.47615155E+05	4.07957628E+06	165
5.48587911E+05	4.07935599E+06	5.47643805E+05	4.07965218E+06	161
5.48592583E+05	4.07943942E+06	5.47650567E+05	4.07973495E+06	160
5.48597439E+05	4.07952279E+06	5.47656149E+05	4.07981809E+06	160
5.48602295E+05	4.07960616E+06	5.47661732E+05	4.07990123E+06	160
5.48607151E+05	4.07968952E+06	5.47667314E+05	4.07998437E+06	160
5.48612007E+05	4.07977289E+06	5.47672896E+05	4.08006752E+06	160
5.48616863E+05	4.07985626E+06	5.47678479E+05	4.08015066E+06	160
5.48621719E+05	4.07993963E+06	5.47684061E+05	4.08023380E+06	160
5.48626574E+05	4.08002300E+06	5.47689643E+05	4.08031694E+06	159
5.48631430E+05	4.08010637E+06	5.47695226E+05	4.08040008E+06	159
5.48636286E+05	4.08018974E+06	5.47700808E+05	4.08048322E+06	159
5.48641142E+05	4.08027311E+06	5.47706390E+05	4.08056636E+06	159
5.48645998E+05	4.08035648E+06	5.47711973E+05	4.08064951E+06	116

Conclusion: Data printed in the tpa output and in *drifts.dat* are identical; subroutine *getdrifts.f* was correctly implemented and works properly.

PL-3: The distribution NumberOfMagmaInducedMechanicalFailuresRemainingInDrift, in the input files of versions 5.0.0b and 5.0.0c, are as follows:

-Version 5.0.0b:

```
loguniform
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]
1.0, 1402.0
```

-Version 5.0.0c:

```
usersuppliedpwisecdf
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]
19
0.      0.000
0.1     0.084
200.    0.094
600.    0.117
1000.   0.141
1400.   0.175
1800.   0.213
2110.   0.257
2111.   0.475
2827.   0.562
3147.   0.588
3148.   0.712
5000.   0.781
6300.   0.813
7800.   0.843
9122.   0.881
9123.   0.967
9444.   0.969
9445.   1.000
```

Conclusion: Visual comparison is confirming (1) old lognormal distribution was replaced with an user-provided one, and (2) two new points (0.0,0.0) were added to the distribution shown in Appendix A.

PL-4: Parameters VolcanicEventDuration and VolcanicEventPower as in the input files of 5.0.0b and 5.0.0c:

-Version 5.0.0b:

```
loguniform
```

```
VolcanicEventDuration[s]
1.8e5, 1.3e6

loguniform
VolcanicEventPower[W]
3.5e9, 5.3e11
```

-Version 5.0.0c:

```
loguniform
VolcanicEventDuration[s]
8.64e4, 2.59e5

loguniform
VolcanicEventPower[W]
9.0e9,  5.0e11
```

Conclusion: New values were correctly implemented in the tpa 5.0.0c input file.

ATTACHMENT B

I. Test Plan for TPA SCR-470

Test Plan Name: Create Minimum and Maximum Values Files of tpa.inp
Tested by: Zbigniew Wojcik **Date:** June 29, 2004
Host Machine: SUN Ultra-4 server: Spock **Host OS:** Sun Solaris 5.8
Baseline Version: TPA 5.0u **Test Version:** TPA 5.0u modified

PROCESS LEVEL (PL) Tests

PL1
Name: Visual inspection of new file tpamin.out with minimum values of tpa.inp.
- Input files or modifications to input files: tpa.inp
- Path for run directory of modified code: ../zwojcik/scr470/tpa50u_m/
- Program modes to be used: NumberOfRealizations =1.
- Pass / fail criteria: The test passes if:
1. The new file tpamin.out is generated by the modified code and is correct. The correctness is checked by visually testing whether tpamin.out has the minimum values of tpa.inp
Test output file tpamin.out is in pl1, and tpa.inp is in tpa_tst in subdirectory ../tpa50u_m/

PL2
Name: Visual inspection of new file tpamax.out with maximum values of tpa.inp.
- Input files or modifications to input files: tpa.inp
- Path for run directory of modified code: ../zwojcik/scr470/tpa50u_m/
- Program modes to be used: NumberOfRealizations =1.
- Pass / fail criteria: The test passes if:
1. The new file tpamax.out is generated by the modified code and is correct. The correctness is checked by visually testing whether tpamax.out has the maximum values of tpa.inp
Test output file tpamax.out is in pl2 in subdirectory ../tpa50u_m/

SYSTEM LEVEL (SL) Tests
SL1:
Name: Compare if files lhs.out, sp.tpa tpameans.out generated by the modified code are the same as generated by the initial code.
Path for run directory of initial code: ../zwojcik/scr470/tpa50u/
Path for run directory of modified code: ../zwojcik/scr470/tpa50u_m/
Paths for archive of results: ../zwojcik/scr470/tpa50u/ and ../zwojcik/scr470/tpa50u_m/
Special input files or modifications to input files: identical tpa.inp in ../zwojcik/scr470/tpa50u/ and ../zwojcik/scr470/tpa50u_m/
Program modes to be used: NumberOfRealizations =1.

- Pass / fail criteria: The test passes if:
1. The modified TPA runs successfully to completion;
2. The output files lhs.out, sp.tpa tpameans.out generated by the modified code are the same as generated by the initial code (except time stamps).
Test output file lhs.out is in lhs_sl in subdirectory ../tpa50u_m/, and test output file sp.tpa is in sp_ sl,
and output file tpameans.out is in tpameans_sl.

SL2:
Name: See if modified TPA runs successfully to completion when using tpamin.out as tpa.inp.
Path for run directory of modified code: ../zwojcik/scr470/tpa50u_m/
Path for archive of results: ../zwojcik/scr470/tpa50u_m/
Special input files or modifications to input files: using tpamin.out as tpa.inp in ../zwojcik/tpa50u_m/
Program modes to be used: NumberOfRealizations =1.
- Pass / fail criteria: The test passes if:
1. The modified TPA runs successfully to completion. Despite of note: "Run Successfully Completed" after subarea 10, there were messages printed to the screen: "IEEE floating-point exception flag raised" and "computing time differences using 2 digit year from subroutine date is not safe after year 2000".
Test input file tpa.inp with tpamin.out is in tpamin_sl in subdirectory ../tpa50u_m/.
The screen output is saved to file out_sl2 in subdirectory ../tpa50u_m/.

SL3:
Name: See if modified TPA runs successfully to completion when using tpamax.out as tpa.inp.
Path for run directory of modified code: ../zwojcik/scr470/tpa50u_m/
Path for archive of results: ../zwojcik/scr470/tpa50u_m/
Special input files or modifications to input files: using tpaminout as tpa.inp in ../zwojcik/scr470/tpa50u_m/
Program modes to be used: NumberOfRealizations =1.
- Pass / fail criteria: The test passes if:
1. The modified TPA runs successfully to completion. Despite of note: "Run Successfully Completed" after subarea 10, there were messages printed to the screen: "IEEE floating-point exception flag raised" and "computing time differences using 2 digit year from subroutine date is not safe after year 2000".
Test input file tpa.inp with tpamax.out is in tpamax_sl in subdirectory ../tpa50u_m/. The screen output is saved to file out_sl3 in subdirectory ../tpa50u_m/.

Combined tests description:

- Objective: Show that the modified TPA code outputs correct new files tpanim.out and tpamax.out, show that outcome files lhs.out, sp.tpa and tpameans.out are the same as generated by the initial code (except time stamps), and that TPA.e runs successfully when using

tpameans.out as tpa.inp, tpamin.out as tpa.inp and tpamax.out as tpa.inp.

- Assumptions: Setup instructions have been carried out.

- Constraints: none

- Output files to compare: new with old lhs.out, sp.tpa, tpameans.out. New tpamin.out, tpamax.out with tpa.inp.

- Pass / fail criteria: The test passes if:
1. The modified TPA runs successfully to completion;
2. The output files lhs.out, sp.tpa generated by the modified code are the same as by the initial code (except time stamps);
3. The output file tpameans.out generated by the modified code are the same as by the initial code (except time stamps);
4. The new files tpanim.out and tpamax.out are generated by the modified code and are correct;
5. The TPA runs successfully to completion when using tpaminout as tpa.inp;
6. The TPA runs successfully to completion when using tpamax.out as tpa.inp.

II. Step by step test procedure:

Subroutine writemeanvalues() was modified to create new files: tpamin.out and tpamax.out. The task was to test the modifications. Looked at the file reader.f to see the modifications to make the new outputs: they were similar to the making the output to the file tpameans.out, the primary goal of the subroutine writemeanvalues() up to now.

Prepared the testbed: I already had the newest version o tpa code, the tpa50u as subdirectory: ../zwojcik/scr470/tpa50u/
The ../zwojcik/scr470/tpa50u/ was treated as the reference before the changes.
Made copy of ../zwojcik/scr470/tpa50u/ into ../zwojcik/scr470/tpa50u_m/:
zwojcik /scr470# cp -r tpa50u tpa50u_m
Copied the modified reader.f into ../zwojcik/scr470/tpa50u_m/ overwriting previous reader.f.
So, the correct reader.f is in subdirectory ../zwojcik/scr470/tpa50u_m/ on SUN under UNIX and on scr470/tpa50u_m/ on CD.
Then installed and executed the pass / fail criteria comparing the ../zwojcik/scr470/tpa50u/ with the modified ../zwojcik/scr470/tpa50u_m/:
1. Compiled ../zwojcik/scr470/tpa50u_m/ by
make
Executed ../zwojcik/scr470/tpa50u_m by
tpa.e
The code executed successfully one realization to completion. The outcomes were normal.
2. Compared the output files lhs.out and sp.tpa of interest from the execution of ../zwojcik/tpa50u/ and the modified ../zwojcik/scr470/tpa50u_m/. The task was done as follow:

zwojcik# cp ../zwojcik/scr470/tpa50u_m/lhs.out lhs_470.out
zwojcik# mv lhs_470.out ../zwojcik/scr470/tpa50u/ .
zwojcik# diff -iw lhs.out lhs_470.out
The outcomes lhs.out and lhs_470.out were identical, there were no time stamps in the files.
zwojcik# cp ../zwojcik/t scr470/pa50u_m/sp.tpa sp_470.tpa
zwojcik# mv sp_470.tpa t ../zwojcik/scr470/tpa50u/ .
zwojcik# diff -i sp.tpa sp_470.tpa
The outcomes sp.tpa sp_470.tpa were the same, except for time stamps in the files in line 3.
3. Compared the output files tpameans.out from the execution of ../zwojcik/scr470/tpa50u/ and the modified ../zwojcik/scr470/tpa50u_m/. The task was done as follow:
zwojcik# cp ../zwojcik/scr470/tpa50u_m/ tpameans.out tpameans_470.out
zwojcik# mv tpameans_470.out ../zwojcik/scr470/tpa50u/ .
zwojcik# diff -i tpameans.out tpameans_470.out
The outcomes tpameans.out and tpameans_470.out were the same, except time stamps in the files in line 7.
4. The files tpamin.out and tpamax.out were created successfully when running tpa.e in ../zwojcik/scr470/tpa50u_m/. Both tpamin.out and tpamax.out were compared visually on the screen with tpa.inp in in ../zwojcik/scr470/tpa50u_m/:
(a) All types constants, iconstants, iFlag were the same in tpamin.out, tpamax.out and tpa.inp;
(b) Types uniform, loguniform, normal, lognormal in tpa.inp were mapped into type constant. The minimum value of two was taken into tpamin.out, and the maximum of two was taken into tpamax.out. The second value is defined as max, and the first value is defined as minimum.
(c) For triangular and logtriangular, the third value (defined as max) was taken into tpamax.out and the first value (defined as minimum) was taken into tpamin.out.
(d) Types beta, finiteexponentail were mapped into type constant. The second value (defined as max) was taken into tpamax.out and the minimum value listed before this maximum was taken into tpamin.out.
(e) Type hazardcurve was mapped into tpamin.out & tpamax.out without a change.
(f) Type correlateinputs was commented out in tpamin.out & tpamax.out, because after converting distributions into constants correlations make no sense: probabilities disappear.
(g) Type exponential was mapped into type constant. The -log(0.0001) / lambda was taken into tpamin.out, where lambda is the value existing in tpa.inp. The -log(0.9999) / lambda was taken into tpamax.out.

The visual testing was simplified: I was carefully looking for about subsequent 3 occurrences of each new type in tpa.inp testing correctness of its mapping into tpamin.out and tpamax.out. I could carefully examine all data specified in tpa.inp, but I understood that all mappings were done by the computer subroutine writemeanvalues() doing everything in the same way. Once one type was mapped, all other occurrences of the same type were mapped in the same way. Ron accepted this simplification of the visual test, in addition, however, that the simplified visual testing would be done the same way also from the end of the files. I did the visual inspection also from the ends of the files.
In addition, the tests passed when using tpamin.out as tpa.inp and independently when using tpamax.out as tpa.inp when executing tpa.e(see points (5) and (6) below).

5. The tpamin.out was used as tpa.inp and then tpa.e was executed successfully to completion in ../zwojcik/scr470/tpa50u_m/.
6. The tpamax.out was used as tpa.inp and then tpa.e was executed successfully to completion in ../zwojcik/scr470/tpa50u_m/.

Overall test status: **PASS.**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): 477	**2. Software Title and Version:** TPA5.0s	**3. Project No:** 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): check_timenextevent.t, check_payload_glass.t, exec.f, invent.f, reader.f, retrieve_input.h, retrieve_input.t, sampler.f, tpa.inp, update_input.h, update_input.t, samplerb.i, samplerd.i, samplere.i, sampleri.i, samplerv.i, samplerw.i.

1) Remove DistanceCutoffForDoseConversionDualityInDCAGS[km] from *tpa.inp.*
2) Two duplicate name error messages in *reader.f* report an incorrect line number.
3) Error message from *reader.f* gives line number off by 1 when number of nuclides is tested against maximum possible. Also, test uses maxnnucl - maxclnuc when it only needs to use maxnnucl.
4) Add checks to prevent divide by 0 for the 2 sampled parameters WastePackagePayload[MTU] and EquivalentMTUPayloadOfGlassPackage[MTU]. Also, check that FractionOfRepositoryWaste InGlassForm[] is between 0.0 and 1.0, inclusive.
5) Error message in *invent.f* (newinventdb) gives the name of the subroutine as cipermtuat emplaceperiso instead of newinventdb.
6) Remove warning messages displayed on screen during run when VolcanismDisruptive ScenarioFlag(yes=1,no=0) is set to 1 and check in code instead. Correct maximum value for TimeOfNextVolcanicEventinRegionOfInterest[yr] and TimeOfNextFaultingEventinRegionOf Interest[yr] if necessary and print message.
7) When TimeOfNextVolcanicEventinRegionOfInterest[yr] is constant and is the same as MaximumTime[yr], with DirectReleaseOnlyFlag[yes=1,np=0] set to 1, TPA code aborts.

5. Change Requested by: Ron Janetzke Date: 11-22-2003	**6. Change Authorized by** (*Software Developer*): Ron Janetzke Date: 11-22-2003 R. Janetzke

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment A.

Affected automated test files: check_timenextevent.t, check_payload_glass.t, retrieve_input.t, and update_input.t

8. Implemented by: Carol S. Scherer Carol S. Scherer	**Date:** 5-05-2004

9. Description of Acceptance Tests: The software was tested in accordance with the Test Plan for TPA SCR #477 (see tp_scr477.wpd). The software, test directories, and test results are contained on a CD labeled "TPA SCR #472 - Test Directories (Code Development)." All tests passed.

10. Tested by: Carol S. Scherer Carol S. Scherer	**Date:** 5-05-2004

CNWRA Form TOP-5 (05/2000)

ATTACHMENT A

Description of Change(s) or Problem Resolution:

1) *Remove DistanceCutoffForDoseConversionDualityInDCAGS[km] from tpa.inp.*

Parameter was commented out in *tpa.inp*.

2) *Two duplicate name error messages in reader.f report an incorrect line number.*

Code was added to the two duplicate nuclide name error checks to display the duplicate name. The 'Look on line . . .' message was changed to 'Look on or above line . . .'.

3) *Error message from reader.f gives line number that is off by 1 when number of nuclides read is tested against maximum number possible. Also, test uses maxnnucl - maxclnuc when it only needs to use maxnnucl.*

The code was displaying the variable 'iline' which had already been incremented. Instead of reporting 'iline', the code now reports 'iline - 1'.

4) *Add checks to prevent divide by 0 the 2 sampled parameters WastePackagePayload[MTU] and EquivalentMTUPayloadOfGlassPackage[MTU]. Also, check that FractionOfRepository WasteInGlassForm[] is between 0.0 and 1.0, inclusive.*

A subroutine called check_payload_glass was added in *reader.f*. It is called by another new subroutine called check_inputs, which is called after tpa.inp is read in. Check_payload_glass includes all three checks.

5) *Error message in invent.f (newinventdb) gives the name of the subroutine as cipermtuat emplaceperiso instead of newinventdb.*

The message was corrected.

6) *Remove warning messages displayed on screen during run when VolcanismDisruptive ScenarioFlag(yes=1,no=0) is set to 1 and check in code instead. Correct maximum value for TimeOfNextVolcanicEventinRegionOfInterest[yr] and TimeOfNextFaultingEventinRegionOfInterest[yr] if necessary and print message.*

The code in *exec.f* that displayed the NOTEs was commented out.

7) *When TimeOfNextVolcanicEventinRegionOfInterest[yr] is set to constant and is the same as MaximumTime[yr], with DirectReleaseOnlyFlag[yes=1,np=0] set to 1, TPA code will abort.*

In exec.f, approximately line 4734, change the code from 'if (tim(ntim) .le.

voltimeofevent) then' to if (tim(ntim) .lt. voltimeofevent) then'. This corrects the problem that made the code crash.

Three new subroutines were added in reader.f: *1) check_inputs* which calls other subroutines that check the input values and corrects them after comparing them to other inputs, if necessary; *2) check_timenextevent* which compares TimeOfNextVolcanicEventinRegionOf Interest[yr] or TimeOfNextFaultingEventinRegionOfInterest[yr] to MaximumTime[yr]; and *3) check_payload_glass*. If TimeOfNextFaultingEventinRegionOfInterest[yr] is a sampled parameter with a maximum time, then this maximum time must be equal to the value for MaximumTime[yr]. If TimeOfNextVolcanicEventinRegionOfInterest[yr] is a sampled parameter with a maximum time, then this maximum time must be less than or equal to the value for MaximumTime[yr]. A check is also made that the minimum time is greater than 0.0. If either value is incorrect, the values are reset to the correct values. The subroutine *check_payload_glass* is also called to check the values input for WastePackagePayload[MTU], EquivalentMTUPayloadOfGlassPackage[MTU], and FractionOfRepositoryWasteInGlassForm[]. The payload input values cannot be 0.0 or less. The fraction must be between 0.0 and 1.0, inclusive.

Check_inputs is called after all of tpa.inp is read but before parameters are sampled. (NOTE: With the addition of *check_inputs*, it is possible to cull error checks out of other routines and add new subroutines in *reader.f* to handle value checks for input parameters. This would have two benefits: 1) error checks are made earlier and if the code is going to be aborted due to an invalid input, the stop will occur before processing of the data occurs; 2) some input value checks are done in multiple places so the total number of checks could be reduced.)

Modifications To Existing Code

Differences between the original code and the code modified for SCR477 are detailed below:

1) exec.f:

```
1828,1850c2251,2270
< c css -c css - 1/27/2004; SCR477:  NOTES no longer needed
c       if( iflagvolcano .eq. 1 ) then
c         print *, ' '
c         print *,
c      &  '***>>> NOTE: When running with volcanism, verify that   <<<***'
c         print *,
c      &  '***>>> the maximum value of the PDF for parameter       <<<***'
c         print *,
c      &  '***>>> TimeOfNextVolcanicEventinRegionOfInterest[yr] is <<<***'
c         print *,
c      &  '***>>> equal to the parameter MaximumTime[yr].          <<<***'
c         print *,
```

```
c     &  '***>>>                                                  <<<***'
c        print *,
c     &  '***>>> Also, verify that the maximum total of both      <<<***'
c        print *,
c     &  '***>>> ejected and failed in drift volcanic failures    <<<***'
c        print *,
c     &  '***>>> not exceed the number of WPs in the subarea.     <<<***'
c        print *, ' '
c        print *, ' '
c      endif
c SCR477:  end change
 1/27/2004; SCR477:  NOTES no longer needed
---
      if( iflagvolcano .eq. 1 ) then
        print *, ' '
        print *,
     &  '***>>> NOTE: When running with volcanism, verify that   <<<***'
        print *,
     &  '***>>> the maximum value of the PDF for parameter       <<<***'
        print *,
     &  '***>>> TimeOfNextVolcanicEventinRegionOfInterest[yr] is <<<***'
        print *,
     &  '***>>> equal to the parameter MaximumTime[yr].          <<<***'
        print *,
     &  '***>>>                                                  <<<***'
        print *,
     &  '***>>> Also, verify that the maximum total of both      <<<***'
        print *,
     &  '***>>> ejected and failed in drift volcanic failures    <<<***'
        print *,
     &  '***>>> not exceed the number of WPs in the subarea.     <<<***'
        print *, ' '
        print *, ' '
      endif

3378,3385c4374,4380
< c css - 12/29/2004; SCR477:
< c                 if (tim(itim) .le. voltimeofevent) then
<                  if (tim(itim) .lt. voltimeofevent) then
< c SCR477: end change
<                    wpsfailedtime(4,1,2) = tim(itim)
<                  else
<                    go to 936
<                  endif
---
> c css - 12/29/2003:  scr477
> c                   if (tim(itim) .le. voltimeofevent) then
>                   if (tim(itim) .lt. voltimeofevent) then
>                      wpsfailedtime(4,1,2) = tim(itim)
>                   else
>                      go to 936
>                   endif
```

2) invent.f

in subroutine newinventdb:

change: “print *, ' ***>>> Error in cipermtuatemplaceperiso <<<***'” and

change: “print *, ' ***>>> Error in INVENT <<<***”

to: “print *, ' ***>>> Error in newinventdb <<<***”

3) reader.f:

```
168a155,158
> c css - 2/13/2004; SCR447 - correct error messages
>       character*6  dup_name
> c SCR477: end change
>

789a760,761
> c css - 2/2/2004; SCR477 - test needs to occur regardless of input type
> c                          so move it further down - see call check_inputs

791,794c763,766
<          if (name .eq.
<      &       'TimeOfNextVolcanicEventinRegionOfInterest[yr]') then
<               timemaxvolcano = xmax
<          end if
---
> c         if (name .eq.
> c     &       'TimeOfNextVolcanicEventinRegionOfInterest[yr]') then
> c              timemaxvolcano = xmax
> c         end if

1253a1212,1213
> c css: 12-31-2003; SCR477: only need to compare against maxnnucl
> cc     &      (nnucl .gt. maxnnucl - maxclnuc) ) then

1258c1215,1216
<      &      (nnucl .gt. maxnnucl - maxclnuc) ) then
---
> c     &      (nnucl .gt. maxnnucl - maxclnuc) ) then
>      &      (nnucl .gt. maxnnucl) ) then

1261c1219,1220
<           print *, ' (nnucl .lt. 1) .or. (nnucl .gt. maxnnucl-maxclnuc)'
---
> c          print *, ' (nnucl .lt. 1) .or. (nnucl .gt. maxnnucl-maxclnuc)'
>           print *, ' (nnucl .lt. 1) .or. (nnucl .gt. maxnnucl)'

1263c1222,1223
<           print *, ' maxnnucl -maxclnuc= ', maxnnucl-maxclnuc
---
> c          print *, ' maxnnucl -maxclnuc= ', maxnnucl-maxclnuc
>           print *, ' maxnnucl = ', maxnnucl

1268c1228
< cc end of change SCR368
---
> c SCR477:  end change

1428c1387,1399
<           print *, ' Look on line = ', iline
---
> c css - 12/31/2003; SCR477:  line # incorrect
```

```
> c          print *, ' Look on line = ', iline
>           i = 2
>           dup_name = '      '
>           do while ((i .le. numclnuc) .and. (dup_name .eq. '      '))
>              if (iinames(i-1) .eq. iinames(i)) then
>                 dup_name = names(ipt(i))
>              end if
>              i = i + 1
>           end do
>           print *, ' Look at or above line = ', iline,
>      &             ' for duplicate name = ', dup_name
> c SCR477:  end change

1616a1574,1581
> c css - 2/2/2004; SCR477 - add test for
TimeOfNextVolcanicEventinRegionOfInterest
> c                          add test for WastePackagePayload[MTU],
> c                          EquivalentMTUPayloadOfGlassPackage[MTU], and
> c                          FractionOfRepositoryWasteInGlassForm[]
> c
> c   SPECIAL TESTS FOR INPUT VALUES
>       call check_inputs()
> c - end change:  SCR477

1973,1982c1917,1929
<         else if( timemax .lt. timemaxvolcano ) then
<            print *, ' '
<            print *, ' ***>>> Error in Reader <<<*** '
<            print *, ' problem with MaximumTime or '
<            print *, ' with TimeOfNextVolcanicEventinRegionOfInterest'
<            print *, '  timemax .lt. timemaxvolcano '
<            print *, ' MaximumTime = ', timemax
<            print *, ' timemaxvolcano = ', timemaxvolcano
<            print *, ' '
<            CALL QUERYSTOP()
---
> c css - 2/2/2004; SCR477 - test moved to subroutine
> c                          check_timenextevent
> c        else if( timemax .lt. timemaxvolcano ) then
> c           print *, ' '
> c           print *, ' ***>>> Error in Reader <<<*** '
> c           print *, ' problem with MaximumTime or '
> c           print *, ' with TimeOfNextVolcanicEventinRegionOfInterest'
> c           print *, '  timemax .lt. timemaxvolcano '
> c           print *, ' MaximumTime = ', timemax
> c           print *, ' timemaxvolcano = ', timemaxvolcano
> c           print *, ' '
> c           CALL QUERYSTOP()
> c SCR477:  end change

4221a4071,4073
> c css - 2/13/2004; SCR447 - correct error messages
>       character*6  dup_name
> c SCR477: end change

4466c4311,4323
<         print *, ' Look on line = ', iline
---
> c css - 12/31/2003; SCR477:  line # incorrect
> c          print *, ' Look on line = ', iline
```

```
>            i = 2
>            dup_name = '        '
>            do while ((i .le. numclnuc) .and. (dup_name .eq. '        '))
>               if (iicldnames(i-1) .eq. iicldnames(i)) then
>                  dup_name = cldnames(ipt(i))
>               end if
>               i = i + 1
>            end do
>            print *, ' Look at or bove line = ', iline,
>      &              ' for duplicate name = ', dup_name
> c SCR477:  end change
```

4) sampler.f:

no modifications to existing code were made - new subroutines were added

5) tpa.inp:

```
6277,6279c6278,6281
< constant
< DistanceCutoffForDoseConversionDualityInDCAGS[km]
< 19.99
---
> * css - 12/31/2003; SCR477 - parameter no longer used
> *constant
> *DistanceCutoffForDoseConversionDualityInDCAGS[km]
> *19.99
```

New Code

The following subroutines and files were added to the **TPA** code:

1. subroutine *check_inputs* in *reader.f*:
2. subroutine *check_timenextevent* in *reader.f*:
3. subroutine *check_payload_glass* in *reader.f*
4. subroutine *retrieve_input* in *sampler.f*:
5. subroutine *update_input* in *sampler.f*:
6. *retrieve_input.h*:
7. *update_input.h*:
8. *check_timenextevent.h*
9. *check_payload_glass.t*
10. *check_timenextevent.t*
11. *retrieve_input.t*
12. *update_input.t*

Note: No .h files were created for *check_inputs* or *check_payload_glass*. No parameters are passed to these subroutines. No .t file was created for *check_inputs*. This routine simply calls other subroutines that perform input value checks.

05/05/4

Test Plan/Report for TPA SCR #477

(Code Development Phase)

Test Plan Name: Correct Errors, Add Error Checks And Remove Obsolete Code And Parameters

Tested By: Carol S. Scherer

Date: May 5, 2004

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0r (4.2 solapps compiler)

Test Version: TPA 5.0r modified (4.2 solapps compiler)

Code Modifications:

The following code modifications were made to **TPA** for SCR #477 (*see scr477.wpd*):

1. The parameter DistanceCutoffForDoseConversionDualityInDCAGS[km] is no longer used and was commented out of *tpa.inp*. Code that used this parameter had been commented out before.

2. The code in *reader.f* that displayed error messages when duplicate names were input for radionuclides reported the wrong line number in *tpa.inp*. Code was added to the two duplicate nuclide name error checks to display the duplicate name. The 'Look on line . . .' message was changed to 'Look on or above line . . .'.

3. The code in *reader.f* that displayed an error when the maximum number of nuclides was exceeded was displaying the variable ***iline*** which had already been incremented and so was off by 1. Instead of reporting ***iline***, the code now reports ***iline - 1***.

4. A subroutine called **check_payload_glass** was added in *reader.f*. It is called by another new subroutine called **check_inputs**, which is called after tpa.inp is read in. **Check_payload_glass** includes checks for WastePackagePayload[MTU] (must be greater than 0.0), EquivalentMTUPayloadOfGlassPackage[MTU] (must be greater than 0.0), and FractionOfRepositoryWasteInGlassForm[] (must be between 0.0 and 1.0, inclusive). The error checks for 0.0 prevent a divide by 0.0 in subsequent code.

5. The error message in invent.f that said 'Error in cipermtuatemplaceperiso' was corrected to read 'Error in newinventdb'.

6. The code in *exec.f* that displayed the NOTEs about TimeOfNextVolcanicEventin RegionOf Interest[yr], MaximumTime[yr], and Waste Packages was commented out. The messages are no longer needed because the conditions are checked automatically by the code.

7. *When TimeOfNextVolcanicEventinRegionOfInterest[yr] is set to constant and is the same as MaximumTime[yr], with DirectReleaseOnlyFlag(yes=1,no=0) set to 1, TPA code will abort. VolcanismDisruptiveScenarioFlag(yes=1,no=0)* must also be set to 1. Two new subroutines were added in reader.f: 1) **check_inputs** which calls other subroutines that check the input values and corrects them after comparing them to other inputs, if necessary; and 2) **check_timenextevent** which compares TimeOfNext VolcanicEventinRegionOfInterest[yr] to MaximumTime[yr]. If TimeOfNextVolcanic Eventin RegionOfInterest[yr] is a sampled parameter with a maximum time, then this maximum time must be less than or equal to the value for MaximumTime[yr]. A check is also made that the minimum time is greater than or equal to 0.0. If either value is incorrect, the values are reset to the correct values. The same checks are made for TimeOfNextFaultingEventinRegionOfInterest[yr], except that the maximum time for this event must be equal to the value for MaximumTime[yr].

   Check_inputs is called after all of *tpa.inp* is read but before parameters are sampled. Two new utility subroutines were added to *sampler.f*: 1) **retrieve_input** and 2) **update_input**. **Retrieve_input** accepts a parameter name, finds the index for that parameter name in the input arrays, and uses the index to retrieve the data from *tpa.inp* associated with that parameter name. **Update_input** is called with modified data values to be stored over the original input values in the input arrays.

Testing Setup:

Directories/paths used for testing:
$HOME = /net/spock/home/cscherer
Path for run directory: ***$HOME/scr477***

Environment variables:

TPA_TEST = $HOME ***/scr477***
TPA_DATA = $HOME ***/scr477***

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 477 - Test Directories (Code Development)*" (attached).

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectory: ***scr477***.

2. In the directory ***scr477***, create the following subdirectories: ***flt1, flt2, flt3, flt4, flt5, slt1, slt2, slt3, slt4, slt5,*** and ***slt6.***

3. Copy **TPA** version 5.0r to the run directory. Compile *tpa.e* using *Makefile4.2*. Save a copy of the executable as *tpa_vr.e*. Save a copy of the original source code file for any file that is modified for SCR477. Save a copy of the original *tpa.inp* as *tpa_vr.inp*.

4. Merge in the changes to *sampler.f* and *reader.f* for version s into the version r files. Save these files as *sampler_tpa50s.f* and *reader_tpa50s.f*. Modify files as described in *scr_477.wpd,* using *sampler_tpa50s.f* and *reader_tpa50s.f* for *sampler.f* and *reader.f*, respectively. Recompile *tpa.e* using *Makefile4.2*. Save a copy of the executable as *tpa_scr477.e*. Save a copy of the modified *tpa.inp* as *tpa_scr477.inp*.

5. Compile and run version r of the TPA code using *tpa_vr.inp*. Save a copy of the output from this run as *tpa_vr.out*.

Functional Level Tests:

These tests are designed to demonstrate that the modified and new code modules are implemented correctly and produce expected results.

1. Name: Test Functionality Of New Subroutines *retrieve_input* And *update_input* Using Sampled Parameter TimeOfNextVolcanicEventinRegionOfInterest[yr]

   Paths for archives of results: ***$HOME /scr477/flt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: make the following changes to *reader_scr477_s.f* and *sampler_scr477_s.f*. Save as *reader_flt1.f* and *sampler_flt1.f*, respectively.

   diff reader_scr477_s.f reader_flt1.f

```
4577a4578,4589
> c SCR477 - begin test
>       print *, 'in check_timenextevent - before call to ' //
>      &         'retrieve_input'
```

```
>       print *, '  ptype  = ', ptype
>       print *, '  pindex = ', pindex
>       print *, '  dp1    = ', dp1
>       print *, '  dp2    = ', dp2
>       print *, '  dp3    = ', dp3
>       print *, '  dp4    = ', dp4
>       print *, '  i1     = ', i2
>       print *, '  i2     = ', i2
> c SCR477 - end test

4579a4592,4603
> c SCR477 - begin test
>       print *, 'in check_timenextevent - after call to ' //
>      &         'retrieve_input'
>       print *, '  ptype  = ', ptype
>       print *, '  pindex = ', pindex
>       print *, '  dp1    = ', dp1
>       print *, '  dp2    = ', dp2
>       print *, '  dp3    = ', dp3
>       print *, '  dp4    = ', dp4
>       print *, '  i1     = ', i2
>       print *, '  i2     = ', i2
> c SCR477 - end test

4644a4669,4680
> c SCR477 - begin test
>       print *, 'in check_timenextevent - before call to ' //
>      &         'update_input'
>       print *, '  ptype  = ', ptype
>       print *, '  pindex = ', pindex
>       print *, '  dp1    = ', dp1
>       print *, '  dp2    = ', dp2
>       print *, '  dp3    = ', dp3
>       print *, '  dp4    = ', dp4
>       print *, '  i1     = ', i2
>       print *, '  i2     = ', i2
> c SCR477 - end test

4646a4683,4694
> c SCR477 - begin test
>       print *, 'in check_timenextevent - after call to ' //
>      &         'update_input'
>       print *, '  ptype  = ', ptype
>       print *, '  pindex = ', pindex
>       print *, '  dp1    = ', dp1
>       print *, '  dp2    = ', dp2
>       print *, '  dp3    = ', dp3
>       print *, '  dp4    = ', dp4
>       print *, '  i1     = ', i2
>       print *, '  i2     = ', i2
> c SCR477 - end test
```

diff sampler_scr477_s.f sampler_flt.f

```
2561a2562,2574
>
> c SCR477 - begin test
>       print *, 'in check_timenextevent - before retrieval'
>       print *, '  ptype  = ', ptype
>       print *, '  pindex = ', pindex
>       print *, '  dp1    = ', dp1
>       print *, '  dp2    = ', dp2
>       print *, '  dp3    = ', dp3
>       print *, '  dp4    = ', dp4
>       print *, '  i1     = ', i2
>       print *, '  i2     = ', i2
> c SCR477 - end test

2598a2612,2623
> c SCR477 - begin test
>       print *, 'in check_timenextevent - after retrieval'
>       print *, '  ptype  = ', ptype
>       print *, '  pindex = ', pindex
>       print *, '  dp1    = ', dp1
>       print *, '  dp2    = ', dp2
>       print *, '  dp3    = ', dp3
>       print *, '  dp4    = ', dp4
>       print *, '  i1     = ', i2
>       print *, '  i2     = ', i2
> c SCR477 - end test

2656a2682,2693
> c SCR477 - begin test
>       print *, 'in update_input - before change'
>       print *, '  pindex = ', pindex
>       print *, '  ptype  = ', ptype
>       print *, '  dp1    = ', dp1
>       print *, '  dp2    = ', dp2
>       print *, '  dp3    = ', dp3
>       print *, '  dp4    = ', dp4
>       print *, '  i1     = ', i2
>       print *, '  i2     = ', i2
> c SCR477 - end test

2700a2738,2749
> c SCR477 - begin test
>       print *, 'in update_input - after change'
>       print *, '  pindex              = ', pindex
>       print *, '  ptype               = ', ptype
>       print *, '  dat1(',pindex,')    = ', dat1(pindex)
>       print *, '  dat2(',pindex,')    = ', dat2(pindex)
>       print *, '  dat3(',pindex,')    = ', dat3(pindex)
>       print *, '  dat4(',pindex,')    = ', dat4(pindex)
>       print *, '  idat1(',pindex,') = ', idat2(pindex)
>       print *, '  idat2(',pindex,') = ', idat2(pindex)
> c SCR477 - end test
```

Program modes to be used: use tpa_scr477.inp and make the modifications shown in the following table:

Test Case	Parameter Type	Parameter Name	Value(s)
flt1a	iflag	VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
	iflag	DirectReleaseOnlyFlag(yes=1,no=0)	1
	constant	TimeOfNextVolcanicEventinRegionOfInterest [yr]	11,000.0
flt1b	iflag	VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
	iflag	DirectReleaseOnlyFlag(yes=1,no=0)	1
	constant	TimeOfNextVolcanicEventinRegionOfInterest [yr]	-1.0
flt1c	iflag	VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
	iflag	DirectReleaseOnlyFlag(yes=1,no=0)	1
	finiteexponential	TimeOfNextVolcanicEventinRegionOfInterest [yr]	100.0,11000.0,1.0e-7
flt1d	iflag	VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
	iflag	DirectReleaseOnlyFlag(yes=1,no=0)	1
	uniform	TimeOfNextVolcanicEventinRegionOfInterest [yr]	100.0,11000.0

Save these input files as *tpa_flt1a.inp*, *tpa_flt1b.inp*, *tpa_flt1c.inp*, and *tpa_flt1d.inp*.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code
  - correctly retrieves and passes input data between subroutines,
  - correctly identifies and corrects invalid input data, and
  - displays a message to the user showing the original and modified data.

- assumptions: none.

- constraints: the files *tpa_flt1a.out, tpa_flt1b.out, tpa_flt1c.out, and tpa_flt1d.out* do not exist in the run directory.

- output files to compare or examine: *tpa_flt1a.out, tpa_flt1b.out, tpa_flt1c.out,* and *tpa_flt1d.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. using the modified files specified above, recompile the **TPA** code and save a copy of the executable as *tpa_flt1.e*
  3. copy *tpa_flt1a.inp* to *tpa.inp*
  4. run *tpa.e* using command "***tpa.e > tpa_flt1a.out***"
  5. copy *tpa_flt1b.inp* to *tpa.inp*
  6. run *tpa.e* using command "***tpa.e > tpa_flt1b.out***"
  7. copy *tpa_flt1c.inp* to *tpa.inp*
  8. run *tpa.e* using command "***tpa.e > tpa_flt1c.out***"
  9. copy *tpa_flt1d.inp* to *tpa.inp*
  10. run *tpa.e* using command "***tpa.e > tpa_flt1d.out***"
  11. copy input and output files to the subdirectory ***flt1***
  12. look at files *tpa_flt1a.out, tpa_flt1b.out, tpa_flt1c.out,* and *tpa_flt1d.out*

- pass/fail criteria: the test passes if:

  1. in each output file, the input data values are reported correctly.
  2. in each output file, invalid input data are flagged and modified.
  3. each time an input value is modified, an appropriate message to the user is displayed.

Results of running test:

PASSED.

2. Name: Test Results of new subroutine *retrieve_input.*

Paths for archives of results: ***$HOME /scr477/flt2***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: use *retrieve_input.t* and recompile **TPA**. There are multiple test cases in *retrieve_input.t* that can be selected individually by the tester. Any combination of the test cases can be selected and run at the same time.

Program modes to be used: use *tpa_scr477.inp*

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to verify that the new and modifed code produces expected results.

- assumptions: test FLT 2 will not be run at the same time as test FLT3; the special *tpa.inp* file used for FLT 3 will cause some FLT 2 tests to fail

- constraints: the file *tpa_flt2.out* does not exist in the run directory.

- output files to compare or examine: *tpa_flt2.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. run *tpa.e* using command "***tpa.e > tpa_flt2.out***"
  3. copy input and output files to ***flt2***
  4. look at the output file

- pass/fail criteria: the test passes if:

  1. in the output file, all test cases are listed as 'PASSED'.

Results of running test:

PASSED.

3. Name: Test Results of new subroutine *update_input*.

Paths for archives of results: ***$HOME /scr477/flt3***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: use *update_input.t* and recompile **TPA**. There are multiple test cases contained in *update_input.t* that can be selected individually by the tester. There are four abort cases in *update_input.f*. No tests after the first abort case will be run.

Program modes to be used: use base case *tpa_scr477.inp* and make the following modifications:

Set TimeOfNextFaultingEventinRegionOfInterest[yr] to 100.0, 9000.0, 2.0e-5.
Set TimeOfNextVolcanicEventinRegionOfInterest[yr] to 100.0, 11000.0, 1.0e-7.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to verify that the new and modified code produces expected results.

- assumptions: test FLT3 will not be run at the same time as test FLT2

- constraints: the file *tpa_flt3.out* does not exist in the run directory.

- output files to compare or examine: *tpa_flt3.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. run *tpa.e* using command "***tpa.e > tpa_flt3.out***"
  3. copy input and output files to ***flt3***
  4. look at the output file

- pass/fail criteria: the test passes if:

  1. in the output file, no test cases are listed as 'FAILED'.

Results of running test:

PASSED.

4. Name: Test Results of new subroutine *check_timenextevent.*

   Paths for archives of results: ***$HOME /scr477/flt4***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: use *check_timenextevent.t* and recompile **TPA**. There are multiple test cases contained in *check_timenextevent.t* that can be selected individually by the tester.

   Program modes to be used: use base case *tpa_scr477.inp* and make the following modifications:

   for test case 1: Set TimeOfNextVolcanicEventinRegionOfInterest[yr] type to normal and values to -10.0, 11000.0; save as *tpa_tnetc1.inp.*

   for test case 2: Leave TimeOfNextVolcanicEventinRegionOfInterest[yr] type as finite exponential and set values to 100.0, 9000.0, 1.0e-7; save as *tpa_tnetc2.inp.*

   for test case 3: Leave TimeOfNextFaultingEventinRegionOfInterest[yr] type as finite exponential and set values to 100.0, 9000.0, 1.0e-7; save as *tpa_tnetc2.inp.*

   for test case 4: Set TimeOfNextFaultingEventinRegionOfInterest[yr] to 100.0, 13000.0, 2.0e-5; save as *tpa_tnetc3.inp.*

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that the new and modified code produces expected results.
   - assumptions: none.
   - constraints: the file *tpa_flt4.out* does not exist in the run directory.
   - output files to compare or examine: *tpa_fl4.out*
   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>

2. run *tpa.e* using command "***tpa.e > tpa_flt4.out***"
3. copy input and output files to ***flt4***
4. look at the output file

- pass/fail criteria: the test passes if:

1. in the output file, all test cases are listed as 'PASSED'.

Results of running test:

PASSED.

5. Name: Test Results of new subroutine *check_payload_glass.*

Paths for archives of results: ***$HOME /scr477/flt5***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: use *check_payload_glass.t* and recompile **TPA**. There are multiple test cases contained in *check_payload_glass.t* that can be selected individually by the tester. There are four abort cases in *check_payload_glass.t.* No test cases after the first abort case will be run.

Program modes to be used: use base case *tpa_scr477.inp* and make the following modifications:

for test case 1: Set WastePackagePayload[MTU] to 0.0; save as *tpa_pgtc1.inp.*

for test case 2: Set EquivalentMTUPayloadOfGlassPackage[MTU] to 0.0; save as *tpa_pgtc2.inp.*

for test case 3: Set FractionOfRepositoryInGlassForm[] to -0.1; save as *tpa_pgtc3.inp.*

for test case 4: Set FractionOfRepositoryInGlassForm[] to 1.1; save as *tpa_pgtc4.inp.*

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:
- objective: to verify that the new and modified code produces expected results.

- assumptions: none.

- constraints: the file *tpa_flt5.out* does not exist in the run directory.

- output files to compare or examine: *tpa_flt5.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. run *tpa.e* using command "***tpa.e > tpa_flt5.out***"
  3. copy input and output files to ***flt5***
  4. look at the output file

- pass/fail criteria: the test passes if:

  1. in the output file, no test cases are listed as 'FAILED'.

Results of running test:

PASSED.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

1. Name: Compare Modified Code To Previous Version Of The Code.

   Paths for archives of results: ***$HOME /scr477/slt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use *tpa_scr477.inp*

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:

- objective: to show that the modified **TPA** code generates the same results as before and the new error handling and display messages are correct.

- assumptions: all setup instructions have been carried out and *tpa_vr.out* exists.

- constraints: the file *tpa_slt1.out* does not exist in the run directory.

- output files to compare or examine: *tpa_slt1.out* and *tpa_vr.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_scr477.e* to *tpa.e*
  3. copy *tpa_scr477.inp tpa.inp*
  4. run *tpa.e* using command "***tpa.e > tpa_slt1.out***"
  5. compare files *tpa_slt1.out* and *tpa_vr.out*
  6. copy input and output files to ***slt1***
  7. look at file *samplpar.hdr*

- pass/fail criteria: the test passes if:

  1. The code runs successfully to completion.

  2. The output files are the same except for time/date stamps.

  3. The sampled parameter DistanceCutoffForDoseConversionDualityInDCAGS[km] is no longer contained in the file *samplpar.hdr*.

Results of running test:

PASSED.

2. Name: Test Removal of Messages From Output Display.

Paths for archives of results: ***$HOME /scr477/slt2***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use base case *tpa_scr477.inp* for the base case run; copy base case *tpa_scr477.inp* to *tpa_slt2.inp* and make the following modifications for the test case run:

Set DirectReleaseOnlyFlag(yes=1,no=0) to 1.
Set VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code generates the same results as the base case except that the displayed messages change in the test case.

- assumptions: none.

- constraints: the file *tpa_slt2.out* does not exist in either the run directory.

- output files to compare or examine: *tpa_slt2.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_scr477.inp* to *tpa.inp*
  3. copy *tpa_scr477.e* to *tpa.e*
  4. run *tpa.e* using command "***tpa.e > tpa_scr477.out***"
  5. copy *tpa_slt2.inp* to *tpa.inp*
  6. run *tpa.e* using command "***tpa.e > tpa_slt2.out***"
  7. copy input and output files to ***slt2***
  8. compare the two output files

- pass/fail criteria: the test passes if:

  1. Both runs complete successfully.

  2. The Notes related to WPs and TimeOfNextVolcanicEventinRegionOfInterest[yr] appear in the base case run but not in the test run. A diff of the two files will produce output like this:

```
3c3
<         Job started: Thu Feb 12 14:24:45 2004
---
```

```
>         Job started: Thu Feb 12 14:30:35 2004
42,52d41
<  ***>>> NOTE: When running with volcanism, verify that   <<<***
<  ***>>> the maximum value of the PDF for parameter       <<<***
<  ***>>> TimeOfNextVolcanicEventinRegionOfInterest[yr] is <<<***
<  ***>>> equal to the parameter MaximumTime[yr].          <<<***
<  ***>>>                                                  <<<***
<  ***>>> Also, verify that the maximum total of both      <<<***
<  ***>>> ejected and failed in drift volcanic failures    <<<***
<  ***>>> not exceed the number of WPs in the subarea.     <<<***
<
<
<
```

Results of running test:

PASSED.

3. Name: Test Correction Of TimeOfNextVolcanicEventinRegionOfInterest[yr] / MaximumTime[yr] Error.

   Paths for archives of results: ***$HOME /scr477/slt3***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use *tpa_vr.inp* for test case a and use *tpa_scr477.inp* for test case b. Both input files should be modifed as follows:

   Set VolcanismDisruptiveScenarioFlag(yes=1,no=0) to 1.
   Set DirectReleaseOnlyFlag(yes=1,no=0) to 1.
   Set TimeOfNextVolcanicEventinRegionOfInterest to constant 10,000.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to show that the modified **TPA** code corrects the error that caused the code to abort and that the modified code no longer displays the Notes about waste packages and time of the next volcanic event

   - assumptions: none.

- constraints: the files *tpa_slt3a_orig.out* and *tpa_slt3b_scr477.out* do not exist in the run directory.

- output files to compare or examine: *tpa_slt3a_orig.out* and *tpa_slt3b_scr477.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_vr.inp* to *tpa.inp*
  3. copy *tpa_vr.e* to *tpa.e*
  4. run *tpa.e* using command "***tpa.e > tpa_slt3a_orig.out***"
  5. copy *tpa_scr477.inp* to *tpa.inp*
  6. copy *tpa_scr477.e* to *tpa.e*
  7. run *tpa.e* using command "***tpa.e > tpa_slt3b_scr477.out***"
  8. copy input and output files to ***slt3***
  9. compare the output files

- pass/fail criteria: the test passes if:

  1. The output file *tpa_slt3a_orig.out* displays the following Note:

```
<   ***>>> NOTE: When running with volcanism, verify that   <<<***
<   ***>>> the maximum value of the PDF for parameter       <<<***
<   ***>>> TimeOfNextVolcanicEventinRegionOfInterest[yr] is <<<***
<   ***>>> equal to the parameter MaximumTime[yr].          <<<***
<   ***>>>                                                  <<<***
<   ***>>> Also, verify that the maximum total of both      <<<***
<   ***>>> ejected and failed in drift volcanic failures    <<<***
<   ***>>> not exceed the number of WPs in the subarea.     <<<***
<
<
<
```

  2. The output file *tpa_slt3a_orig.out* shows that the run failed, displaying a message like the following:

```
<    *** failed WPs:    0  out of   1462 ***
<   exec: calling ebsrel
<         ebsrel: running spent fuel waste form
<                          There is no EBS release
<   exec: calling uzft
<   ***>>> error in UZFT <<<***
<   Matrix infiltration is too low for the
<   Van Genuchten curve from DCM3D
<   infil(itime)=  0.
<   time=  0.
```

3. The output file *tpa_slt3b_scr477.out* shows that the run completed successfully and that neither the Note from 1. nor the error message from 2. above appears.

Results of running test:

PASSED.

4. Name: Test Payload and Glass Fraction Error Traps

Paths for archives of results: ***$HOME /scr477/slt4***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_scr477.inp;* make four copies and save as *tpa_slt4a.inp*, *tpa_slt4b.inp*, *tpa_slt4c.inp*, and *tpa_slt4d.inp*; make the following modifications:

tpa_slt4a.inp:
Set WastePackagePayload[MTU] to 0.0.

tpa_slt4b.inp:
Set EquivalentMTUPayloadOfGlassPackage[MTU] = 0.0.

tpa_slt4c.inp:
Set FractionOfRepositoryWasteInGlassForm[] = -0.1.

tpa_slt4d.inp:
Set FractionOfRepositoryWasteInGlassForm[] = 1.1.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code error traps work correctly.

- assumptions: none.

- constraints: the files *tpa_slt4a.out, tpa_slt4b.out, tpa_slt4c.out,* and *tpa_slt4d.out* do not exist in the run directory.

```
=====================================================================

  ***>>> Error in check_payload_glass <<<***
  FractionOfRepositoryWasteInGlassForm[] must be a value between 0.0 and 1.0,
inclusive
  FractionOfRepositoryWasteInGlassForm[] =    -1.0000000000000D-01
```

4. For test case d, the run aborts and a message like the following is displayed:

```
=====================================================================
          exec: Welcome to TPA Version 5.0r
        Job started: Fri Feb 13 16:10:45 2004
=====================================================================

  ***>>> Error in check_payload_glass <<<***
  FractionOfRepositoryWasteInGlassForm[] must be a value between 0.0 and 1.0,
inclusive
  FractionOfRepositoryWasteInGlassForm[] =     1.1000000000000
```

Results of running test:

PASSED.

5. Name: Test Correction Of Number Of Nuclides Error Message

Paths for archives of results: ***$HOME /scr477/slt5***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: copy *tpa_scr477.inp* to *tpa_slt5.inp* and make the following modification:

Set the number of nuclides to 44.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code displays the correct error message
- assumptions: none.

- constraints: the file *tpa_slt5.out* does not exist in the run directory.

- output files to compare or examine: *tpa_slt5.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_slt5.inp* to *tpa.inp*
  3. copy *tpa_scr477.e* to *tpa.e*
  4. run *tpa.e* using command "***tpa.e > tpa_slt5.out***"
  5. copy input and output files to ***slt5***
  6. look at output file

- pass/fail criteria: the test passes if:

  1. The run aborts and a message like the following is displayed:

```
=====================================================================
          exec: Welcome to TPA Version 5.0r
        Job started: Fri Feb 13 12:42:10 2004
=====================================================================

  ***>>>  Error in Reader <<<***
  (nnucl .lt. 1) .or. (nnucl .gt. maxnnucl)
  nnucl    =   44
  maxnnucl =   43
  Look on Line Number =   307
```

Results of running test:

PASSED.

6. Name: Test Correction Of Duplicate Name Error Message

   Paths for archives of results: ***$HOME /scr477/slt6***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: copy *tpa_scr477.inp* to *tpa_slt6a.inp* and *tpa_slt6b.inp* and make the following modifications:

   for *tpa_slt6a.inp*: change Pb210 to Np237 in chain 5 of the acqueousnuclides list

for *tpa_slt6b.inp*: change Ra226 to Np237 in chain 5 of the colloidalnuclides list

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code displays the correct error messages

- assumptions: none.

- constraints: the files *tpa_slt6a.out* and *tpa_slt6b.out* do not exist in the run directory.

- output files to compare or examine: *tpa_slt6a.out* and *tpa_slt6b.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_scr477.e* to *tpa.e*
  3. copy *tpa_slt6a.inp* to *tpa.inp*
  4. run *tpa.e* using command "***tpa.e > tpa_slt6a.out***"
  5. copy *tpa_slt6b.inp* to *tpa.inp*
  6. run *tpa.e* using command "***tpa.e > tpa_slt6b.out***"
  7. copy input and output files to ***slt6***
  8. look at the output files

- pass/fail criteria: the test passes if:

  1. For test case a, the run aborts and a message like the following is displayed:

```
=====================================================================
          exec: Welcome to TPA Version 5.0r
        Job started: Fri Feb 13 13:59:55 2004
=====================================================================

  ***>>> Error in Reader <<<***
  list of aqueous nuclide names has duplicate
   1 name = Cm246
   2 name = U238
   3 name = Cm245
   4 name = Am241
   5 name = Np237
   6 name = Am243
   7 name = Pu239
   8 name = Pu240
   9 name = U234
```

```
 10 name = Th230
 11 name = Ra226
 12 name = Np237
 13 name = Cs135
 14 name = I129
 15 name = Tc99
 16 name = Ni59
 17 name = C14
 18 name = Se79
 19 name = Nb94
 20 name = Cl36
Look at or above line =   360 for duplicate name = Np237
```

2. For test case b, the run aborts and a message like the following is displayed:

```
=========================================================================
          exec: Welcome to TPA Version 5.0r
        Job started: Fri Feb 13 13:59:27 2004
=========================================================================

  ***>>> Error in Reader <<<***
  list of colloidal nuclide names has duplicate
   1 name = Jc246
   2 name = U238
   3 name = Jc245
   4 name = Ja241
   5 name = Np237
   6 name = Ja243
   7 name = Jp239
   8 name = Jp240
   9 name = Jt230
   10 name = Np237
   11 name = Pb210
  Look at or bove line =   390 for duplicate name = Np237
```

Results of running test:

PASSED.

NOTES:

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-478	**2. Software Title and Version:** **TPA 5.0s**	**3. Project No:** 20.06002.01.113
4. Affected Software Module(s), Description of Problem(s): *weldfail.f, ebsrel.f, nfenv.f, failt.f, ebsfail.f, exec.f,* and *corrosn.f* See attachment A.		
5. Change Requested by: O. Pensado Date: 2-23-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date:2-23-2004	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): 1. Updated equation for corrosion potential. See attachment B for equation and parameter mapping. 2. Introduced Arrhenius dependence of the passive current density on the temperature. See attachment B . 3. Introduced additional constraint to localized corrosion. Localized corrosion is assumed to occur if the ratio of inhibitor to chloride is low, plus the other requirements for localized corrosion.		
8. Implemented by: R. Janetzke Z. Wojcik O. Pensado	**Date:** 5-25-04	
9. Description of Acceptance Tests: See attached CD "SCR478 Test Plan".		
10. Tested by: Marty Menchaca Femi Osidele	**Date:** 9-9-04	

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR478

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)	Distribution	Range	Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)
Add	EBSFAIL	OuterActivationEnergyPassiveCurrDens[J/mol]		constant	4.47E+04		OPR
Add	EBSFAIL	InnerActivationEnergyPassiveCurrDens[J/mol]	Activation energy for Arrhenius dependence of passive current density on temperature.	constant	4.47E+04	Pensado, O., D.S. Dunn, G.A. Cragnolino, V. Jain. Passive Dissolution of Container Materials ——Modeling and Experiments. CNWRA, San Antonio, Texas. CNWRA 2003-01. 2002.	OPR

Add	EBSFAIL	RefTemperaturePassiveCurrDens[K]	Reference temperature to define Arrhenius dependence of passive current density on temperature.	constant	3.68E+02	Pensado, O., D.S. Dunn, G.A. Cragnolino, V. Jain. Passive Dissolution of Container Materials ——Modeling and Experiments. CNWRA, San Antonio, Texas. CNWRA 2003-01. 2002.	OPR
Add	EBSFAIL	TransitionLowHighpH	Two different set of parameters are used to compute the corrosion potential. This pH parameter defines the transition pH to select the appropriate set of parameters.	constant	6	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR
Add	EBSFAIL	OuterChargeTransferCoefReductionReactHighpH	Charge transfer coefficient for reduction reaction, high pH range. Parameter used to compute the corrosion potential.	constant	0.0248	Fitting corrosion potential to experimental data.	OPR
Add	EBSFAIL	OuterChargeTransferCoefReductionReactLowpH	Charge transfer coefficient for reduction reaction, low pH range. Parameter used to compute the corrosion potential.	constant	0.01287	Fitting corrosion potential to experimental data.	OPR

Add	EBSFAIL	OuterReferenceCurrReductionReactHighpH[C/(m2*yr)]	Reference current density to compute the cathodic current density due to the main reduction reaction (e.g. oxygen reduction). This cathodic current density is used to compute the corrosion potential. High pH range.	constant	5.51E+09	Fitting corrosion potential to experimental data.	OPR
Add	EBSFAIL	OuterReferenceCurrReductionReactLowpH[C/(m2*yr)]	Reference current density to compute the cathodic current density due to the main reduction reaction (e.g. oxygen reduction). This cathodic current density is used to compute the corrosion potential. Low pH range.	constant	7.57E+09	Fitting corrosion potential to experimental data.	OPR
Add	EBSFAIL	OuterActivationEnergyReductionReactHighpH[J/mole]	Activation energy for Arrhenius dependence of cathodic current density on temperature. High pH range.	constant	40000	Parameter called OuterWPActivationEnergyforOxygenReduction[J/mole] in TPA 4.0. Assumed based on Calvo (1979) A value of 40000 J/mole does reproduce the temperature dependence noted in the laboratory of the corrosion potential.	OPR

Add	EBSFAIL	OuterActivationEnergyReductionReactLowpH[J/mole]	Activation energy for Arrhenius dependence of cathodic current density on temperature. Low pH range.	constant	40000	Parameter called OuterWPActivationEnergyforOxygenReduction[J/mole] in TPA 4.0. Assumed based on Calvo (1979) A value of 40000 J/mole does reproduce the temperature dependence noted in the laboratory of the corrosion potential.	OPR
Add	EBSFAIL	OuterEffectiveReactionOrderHHighpH	Reaction order with respect to hydroxil ion (H+ or protons). Parameter used to compute the cathodic current density, used to compute the corrosion potential. High pH range	constant	0.01897	Fitting corrosion potential to experimental data.	OPR
Add	EBSFAIL	OuterEffectiveReactionOrderHLowpH	Reaction order with respect to hydroxil ion (H+ or protons). Parameter used to compute the cathodic current density, used to compute the corrosion potential. Low pH range	constant	0.0256	Fitting corrosion potential to experimental data.	OPR

Add	EBSFAIL	InnerChargeTransferCoefReductionReactHighpH	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	0.0248	Same value for "Outer" container employed. This parameter is not important, as no credit is assigned to inner container.	OPR
Add	EBSFAIL	InnerChargeTransferCoefReductionReactLowpH	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	0.01287	Same value for "Outer" container employed. This parameter is not important, as no credit is assigned to inner container.	OPR
Add	EBSFAIL	InnerReferenceCurrReductionReactHighpH[C/(m2*yr)]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	5.51E+09	Same value for "Outer" container employed. This parameter is not important, as no credit is assigned to inner container.	OPR
Add	EBSFAIL	InnerReferenceCurrReductionReactLowpH[C/(m2*yr)]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	7.57E+09	Same value for "Outer" container employed. This parameter is not important, as no credit is assigned to inner container.	OPR

Add	EBSFAIL	InnerActivationEnergy ReductionReactHighp H[J/mole]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	40000	Same value for "Outer" container employed. This parameter is not important, as no credit is assigned to inner container.	OPR
Add	EBSFAIL	InnerActivationEnergy ReductionReactLowp H[J/mole]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	40000	Same value for "Outer" container employed. This parameter is not important, as no credit is assigned to inner container.	OPR
Add	EBSFAIL	InnerEffectiveReaction OrderHHighpH	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	0.01897	Same value for "Outer" container employed. This parameter is not important, as no credit is assigned to inner container.	OPR
Add	EBSFAIL	InnerEffectiveReaction OrderHLowpH	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	0.0256	Same value for "Outer" container employed. This parameter is not important, as no credit is assigned to inner container.	OPR

Add	EBSFAIL	OuterInhibitingNitrateToCl	Nitrate to chloride concentration ratio for computation of action of inhibitors. Below this ratio, the repassivation potential is assumed to increase linearly with the ratio up to OuterDeltaEcritInh[mV]. Above this ratio, the increase in the repassivatio	constant	0.1	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR
Add	EBSFAIL	OuterInhibitingCarbonateToCl	Carbonate to chloride concentration ratio for computation of action of inhibitors. Below this ratio, the repassivation potential is assumed to increase linearly with the ratio up to OuterDeltaEcritInh[mV]. Above this ratio, the increase in the repassivat	constant	0.1	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR
Add	EBSFAIL	OuterInhibitingSulfateToCl	Sulfate to chloride concentration ratio for computation of action of inhibitors. Below this ratio, the repassivation potential is assumed to increase linearly with the ratio up to OuterDeltaEcritInh[mV]. Above this ratio, the increase in the repassivatio	constant	0.5	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR

Add	EBSFAIL	OuterDeltaEcritInh[mV]	Maximum increase in the repassivation potential due to the action of inhibitors.	constant	800	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR
Add	EBSFAIL	InnerInhibitingNitrateToCl	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	1.00E+10	Arbitrarily high value to avoid any effect of inhibitors on the localized corrosion of the inner waste package (no credit is given to inner waste package protection)	OPR
Add	EBSFAIL	InnerInhibitingCarbonateToCl	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	1.00E+10	Arbitrarily high value to avoid any effect of inhibitors on the localized corrosion of the inner waste package (no credit is given to inner waste package protection)	OPR

Add	EBSFAIL	InnerInhibitingSulfateToCl	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	1.00E+10	Arbitrarily high value to avoid any effect of inhibitors on the localized corrosion of the inner waste package (no credit is given to inner waste package protection)	OPR
Add	EBSFAIL	InnerDeltaEcritInh[mV]	The prefix "Inner" refers to the inner waste package. See analogous parameter for the "Outer" waste package for parametere definition.	constant	0.00E+00	Zero value selected to avoid any effect of inhibitors on the localized corrosion of the inner waste package (no credit is given to inner waste package protection)	OPR
Add	EBSFAIL	WeldInhibitingNitrateToCl	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.3	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR

Add	EBSFAIL	WeldInhibitingCarbonateToCl	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.1	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR
Add	EBSFAIL	WeldInhibitingSulfateToCl	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	0.5	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR
Add	EBSFAIL	WeldDeltaEcritInh[mV]	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	constant	800	Dunn D.S., L. Yang, C. Wu, and G.A. Cragnolino. Effect of Inhibiting Oxyanions on the Localized Corrosion Susceptibility of Waste Package Container Materials. Submitted to International Symposium on the Scientific Basis for Nuclear Waste Management XXVI	OPR

Add	EBSFAIL	WeldCritChlorideConc [mol/L]	The prefix "Weld" refers to weld areas on the waste package. See analogous parameter for the "Outer" waste package for parameter definition.	loguniform	0.001, 0.25	Dunn, D.S., D. Daruwalla, Y.-M. Pan. Effect of Fabrication Processes on Material Stability -- Characterization and Corrosion. CNWRA 2004-01. CNWRA: San Antonio, Texas; October 2003. Loguniform distribution is conservative since low values are frequently	OPR
	NFENV	RewettingHumidity	Humidity at the WP surface at which it is assumed that further evaporation is not significant.	uniform	0.95,0.98	Reasonable selection. Selection of higher values (close to 1) is conservative. The effect of this parameter is extending the time localized corrosion could occur (Environment II). The higher the value of this parameter, the longer is the critical perio	OPR
	NFENV	EnvironmentI_FI[mol/L]	Fluoride concentration during environment I on the drip shield surface.	constant	0.00001	Formation of significant concentration of fluoride due to deliquescence processes of salts in dust is unlikely. A low value of the fluoride concentration is selected to indicate that fluoride enhancing of the titanium corrosion rate during environment I i	OPR

	NFENV	EnvironmentI_Cl[mol/L]	Chloride concentration during environment I on the waste package surface.	constant	1.0	Solutions during Environment I are the result of deliquescence of salts in dust or mixing of dust with condensates. There is apparent abundance of nitrate compounds in dust. Therefore, localized corrosion during Environment I is unlikely. This parameter	OPR
Add	NFENV	EnvironmentI_pH[]	pH during environment I on the waste package surface.	constant	7	Solutions during Environment I are the result of deliquescence of salts in dust or mixing of dust with condensates. There is apparent abundance of nitrate compounds in dust. Therefore, localized corrosion during Environment I is unlikely. This parameter	OPR
Add	NFENV	EnvironmentI_NO3[mol/L]	Nitrate concentration during environment I on the waste package surface.	constant	1.0	Solutions during Environment I are the result of deliquescence of salts in dust or mixing of dust with condensates. There is apparent abundance of nitrate compounds in dust. Therefore, localized corrosion during Environment I is unlikely. This parameter	OPR

Add	NFENV	EnvironmentI_CO3[mol/L]	Carbonate concentration during environment I on the waste package surface.	constant	0.0	Solutions during Environment I are the result of deliquescence of salts in dust or mixing of dust with condensates. There is apparent abundance of nitrate compounds in dust. Therefore, localized corrosion during Environment I is unlikely. This parameter	OPR
Add	NFENV	EnvironmentI_SO4[mol/L]	Sulfate concentration during environment I on the waste package surface.	constant	0.0	Solutions during Environment I are the result of deliquescence of salts in dust or mixing of dust with condensates. There is apparent abundance of nitrate compounds in dust. Therefore, localized corrosion during Environment I is unlikely. This parameter	OPR
Add	NFENV	EnvironmentI_Wastepackage_DeltaECrit[VSHE]	Increase in the repassivation potential due to secondary factors such as microbial action or unaccounted processes during Environment I. Value used to construct input file deltaec.inp for failt	constant	0.0	Action of secondary processes increasing the repassivation potential is disregarded in the base case.	OPR

Add	NFENV	EnvironmentII_Fl[mol/L]	Fluoride concentration during environment II on the drip shield surface.	constant	1.0e-5	Pabalan R.T., Yang L.,and Browning L.(2002) Effects of Salt Formation on the Chemical Environment of Drip Shields and Waste Packages at the Proposed Nuclear Waste Repository at Yucca Mountain, Nevada. CNWRA report 2002-03. Chapter 11	OPR
Add	NFENV	EnvironmentII_Cl[mol/L]	Chloride concentration during environment II on the waste package surface.	usersupplie dpwisecdf	10 0.0, 0.0 0.45, 0.1620 0.95, 0.3175 1.84, 0.3721 1.98, 0.4891 1.99, 0.7042 2.23, 0.9757 2.57 0.9836 3.1, 0.9978 3.82, 1.0	Chapter 3 of the Risk Analysis for Risk Insights Report.	OPR
Add	NFENV	EnvironmentII_pH[]	pH during environment II on the waste package surface.	usersupplie dpwisecdf	6 5.902817, 0.0 6.05, 0.0022 7.0, 0.0164 7.23, 0.0243 8.83, 0.0789 8.84, 1.0	Chapter 3 of the Risk Analysis for Risk Insights Report.	OPR

Add	NFENV	EnvironmentII_NO3[mol/L]	Nitrate concentration during environment II on the waste package surface.	usersupplied pwisecdf	10 0.0, 0.0 0.03, 0.162 0.06, 0.2166 0.07, 0.4881 0.14, 0.6051 0.18, 0.613 0.19, 0.8281 0.21, 0.8303 0.39, 0.8445 0.41, 1.0	Chapter 3 of the Risk Analysis for Risk Insights Report.	OPR
Add	NFENV	EnvironmentII_CO3[mol/L]	Carbonate concentration during environment II on the waste package surface.	constant	0.0	The precense of carbonate is conservatively disregarded in the base case.	OPR
Add	NFENV	EnvironmentII_SO4[mol/L]	Sulfate concentration during environment II on the waste package surface.	constant	0.0	The precense of sulfate is conservatively disregarded in the base case.	OPR
Add	NFENV	EnvironmentII_Waste package_DeltaECrit[VSHE]	Increase in the repassivation potential due to secondary factors such as microbial action or unaccounted processes during Environment II. Value used to construct input file deltaec.inp for failt	constant	0.2	Action of secondary processes increasing the repassivation potential is disregarded in the base case.	OPR

Add	NFENV	EnvironmentIII_Fl[mol/L]	Fluoride concentration during environment III on the drip shield surface (seepage composition)	constant	4.08e-4	Supplemental Science and Performance Analyses Volume 1 Scientific Bases and Analyses. Rev. 00 U.S. Department of Energy TDR-MGR-MD-000007 Las Vegas, NV; June 2001. Page 6T-4, Table 6.3.1 - 6.2.	OPR
Add	NFENV	EnvironmentIII_Cl[mol/L]	Chloride concentration during environment III on the waste package surface (seepage composition).	constant	6.65e-3	Supplemental Science and Performance Analyses Volume 1 Scientific Bases and Analyses. Rev. 00 U.S. Department of Energy TDR-MGR-MD-000007 Las Vegas, NV; June 2001. Page 6T-4, Table 6.3.1 - 6.2. Localized corrosion is assumed not to occur during Period II	OPR
Add	NFENV	EnvironmentIII_pH[]	pH during environment III on the waste package surface (seepage composition).	constant	8.37e0	Supplemental Science and Performance Analyses Volume 1 Scientific Bases and Analyses. Rev. 00 U.S. Department of Energy TDR-MGR-MD-000007 Las Vegas, NV; June 2001. Page 6T-4, Table 6.3.1 - 6.2. Localized corrosion is assumed not to occur during Period III	OPR

Add	NFENV	EnvironmentIII_NO3[mol/L]	Nitrate concentration during environment III on the waste package surface (seepage composition).	constant	6.65e-3	Assumed value. It is assumed that localized corrosion does not occur during Period III due to dilute nature of seepage solutions.	OPR
Add	NFENV	EnvironmentIII_CO3[mol/L]	Carbonate concentration during environment III on the waste package surface (seepage composition).	constant	2.11e-3	Supplemental Science and Performance Analyses Volume 1 Scientific Bases and Analyses. Rev. 00 U.S. Department of Energy TDR-MGR-MD-000007 Las Vegas, NV; June 2001. Page 6T-4, Table 6.3.1 - 6.2. Localized corrosion is assumed not to occur during Period I	OPR
Add	NFENV	EnvironmentIII_SO4[mol/L]	Sulfate concentration during environment III on the waste package surface (seepage composition).	constant	0.0	Assumed value. It is assumed that localized corrosion does not occur during Period III due to dilute nature of seepage solutions. The precise value of this parameter is not important.	OPR

Add	NFENV	EnvironmentIII_Waste package_DeltaECrit[V SHE]	Increase in the repassivation potential due to secondary factors such as microbial action or unaccounted processes during Environment III. Value used to construct input file deltaec.inp for failt	constant	0.0	Action of secondary processes increasing the repassivation potential is disregarded in the base case.	OPR
Add	NFENV	SeepageThresholdT[C]		constant	100.0		OPR
Add	NFENV	FlagSeepageThreshol d[]		iflag	1		OPR
Delete	NFENV	IndriftEvaporationTem perature[C]					OPR
Delete	NFENV	Indrift_Cl_PreTemper aturePeak[mol/L]					OPR
Delete	NFENV	Indrift_Fl_PreTempera turePeak[mol/L]					OPR
Delete	NFENV	Indrift_pH_PreTemper aturePeak[mol/L]					OPR
Delete	NFENV	Indrift_CO3_PreTemp eraturePeak[mol/L]					OPR
Delete	NFENV	Indrift_Cl_PostTemper aturePeak[mol/L]					OPR
Delete	NFENV	Indrift_Fl_PostTemper aturePeak[mol/L]					OPR
Delete	NFENV	Indrift_pH_PostTempe raturePeak[mol/L]					OPR

Delete	NFENV	Indrift_CO3_PostTemperaturePeak[mol/L]					OPR
Delete	DSFAIL	Wastepackage_DeltaECrit_PreTemperaturePeak[VSHE]					OPR
Delete	DSFAIL	Wastepackage_DeltaECrit_PostTemperaturePeak[VSHE]					OPR
Delete	EBSFAIL	OuterWPBetaKineticsParameterfor Oxygen					OPR
Delete	EBSFAIL	InnerWPBetaKineticsParameterforOxygen					OPR
Delete	EBSFAIL	OuterWPRateConstantforOxygenReduction[coulomb-m/mole/yr]					OPR
Delete	EBSFAIL	OuterWPActivationEnergyforOxygenReduction[J/mole]					OPR
Delete	EBSFAIL	InnerWPRateConstantforOxygenReduction[coulomb-m/mole/yr]					OPR
Delete	EBSFAIL	InnerWPActivationEnergyforOxygenReduction[J/mole]					OPR
Delete	EBSFAIL	StandardExchangeCurrentDensityforOxygenReduction[C/(m^2yr)]					OPR
Delete	EBSFAIL	EquilibriumPotentialOxygenReduction[VSHE]					OPR

Attachment A

Affected Software Module(s), Description of Problem(s):

1. Introduced temperature dependence of anodic current density in Arrhenius form. This temperature dependence is needed to improve corrosion potential estimates. Affected modules: *weldfail.f* and *failt.f.*

2. Replace equations to compute corrosion potential for better consistency with experimental data. Currently, the corrosion potential is conservatively overestimated. Affected modules: *weldfail.f* and *failt.f.*

3. Introduced inhibitors to localized corrosion. Experimentally it is known that localized corrosion is not activated if inhibitors are present in the system above a threshold value. Affected modules: *weldfail.f* and *failt.f.*

4. Introduce a new parameter **SeepageThresholdT[C]**. It will be assumed that when the drift wall temperature is above **SeepageThresholdT[C]**, seepage cannot contact drip shields or waste packages. **Qhit** and **Qmiss** should be modified accordingly (**Qhit** = 0 if the drift wall temperature is above the threshold). Affected modules: *nfenv.f* and *releaset.f*

5. Introduce a flag, **FlagSeepageThreshold**, to activate use of the **SeepageThresholdT[C]**. The intent of this flag is to recover previous code computations if desired. Affected modules: *nfenv.f* and *releaset.f.* The **SeepageThresholdT[C]** should be applied on all refluxing models.

6. Implement logic to divide near-field chemistry into 3 periods: I) deliquescence, II) direct seepage contact + evaporation, and III) re-wetting. Affected modules: *nfenv.f.* Introduce new parameter named **RewettingHumidity** to define the end of period II or start of period III.

7. Introduce inhibiting oxyanions to be tracked by *nfenv.rlt*: nitrate, carbonate, sulfate. Define a new column in the input file *ebstrhc.inp* with an effective inhibitor concentration. The effective inhibitor concentration is modeled as a linear combination of the relevant inhibiting oxyanions. Affected module: *nfenv.f*

Attachment B

1. Passive current density as a function of temperature

$$I_a(T) = I_a^o \exp\left[-\frac{E_o}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}}\right)\right] \qquad [1]$$

Parameter mapping

Note: Inner overpack and outer overpack have independent values of the parameters. Weld parameters are assumed to be the same of outer overpack parameters.

Parameter	tpa.inp	Distribution	Value
I_a^o	AA_1_1[C/m2/yr]	triangular	1.6E3, 3.2E3, 6.4E3
I_a^o	AA_2_1[C/m2/yr]	constant	1.00E+04
	NEW PARAMETERS		
E_o	OuterActivationEnergyPassiveCurrDens[J/mol]	constant	4.47E+04
E_o	InnerActivationEnergyPassiveCurrDens[J/mol]	constant	4.47E+04
T_{ref}	RefTemperaturePassiveCurrDens[K]	constant	3.68E+02

2. New equation for the corrosion potential

$$i_r(E_{corr},T) = -\frac{i_r^{ef}\dfrac{C_{O_2}^{bulk}(T)}{C_{O_2}^{bulk}(T_{ref})} e^{-\frac{E_a}{RT}} e^{-\frac{Z_r\beta_r^{ef}F}{RT}E_{corr}} \left[H^+\right]^{n_H^{ef}} pO_2^{\,n_O^{ef}}}{1 + \dfrac{\delta\, i_r^{ef}}{4F\phi\tau\, D_{O_2}(T)C_{O_2}^{bulk}(T_{ref})} e^{-\frac{E_a}{RT}} e^{-\frac{Z_r\beta_r^{ef}F}{RT}E_{corr}} \left[H^+\right]^{n_H^{ef}} pO_2^{\,n_O^{ef}}} \qquad [2]$$

Same previous equations were used to define the oxygen concentration and oxygen diffusion coefficient as functions of the temperature. The total partial cathodic current density is computed as

$$I_{cath}(E_{corr},T) = I_r(E_{corr},T) + I_{H_2O}(E_{corr},T) \qquad [3]$$

The same previous equation of cathodic current density due to water reduction as a function of the corrosion potential was used. The corrosion potential is found as a numeric solution to the equation

$$I_a(T) + I_{carh}(E_{corr}, T) = 0 \qquad [4]$$

Experimentally, it has been found that the corrosion potential tends to be higher at lower pH values. This transition was modeled by selecting two sets of kinetic parameters, one set corresponding to the low-pH xregime, and a second set for the high-pH regime. The pH of transition is around 6.

Parameter mapping

Note: Inner overpack and outer overpack have independent values of the parameters. Weld parameters are assumed to be the same of outer overpack parameters.

Parameter	tpa.inp	Distribution	Value
	OuterWPBetaKineticsParameterforWater	constant	0.5
	InnerWPBetaKineticsParameterforWater	constant	0.5
	OuterWPRateConstantforWaterReduction[coulomb-m/m^2/yr]	constant	0
	OuterWPActivationEnergyforWaterReduction[J/mole]	constant	25000
	InnerWPRateConstantforWaterReduction[coulomb-m/m^2/yr]	constant	3.2
	InnerWPActivationEnergyforWaterReduction[J/mole]	constant	25000
	NEW PARAMETERS		
	TransitionLowHighpH	constant	6.0
β_r^{ef}	OuterChargeTransferCoefReductionReactHighpH	constant	0.0248
β_r^{ef}	OuterChargeTransferCoefReductionReactLowpH	constant	0.01287
i_r^{ef}	OuterReferenceCurrReductionReactHighpH[C/(m2*yr)]	constant	5.51E+09
i_r^{ef}	OuterReferenceCurrReductionReactLowpH[C/(m2*yr)]	constant	7.57E+09
E_a	OuterActivationEnergyReductionReactHighpH[J/mole]	constant	40000
E_a	OuterActivationEnergyReductionReactLowpH[J/mole]	constant	40000
n_H^{ef}	OuterEffectiveReactionOrderHHighpH	constant	0.01897
n_H^{ef}	OuterEffectiveReactionOrderHLowpH	constant	0.0256
n_o^{ef}	Not defined by user but in ebsfail.def	constant	0.0248
n_o^{ef}	Not defined by user but in ebsfail.def	constant	0.01287
β_r^{ef}	InnerChargeTransferCoefReductionReactHighpH	constant	0.0248
β_r^{ef}	InnerChargeTransferCoefReductionReactLowpH	constant	0.01287
i_r^{ef}	InnerReferenceCurrReductionReactHighpH[C/(m2*yr)]	constant	5.51E+09
i_r^{ef}	InnerReferenceCurrReductionReactLowpH[C/(m2*yr)]	constant	7.57E+09
E_a	InnerActivationEnergyReductionReactHighpH[J/mole]	constant	40000
E_a	InnerActivationEnergyReductionReactLowpH[J/mole]	constant	40000
n_H^{ef}	InnerEffectiveReactionOrderHHighpH	constant	0.01897
n_H^{ef}	InnerEffectiveReactionOrderHLowpH	constant	0.0256
n_o^{ef}	Not defined by user but in ebsfail.def	constant	0.0248
n_o^{ef}	Not defined by user but in ebsfail.def	constant	0.01287
	END OF NEW PARAMETERS		
δ_1	ThicknessOfWaterFilm[m]	constant	0.0
δ_2	WPsurfaceScaleThickness[m]	constant	0.0
ϕ	TortuosityOfScaleonWP	constant	1.0
τ	PorosityOfScaleonWP	constant	1.0
δ	$\max(\delta_1,\delta_2)$		

DELETE PARAMETERS

OuterWPBetaKineticsParameterforOxygen
InnerWPBetaKineticsParameterforOxygen
OuterWPRateConstantforOxygenReduction[coulomb-m/mole/yr]
OuterWPActivationEnergyforOxygenReduction[J/mole]
InnerWPRateConstantforOxygenReduction[coulomb-m/mole/yr]
InnerWPActivationEnergyforOxygenReduction[J/mole]
StandardExchangeCurrentDensityforOxygenReduction[C/(m^2 yr)]
EquilibriumPotentialOxygenReduction[VSHE]

Comparison of corrosion potential to experimental data selecting AA_1_1[C/m2/yr] = 3.2E3

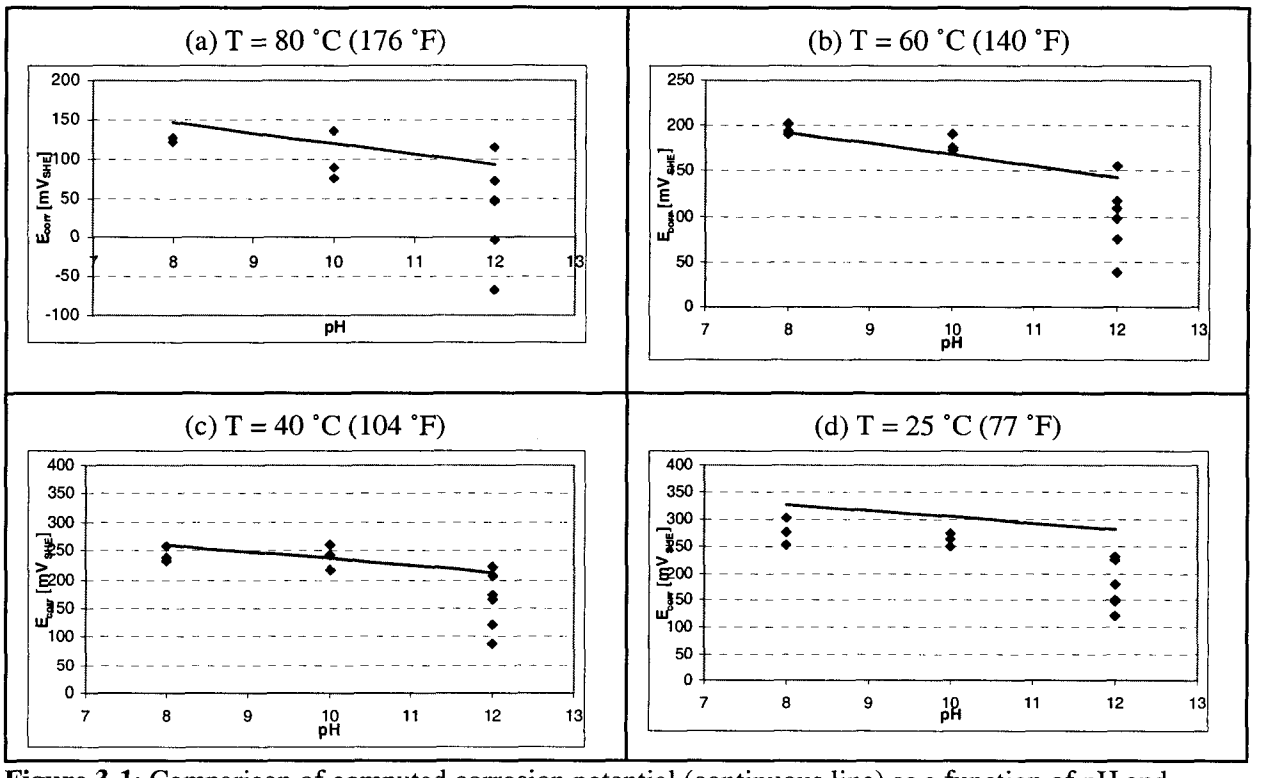


Figure 3-1: Comparison of computed corrosion potential (continuous line) as a function of pH and temperature to experimental data (diamonds) for (a) 80 °C (176 °F), (b) 60 °C (140 °F), (c) 40 °C (104 °F), and (d) 25 °C (77 °F). The figure contains experimental corrosion potentials from multiple specimens in 4 M NaCl solution, determined after approximately 1 day exposure.

3. Localized corrosion inhibitors

Localized corrosion is assumed to initiate if

i) chloride concentration greater than a minimum value:

$$[Cl^-] \geq Cl_{crit} \qquad [5]$$

ii) corrosion potential greater than the repassivation potential
iii) Inhibitor to chloride ratio less than a threshold value, ω_N

The effective inhibitor concentration is computed as

$$inh = [NO_3^-] + \frac{\omega_N}{\omega_C}[CO_3^{2-}] + \frac{\omega_N}{\omega_S}[SO_4^{2-}] \qquad [6]$$

The following is a necessary condition for localized corrosion

$$\frac{inh}{[Cl^-]} < \omega_N \qquad [7]$$

Localized corrosion is assumed not to occur if the previous inequality is not satisfied.

Parameter mapping

Note: Inner overpack, outer overpack, and weld area have all independent parameters.

ALL PARAMETERS IN TABLE ARE NEW.

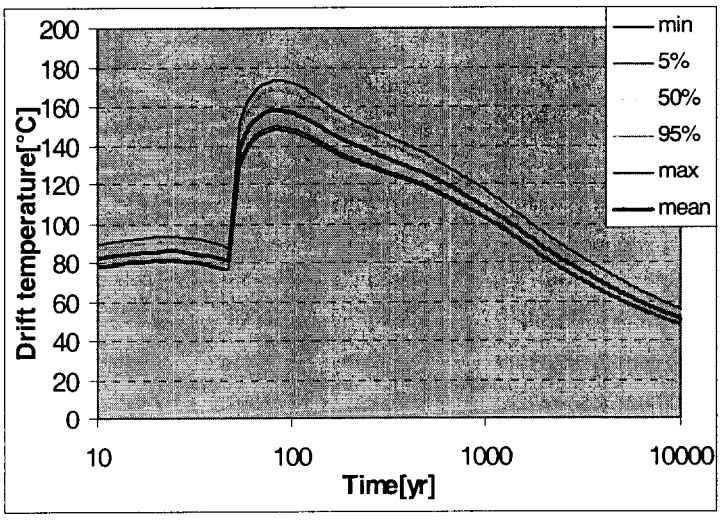
Parameter	**tpa.inp**	**Distribution**	**Value**
Cl_{crit}	CritChlorideConcForFirstLayer[mol/L]	constant	0.5
Cl_{crit}	CritChlorideConcForSecondLayer[mol/L]	constant	1E-10
ω_N	OuterInhibitingNitrateToCl	constant	0.1
ω_C	OuterInhibitingCarbonateToCl	constant	0.1
ω_S	OuterInhibitingSulfateToCl	constant	0.5
ω_N	InnerInhibitingNitrateToCl	constant	1.00E+10
ω_C	InnerInhibitingCarbonateToCl	constant	1.00E+10
ω_S	InnerInhibitingSulfateToCl	constant	1.00E+10
Cl_{crit}	WeldCritChlorideConc[mol/L]	loguniform	0.001, 0.25
ω_N	WeldInhibitingNitrateToCl	constant	0.3
ω_C	WeldInhibitingCarbonateToCl	constant	0.1
ω_S	WeldInhibitingSulfateToCl	constant	0.5

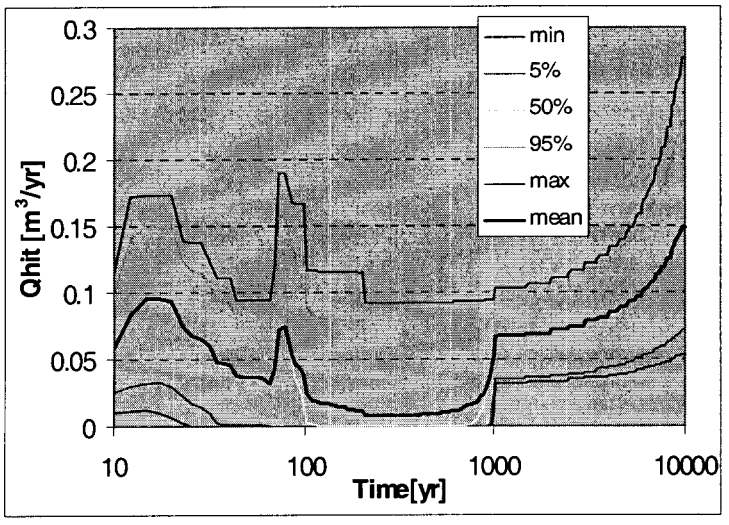
4. New parameter: SeepageThresholdT[C]

Water reaching the drifts and potentially hitting the drip shields: Qhit[m^3/yr].

After drip shield and waste package failure, the water available for transport equals Fmult × Fow × Qhit

TPA 5.0q results:





From the reflux model, the above plot indicates that some realizations (20% ??) have Qhit > 0 at drift wall temperatures a way above the boiling temperature of water.

The modified abstraction will assume that when the drift wall temperature is above SeepageThresholdT[C], seepage cannot contact drip shields or waste packages:

Qhit = 0 if T(drift wall) > SeepageThresholdT[C]

5. Introduce flag: FlagSeepageThreshold

Flag FlagSeepageThreshold will be used to activate use of the SeepageThresholdT[C]. The intent of this flag is to recover previous code computations if desired.

6. Near-field chemistry Environments

Environment I: Deliquescence period
(Relative humidity ≥ CriticalRelativeHumidityAqueousCorrosion) AND {(Drip shield intact) OR (Qhit = 0)}

Environment II: Direct-seepage period + evaporation
(Relative humidity ≥ CriticalRelativeHumidityAqueousCorrosion) AND (Drip shield failed) AND (Qhit > 0) AND (Relative humidity < RewettingHumidity)

Environment III: Re-wetting period
(Drip shield failed) AND (Qhit > 0) AND (Relative humidity ≥ RewettingHumidity)

CODE LOGIC FOR WP CHEMISTRY

IF (Relative humidity < CriticalRelativeHumidityAqueousCorrosion) THEN
    DRY PERIOD
    Apply dry oxidation of WP
ELSEIF (Drip shield intact) OR (Qhit = 0) THEN
    Environment I
    Waste package will exhibit aqueous corrosion
    Use <u>dust deliquescence chemistry</u> or *<u>dust condensate mixing chemistry</u>*
    This period could be the dominating period if the drip shield fails until late in the compliance period.
  ELSEIF (Relative humidity < RewettingHumidity) THEN
      Environment II
      Waste package will exhibit aqueous corrosion
      Use <u>evaporated chemistry</u>
    ELSE
      Environment III
      Waste package will exhibit aqueous corrosion
      Use <u>diluted pore-water chemistry</u>
ENDIF

CODE LOGIC FOR DRIP SHIELD CHEMSITRY

IF (Relative humidity < CriticalRelativeHumidityAqueousCorrosion) THEN

DRY PERIOD

Define fluoride concentration as $[F^-] = 0.0$

ELSEIF (Qhit = 0) THEN

Environment I

Drip shield will exhibit aqueous corrosion.

From conversations with L. Browning, there are no brines with free fluoride.

The fluoride concentration will be most likely zero in this period., but the user defines this concentration in tpa.inp.

ELSEIF (Relative humidity < RewettingHumidity) THEN

Environment II

Use <u>*evaporated chemistry*</u>

ELSE

Environment III

Use <u>*diluted pore-water chemistry*</u>

ENDIF

SEQUENCE IN TPA CODE

1. Call nfenv to define temperatures, relative humidity, and fluoride concentration. If necessary, use fake values (e.g., 0.0) of chloride and other chemical components, as are not used by the mechfail+dsfail modules.

2. Call drip shield modules (mechfail + dsfail)

3. Call part 2 of nfenv to define the input files chlrdmf.dat, ebstrhc.inp, deltaec.inp (containing chloride and inhibitor concentrations).

4. Call failt

Question: at what moment in this process is created the nfenv.rlt file?

The nfenv.rlt file must contain concentrations defined after step 3.

NEW PARAMETERS

RewettingHumidity ~ uniform(0.95,0.98) ??

EnvironmentI_F[mol/L]
EnvironmentI_Cl[mol/L]
EnvironmentI_pH[]
EnvironmentI_NO3[mol/L]
EnvironmentI_CO3[mol/L]
EnvironmentI_SO4[mol/L]
EnvironmentI_Wastepackage_DeltaECrit[VSHE] : used to construct input file deltaec.inp for failt

EnvironmentII_F[mol/L]
EnvironmentII_Cl[mol/L]
EnvironmentII_pH[]
EnvironmentII_NO3[mol/L]
EnvironmentII_CO3[mol/L]
EnvironmentII_SO4[mol/L]
EnvironmentII_Wastepackage_DeltaECrit[VSHE] : used to construct input file deltaec.inp for failt

EnvironmentIII_F[mol/L]
EnvironmentIII_Cl[mol/L]
EnvironmentIII_pH[]
EnvironmentIII_NO3[mol/L]
EnvironmentIII_CO3[mol/L]
EnvironmentIII_SO4[mol/L]
EnvironmentIII_Wastepackage_DeltaECrit[VSHE] : used to construct input file deltaec.inp for failt

DELETE PARAMETERS
IndriftEvaporationTemperature[C]
Indrift_Cl_PreTemperaturePeak[mol/L]
Indrift_Fl_PreTemperaturePeak[mol/L]
Indrift_pH_PreTemperaturePeak[]
Indrift_pH_PreTemperaturePeak[]
Indrift_CO3_PreTemperaturePeak[mol/L]
Indrift_Cl_PostTemperaturePeak[mol/L]
Indrift_Fl_PostTemperaturePeak[mol/L]
Indrift_pH_PostTemperaturePeak[]
Indrift_CO3_PostTemperaturePeak[mol/L]
Wastepackage_DeltaECrit_PreTemperaturePeak[VSHE]
Wastepackage_DeltaECrit_PostTemperaturePeak[VSHE]

DELETE INPUT FILES
multibe.dat, multiaf.dat
multibe.dat is never used in the TPA code
multiaf.dat was intended to define pore-water concentrations as functions of time. Such functions appear irrelevant. The input file should be replaced by the above input parameters for Environment III.

7. New format of the file ebstrhc.inp

```
timr        tcan        tavg        humd      pH    inh
201         201         201         201       201   201
0.          38.5707     20.         0.1025    7.    0.
2.3102      79.175      66.7504     0.177     7.    0.
4.6744      88.8793     77.8903     0.194     7.    0.
7.094       92.9224     82.8086     0.2031    7.    0.
9.5702      94.9829     85.4978     0.2093    7.    0.
12.1044     96.1716     87.1926     0.214     7.    0.
14.698      96.8702     88.3192     0.2179    7.    0.
.
.
.
10000.      51.364      50.9932     0.9819    7.    0.0001
```

The column with the inhibitor concentration, inhconc, is computed, within the nfenv module, as

$$inh = [NO_3^-] + \frac{\omega_N}{\omega_C}[CO_3^{2-}] + \frac{\omega_N}{\omega_S}[SO_4^{2-}] \qquad [8]$$

Test Plan for TPA SCR#478

Test Plan Name:

Tested By: Jose M. Menchaca, and Olufemi Osidele Date: September 9, 2004

Host Machine: SUN Ultra-4 server: Spock Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0s Test Version: TPA 5.0x

Process Level (PL) Tests

PL-1. Name:
Path for run directory: ~jmench/tpa50x/meanvalueRuns/SCR-478
~oosidele/tpa50x/ for Item 6
Path for archive of results: ~jmench/tpa50x/meanvalueRuns/SCR-478
Environment variables: setenv TPA_TEST ~/tpa50x
setenv TPA_DATA ~/tpa50x
Special input files or modifications to input files required :
Item3 and Item7 - forced Environment III values by forcing Drip Shield failure and reducing Rewetting Humidity. Pertinent Lines in the tpa.inp file:

```
constant
DripShieldThickness[m]
0.000

constant
RewettingHumidity[]
0.50

Item5 - Turn Seepage Threshold flag off.
```

Pertinent Lines in the tpa.inp file:

```
FlagSeepageThreshold[]
0
.
```

Special diagnostic code modifications required :modified fortran files as needed for verification purposes.

Corrected repository temperature and seepage threshold temperature calculations in exec.f.

Item 1: Modified corrosn.f to write the value of temperature and the current density at the given temperature.

Item 2: Modified corrosn.f to printout the following values:

piv
pH
Temperature
CorrosionPotential,e
pO2
cO2bulk(T,pO2)

cO2bulk(ReferenceTemperature,pO2)

Item 3: Modified ebsfail.f to printout the following values:

wnwc	Ratio of inhibiting nitrate to Cl to inhibiting carbonate to Cl
inhToCl2	inhibiting nitrate to Cl
inhcToCl2	inhibiting carbonate to Cl
wnws	Ratio of inhibiting nitrate to Cl to inhibiting sulfate to Cl
inhsToCl2	inhibiting sulfate to Cl
it	time
inhEff	Effective inhibitor concentration
no3(it)	time dependent nitrogen concentration of water
co3(it)	time dependent carbonate concentration of water
so4(it)	time dependent sulphur concentration of water

Item 6: The file nfenv.f was modified to write the following values to screen: time index, relative humidity, flow rate, period, Cl^- cnd Fl^- concentration. Also, to force Period III, nfenv.f was modified to increase the relative humidity to greater than the rewetting humidity.

Program modes to be used (append flags, scenario/model switches, etc.): Default values
Utility scripts needed to perform the test:
Utility codes needed in the analysis of the test data: Microsoft Excel®

Test Description:
1. Temperature dependence of anodic current density.

Objective: to assure that temperature dependence on anodic current density (as expressed in the equation below) has been properly implemented.

$$I_a(T) = I_a^o \exp\left[-\frac{E_o}{R}\left(\frac{1}{T}-\frac{1}{T_{ref}}\right)\right]$$

Assumptions: The following assumptions were made when implementing the above equation into the Excel® spreadsheet calculations:

Passive current Density, $I^0_a = 9{,}300$
Outer Overpack Activation Energy, $E_0 = 44{,}700$
Inner Overpack Activation Energy, $E_0 = 44{,}700$
Current Density Reference Temperature, $T_{ref} = 368K = 95°C$
Gas Constant, R = 8.3144
Temperature range of T = 273.15K - 473.15K

=E$5*EXP(-F$5*(1/B2-1/H$5)/8.3144)

Constraints:

Output files to compare or examine: Item_01.xls and failt.out

Step by step test procedure to be used:

1. Using the values listed in the "Assumptions" section above, produce a detailed curve (using Microsoft Excel®) showing the anodic current density dependence on temperature.

2. Run the tpa50x code for a mean value case.

3.Read the failt.out file into an Excel® spreadsheet and plot the current density versus temperature and compare the results with the current density versus temperature graph produced in Item_01.xls.

Pass fail criteria: Calculated values in spreadsheet are the same as in TPA output.

PASS

2. Equations computing corrosion potential.

Objective: To assure that the equation for computing corrosion potential (as expressed below) is implemented correctly.

$$i_r(E_{corr},T) = -\frac{i_r^{ef}\dfrac{C_{O_2}^{bulk}(T)}{C_{O_2}^{bulk}(T_{ref})}e^{-\frac{E_a}{RT}}e^{-\frac{Z_r\beta_r^{ef}F}{RT}E_{corr}}\left[H^+\right]^{n_H^{ef}}pO_2^{n_O^{ef}}}{1+\dfrac{\delta\, i_r^{ef}}{4F\phi\tau\, D_{O_2}(T)C_{O_2}^{bulk}(T_{ref})}e^{-\frac{E_a}{RT}}e^{-\frac{Z_r\beta_r^{ef}F}{RT}E_{corr}}\left[H^+\right]^{n_H^{ef}}pO_2^{n_O^{ef}}}$$

Assumptions: The following assumptions were made concerning values used in the caculations:

OuterChargeTransferCoefReductionReactHighpH = 0.0248
OuterChargeTransferCoefReductionReactLowpH = 0.01287
OuterChargeTransferCoefReductionReactHighpH = 5.51E+09
OuterChargeTransferCoefReductionReactLowpH = 7.57E+09
OuterActivationEnergyReductionReactHighpH = 40000
OuterActivationEnergyReductionReactLowpH = 40000
OuterEffectiveReactionOrderHighpH = 0.01897
OuterEffectiveReactionOrderLowpH = 0.0256
reactOrderO2Hi = 0.0248
reactOrderO2Lo = 0.01287
GasConstant = 8.3144
FaradayConstant = 96485
ElectronsRedReactHi = 4
ElectronsRedReactLo = 4
pO2 = 0.21
cO2bulk(ReferenceTemperature,pO2) = 0.268218
ThicknessOfWaterFilm = 0
WPSurfaceScaleThickness = 0

See SCR-478 for parameter to symbol equivalence in the equation.

Constraints:

Since δ is the greater of the "thickness of water film' and "WP surface scale thickness" which are both equal to 0, $\delta = 0$. This means that the entire denominator of the equation is equal to 1, therefore the only part of the equation that has been implemented in the code and the only portion of the equation that has been tested is the numerator.

Output files to compare or examine: failt.out and Scr478.xls

Step by step test procedure to be used

1. Using the values listed in the "Assumptions" section above, calculate partial cathodic current density (using Microsoft Excel®) for values of corrosion potential ranging from -5 to +5 in increments of 1.

2. Run the tpa50x code for a mean value case.

3. Compare the results of the Excel® spreadsheet calculations with the output from the modified failt.out output file.

Pass fail criteria: Calculated values in the spreadsheet are the same (within several significant figures) as in failt.out output file. Additionally, assure that the parameters listed in the **DELETE PARAMETERS** section of item 2 are deleted from the source code and from the tpa.inp files.

PASS on calculations

FAIL on deleted parameters.

The parameters listed below were still present in the TPA 5.0x version of the tpa.inp file and will be deleted in SCR-519:

OuterWPBetaKineticsParameterforOxygen
InnerWPBetaKineticsParameterforOxygen
OuterWPRateConstantforOxygenReduction[coulomb-m/mole/yr]
OuterWPActivationEnergyforOxygenReduction[J/mole]
InnerWPRateConstantforOxygenReduction[coulomb-m/mole/yr]
InnerWPActivationEnergyforOxygenReduction[J/mole]
StandardExchangeCurrentDensityforOxygenReduction[C/(m^2 yr)]
EquilibriumPotentialOxygenReduction[VSHE]

3 and 7. Inhibitors to localized corrosion and inhibiting oxyanions.

Objective: To assure that the portion of the equation dealing with inhibitors to corrosion and the inhibiting oxyanions (as shown in the equation below) are properly implemented.

$$inh = [NO_3^-] + \frac{\omega_N}{\omega_C}[CO_3^{2-}] + \frac{\omega_N}{\omega_S}[SO_4^{2-}]$$

Assumptions:

OuterInhibitingNitrateToCl (inhToCl2) = 0.1
OuterInhibitingCarbonateToCl (inhcToCl2) = 0.1
OuterInhibitingSulfateToCl (inhsToCl2) = 0.5
InnerInhibitingNitrateToCl (inhToCl2) = 1.0×10^{10}
InnerInhibitingCarbonateToCl (inhcToCl2) = 1.0×10^{10}
InnerInhibitingSulfateToCl (inhsToCl2) = 1.0×10^{10}
WeldInhibitingNitrateToCl (inhToCl2) = 0.3
WeldInhibitingCarbonateToCl (inhcToCl2) = 0.1
WeldInhibitingSulfateToCl (inhsToCl2) = 0.5

Constraints:

Output files to compare or examine: ebstrhc.inp (last column contains the inhibitor data) and Scr478.xls.

Step by step test procedure to be used:

1. Using the values listed in the "Assumptions" section above, calculate the effective inhibitor concentration for the known values of inhibiting nitrate, carbonate, and sulfate. The known values of the inhibitors are printed out in the tpa.out file with the modified ebsfail.f file.

2. Run the tpa50x code for a mean value case.
Additionally run a case with the no Drip Shield and with the rewetting humidity lowered to 50% to force environment III conditions to exercise values not used in the normal mean value case.

3. Compare the results of the Excel® spreadsheet calculations with the output from the modified tpa.out output file.

Pass fail criteria: Calculated values in the spreadsheet are the same (within several significant figures) as in tpa.out output file.

Item 3: **PASS**

Item 7: **PASS**

4 and 5. SeepageThresholdT parameter and FlagSeepageThreshold.

Objective: To assure that the seepage threshold temperature parameter, SeepageThresholdT, and the corresponding seepage threshold flag, FlagSeepageThreshold, are properly implemented.

Assumptions:

Constraints:

Output files to compare or examine: nfenv.rlt from each run.

Step by step test procedure to be used

1. Run a meanvalue base case run with the FlagSeepageThreshold set to 1, that is, turnded on.

2. Run a meanvalue base case run with the FlagSeepageThreshold set to 0, that is, turnded off.

3. Read the time, repository temperature (temprep) and water hitting the wastepackage (qm3hit) columns from the "Flag On" nfenv.rlt file and the water hitting the wastepackage (qm3hit) from the "Flag Off" nfenv.rlt file.

4. Create an x-y plot of time versus temperature and time versus "water hitting the waste package" using the dual units feature of Excel.

Pass fail criteria

Item 4. To verify that the seepage threshold temperature parameter is properly implemented , observe the graph created in step 4 above and affirm that anytime that the repository temperature exceeds 100° C (or whatever value the threshold is set to), the water hitting the waste package is zero. If this is the case then Item 4 is passed

Item 5. To verify that the seepage threshold temperature flag has been properly implemented, observe the graph produced in step 4 above and affirm that there are times near the 100° C transition point where there is water hitting the waste package. If this is the case then Item 5 is passed.

6. Logic to divide near-field chemistry into three periods.

Objective: To assure that the three periods used to analyze near-field chemistry for the waste packages and drip shield are properly implemented. Code logic should divide near-field chemistry into 3 periods: (i) Period I: deliquescence, (ii) Period II: direct seepage contact & evaporation, and (iii) Period III: re-wetting. Affected module: nfenv.f. A new parameter (RewettingHumidity) ws introduced to define the end of Period II or start of Period III.

Assumptions: none

Constraints: none

Output files to compare or examine: none

Step by step test procedure to be used

1. Copy and paste screen output into Microsoft Excel spreadsheet and parse the value fields

2. Implement the IF_THEN_ELSE logic independently in Excel (see attached spreadsheet file:
scr478_6_test.xls).

Pass fail criteria: Check that the periods assigned to each time index in the TPA output correspond to those assigned in the spreadsheet calculations. Additionally, assure that the

parameters listed in the **DELETE PARAMETERS** section of item 6 are deleted from the source code and from the tpa.inp files and that the files listed in the **DELETE INPUT FILES** section of item 6 are deleted from the data subdirectory of tpa 5.0x.

PASS on logic and calculations

FAIL on deletion of parameters.

The parameters listed below were still present in the TPA 5.0x version of the tpa.inp file and will be deleted in SCR-519:

IndriftEvaporationTemperature[C]
Indrift_Cl_PreTemperaturePeak[mol/L]
Indrift_Fl_PreTemperaturePeak[mol/L]
Indrift_pH_PreTemperaturePeak[]
Indrift_pH_PreTemperaturePeak[]
Indrift_CO3_PreTemperaturePeak[mol/L]
Indrift_Cl_PostTemperaturePeak[mol/L]
Indrift_Fl_PostTemperaturePeak[mol/L]
Indrift_pH_PostTemperaturePeak[]
Indrift_CO3_PostTemperaturePeak[mol/L]
Wastepackage_DeltaECrit_PreTemperaturePeak[VSHE]
Wastepackage_DeltaECrit_PostTemperaturePeak[VSHE]

FAIL on deletion of input files

The files listed below were still in the data subdirectory of TPA 5.0x and will be deleted in SCR-519.

data/multifaf.dat
data/multifbe.dat

Notes:

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-480	2. Software Title and Version: TPA 5.0w	3. Project No: 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): *nfenv.f, seismo2.f, mechfail.f, tpa.inp, driftcmn.i, exec.f, nrutil.f, ebsrel.f, ebsfail.f, ashplumo.f, execa.i*, and *zbrent.f*

The mechanical failure modules (*seismo2.f* and *mechfail.f*) calculate the degradation for the drift versus time. However, the current TPA code does not use this drift degradation to determine a diameter for natural backfill. In addition, the current TPA code uses only an emplaced backfill thickness within its thermal models. The TPA code needs to be modified to use the drift degradation and generate a diameterA(top) and a diameterB(sides) for natural backfill. The thermal models need to be updated to account for the accumulation of rubble above the drip shield.

5. Change Requested by: D. Gute, S. Mohanty, R. Fedors Date: 4-14-2004	6. Change Authorized by (*Software Developer*): R. Janetzke Date:4-15-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See attachment A, 7-Description of Changes

8. Implemented by: G. Adams	Date: 7-27-2004

9. Description of Acceptance Tests:

See attachment B, 9A-Test Plan for SCR480

See attachment C, 9B-Test Results for SCR480

10. Tested by: Albert Lozano	Date: September 22, 2004

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR480

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)	Distribution	Range	Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)
Add	NFENV	SelectThermalModel(1,2)	Thermal model 1 is a linear model, Thermal model 2 is an iterative model. Both models account for the presence of backfill.	iconstant	1	Allows the user to select between thermal models	*GRA*
Add	NFENV	FractionAllowedToDegrade[]	Used only in thermal model 1. Represents the fraction of the drift allowed to degrade and generate natural backfill.	constant	0.25	Used to represent the elliptical degradation of the drift and the accumulation of natural backfill on the sides of the drip shield first.	GRA

Add	NFENV	SelectParticleModel(1,2)	Used only in thermal model 2. Selects a particle model in which backfill parameters are calculated in particle model 1 or directly substituted in particle model 2.	iconstant	1	Allows the user to select between particle models.	GRA
Add	NFENV	KinematicViscosity[m^2/s]	Corresponds to 450K	constant	32.39e-6		SM
Add	NFENV	ThermalDiffusivity[m^2/s]	Corresponds to the thermal diffusivity calculated from the thermal conductivity using density and heat capacity at 450K. A density of 0.774 kg/m^3 and a heat capacity of 1.021 KJ/Kg-K.	constant	3.417e-4		SM
Add	NFENV	VolumeOfThermalExpansion[1/K]	Volume of thermal expansion of air	constant	2.85e-3		GRA
Add	NFENV	BackfillParticleDiameter[m]		uniform	0.1, 0.5		SM or GO
Add	NFENV	BackfillPorosity[]	Porosity of the backfill	uniform	0.1, 0.6		SM or GO
Add	NFENV	ThermalConductivityOfAir[W/(m-C)]	Thermal conductivity of air	constant	37.3e-3		SM or GO
Add	NFENV	TortuosityOfBackfill[]		uniform	1.25, 3.0		SM or GO
Add	NFENV	SortingCoefficient[]	Trask Sorting Coefficient	constant	2.0		SM or GO

Add	NFENV	SkewnessOfDistribution[ ]	Only used in particle model 2. Calculated in particle model 1.	uniform	0.0, 1.5		SM or GO
Add	NFENV	CoefficientOfVariation[]	Only used in particle model 2. Calculated in particle model 1.	uniform	0.1, 0.6		SM or GO
Add	NFENV	EmissivityOfBackfill[-]		constant	0.8		GRA
Modify From	NFENV	ThermalConductivityOfBackfill[W/(m-C)]		constant	0.27		GRA
Modify To	NFENV	ThermalConductivityOfBackfill[W/(m-C)]		uniform	0.12, 0.45		GRA

Attachment A

7 - Description of Change(s) or Problem Resolution

Two thermal models were incorporated into the TPA code. The first model is a linearized thermal model and is documented in *Temperature and Relative Humidity along Heated Drifts with and without Drift Degradation,* June 2004. The model implemented in the code was expanded to include three parallel paths instead of the two parallel paths shown in the document. The three parallel paths are: 1) the heat transfer pathway through the invert, 2) the heat transfer pathway through the drip shield and backfill in a region of the drift not allowed to degrade, and 3) the heat transfer pathway through the drip shield and backfill in a region of the drift allowed to degrade. The second thermal model is documented in chapter 12 of the *Risk Analysis for Risk Insights Progress Report,* July 31, 2004. This model accounts for convection and conduction through the backfill material. Within this model, the permeability of the backfill material is calculated using two separate particle models. The first particle model calculates the permeability from the median particle diameter and Trask sorting coefficient. The second particle model bypasses some of the calculations in the first particle model and allows the user to directly enter the coefficient of variation of the particle size distribution and the skewness of the particle size distribution. In addition, in this second model, the mean particle diameter is input instead of the median particle diameter.

In order to support these changes, the following parameters were added to *tpa.inp*:

```
iconstant
SelectThermalModel(1,2)
1
**
** FractionAllowedToDegrade is only used in thermal model 1
constant
FractionAllowedToDegrade[]
0.25
**
** Particle model 1 is the base permeability calculation
** Particle model 2 uses parameter substitution to calculate permeability
iconstant
SelectParticleModel(1,2)
1
**
constant
KinematicViscosity[m^2/s]
32.39e-6
**
constant
ThermalDiffusivity[m^2/s]
3.417e-4
**
constant
VolumeOfThermalExpansion[1/K]
2.85e-3
**
**
** For particle model 1, the BackfillParticleDiameter is the median
```

```
** For particle model 2, the BackfillParticleDiameter is the mean
uniform
BackfillParticleDiameter[m]
0.1,0.5
**
uniform
BackfillPorosity[]
0.1,0.6
**
constant
ThermalConductivityOfAir[W/(m-C)]
37.3e-3
**
uniform
TortuosityOfBackfill[]
1.25,3.0
**
constant
SortingCoefficient[]
2.0
**
** SkewnessOfDistribution and CoefficientOfVariation are used
** in particle model 2
uniform
SkewnessOfDistribution[]
0.0,1.5
**
uniform
CoefficientOfVariation[]
0.1,0.6
**
```

The following parameter was modified in *tpa.inp*: (It was formerly a constant of 0.27 and was modified to be a uniform distribution between 0.12 and 0.45.)

```
**constant
uniform
ThermalConductivityOfBackfill[W/(m-C)]
0.12, 0.45
**0.27
```

The base case TPA thermal model is thermal model 1 with the fraction of the drift allowed to degrade equal to 0.25. Note that when the fraction of the drift allowed to degrade equals the circumferential fraction not covered by the floor/invert (currently 0.75), the three heat transfer pathways become just two pathways since all of the non-invert region is allowed to degrade instead of just a portion of it.

Attachment B

9A - Test Plan for TPA SCR#480

Test Plan Name: Thermal Models and Drift Shield Degradation

Tested By:	Albert S. Lozano	Date: September 22, 2004	
Host Machine:	Spock	Host OS:	Solaris
Baseline Version:	tpa50w	Test Version:	tpa50x

Process Level (PL) Tests

Create a directory containing the baseline (previously tested) source code.
Create a directory containing the baseline runtime and related files.

Create a directory containing the modified source code.
Create a directory containing the modified runtime and related files.

Create Environment Variables:
TPA_TEST
TPA_DATA

PL - 1 Modification of *tpa.inp* file to incorporate 13 new parameters.

Special input files or modifications to input files required : Addition of new parameters to *tpa.inp*
Special diagnostic code modifications required : None
Program modes to be used (append flags, scenario/model switches, etc.): None
Utility scripts needed to perform the test: None
Utility codes needed in the analysis of the test data: Text Editor
Test description:
- objective

Verify that thirteen new TPA parameters were added to the *tpa.inp* file. They are SelectThermalModel(1,2), FractionAllowedToDegrade[], SelectParticleModel(1,2), KinematicViscosity[m^2/s], ThermalDiffusivity[m^2/s], VolumeOfThermalExpansion[1/K], BackfillParticleDiameter[m], BackfillPorosity[], ThermalConductivityOfAir[W/(m-C)], TortuosityOfBackfill[], SortingCoefficient[], SkewnessOfDistribution[], and CoefficientOfVariation[]. The TPA parameter ThermalConductivityOfBackfill[W/(m-C)] was changed from a constant to a uniform distribution.

- assumptions: None
- constraints: None
- output files to compare or examine: *tpa.inp*
- step by step test procedure to be used: Observation

- pass fail criteria: If parameters are included in the *tpa.inp* file, then the test passes.

PL - 2 Modification of TPA code to use drift degradation and generate a diameter A (top) and a diameter B(sides) for natural backfill as a function of time

Special input files or modifications to input files required : *tpa.inp*
Special diagnostic code modifications required : Added print statements to *exec.f*
Program modes to be used (append flags, scenario/model switches, etc.): None
Utility scripts needed to perform the test: None
Utility codes needed in the analysis of the test data: Text Editor and Excel
Test description:
- objective
Verify that the code generates a diameter A(top) and a diameter B(sides) of natural backfill as a function of time for three cases.
A. No Disruptive Events
B. Mechanical Degradation
C. Full Wedge
D. Emplacement with fixed thickness

- assumptions: None
- constraints: None
- output files to compare or examine: *equiv.rlt, tpa.out*
EquivalentRadiusDriftArea.xls
- step by step test procedure to be used: A - Examine *tpa.out* temporary prints
B,C,D - Examine the *equiv.rlt* and compare the results to the spreadsheet values.

- pass fail criteria: A- Diameter A and B are 2*(DripShield Radius + Thickness)
Diameter A and diameter B = 2.78 m
B,C - If the spreadsheet values agree with the run, the test passes.
D - Diameter A and B =2.75+.03+2*(.5) =3.78 m

PL - 3 Thermal Models Support Accumulation of Rubble Over Drip Shield

Special input files or modifications to input files required : *tpa.inp*
Special diagnostic code modifications required : None
Program modes to be used (append flags, scenario/model switches, etc.): None
Utility scripts needed to perform the test: None
Utility codes needed in the analysis of the test data: Text Editor, Excel Spreadsheets
Test description:
- objective

Verify that the thermal models use the time variant diameterA(top) and diameterB(sides) of the backfill.

- assumptions: None
- constraints: None
- output files to compare or examine:
- step by step test procedure to be used: During the software development phase, several spreadsheets were developed to assure that the code correctly implemented the thermal models.

  Various TPA runs were executed and the resultant files were stored in directories, *nfenviterative*, *nfenvlinear*, and *wedge*..
- pass fail criteria: If the results of the spreadsheet values agree with the run, then the test passes.

System Level (SL) Tests

SL-1. No system level tests were performed.

SL-2.

Notes:

Attachment C

9B - Test Results for TPA SCR#480

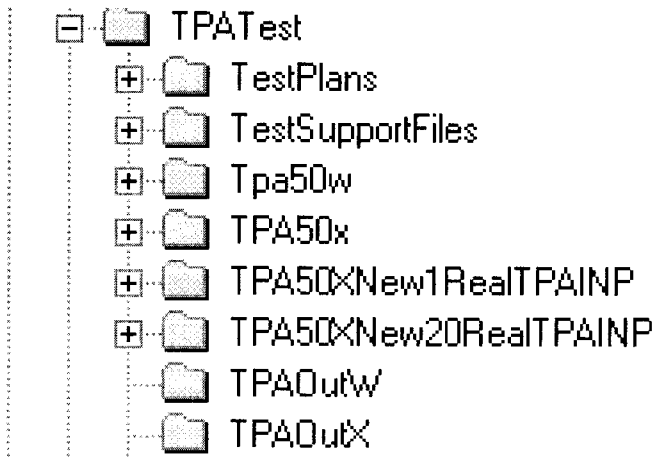
Test Plan Name:	Thermal Models and Drift Shield Degradation	
Tested By:	Albert S. Lozano	Date: September 22, 2004
Host Machine:	Spock	Host OS:
Baseline Version:	tpa50w	Test Version: tpa50x

Process Level (PL) Tests

The following directories were created on "spock" for the tpa50w and tpa50x versions.
`/home/alozano/tpa5/tpa50w`
`/home/alozano/tpa5/tpa50x`

The following environment variables were created on "spock".
TPA_TEST=/home/alozano/tpa5/tpa50x
TPA_DATA=/home/alozano/tpa5/tpa50x

In addition to these images of these two directories and other support directories were created on Adriana for ease of documentation into the word perfect documents.
This directory tree starts at `D:\alozano\tpatest`



PL - 1 Modification of tpa.inp file to incorporate 13 new parameters.

Verify that thirteen new tpa parameters were added to the *tpa.inp* file. They are SelectThermalModel(1,2), FractionAllowedToDegrade[], SelectParticleModel(1,2), KinematicViscosity[m^2/s], ThermalDiffusivity[m^2/s], VolumeOfThermalExpansion[1/K], BackfillParticleDiameter[m], BackfillPorosity[], ThermalConductivityOfAir[W/(m-C)], TortuosityOfBackfill[], SortingCoefficient[], SkewnessOfDistribution[], and

CoefficientOfVariation[]. The TPA parameter ThermalConductivityOfBackfill[W/(m-C)] was changed from a constant to a uniform distribution as described in SCR 480.

The following was copied from *tpa.inp* file for x version

```
** GADAMS PA-SCR-480 7-19-04: Select the model used to calculate
** indrift temperatures, Model 1 is a linearized model and Model 2
** is an iterative model.
iconstant
SelectThermalModel(1,2)
1
**
** FractionAllowedToDegrade is only used in thermal model 1
constant
FractionAllowedToDegrade[]
0.25
**
** GADAMS PA-SCR-480 7-19-04: End of change
**
** GADAMS PA-SCR-480 7-20-04: Added parameters associated with
** iterative model
** Particle model 1 is the base permeability calculation
** Particle model 2 uses parameter substitution to calculate permeability
iconstant
SelectParticleModel(1,2)
1
**
constant
KinematicViscosity[m^2/s]
32.39e-6
**
constant
ThermalDiffusivity[m^2/s]
3.417e-4
**
constant
VolumeOfThermalExpansion[1/K]
2.85e-3
**
**
** For particle model 1, the BackfillParticleDiameter is the median
** For particle model 2, the BackfillParticleDiameter is the mean
uniform
BackfillParticleDiameter[m]
0.1,0.5
**
uniform
BackfillPorosity[]
0.1,0.6
**
constant
ThermalConductivityOfAir[W/(m-C)]
37.3e-3
**
uniform
TortuosityOfBackfill[]
1.25,3.0
**
```

```
constant
SortingCoefficient[]
2.0
**
** SkewnessOfDistribution and CoefficientOfVariation are used
** in particle model 2
uniform
SkewnessOfDistribution[]
0.0,1.5
**
uniform
CoefficientOfVariation[]
0.1,0.6
**
** GADAMS PA-SCR-480 7-20-04: End of change
**
```

```
** GADAMS PA-SCR-480 7-17-04: Added emissivity of backfill material
constant
EmissivityOfBackfill[-]
0.8
**
```

```
** GADAMS PA-SCR-480 7-27-04: Changed thermal conductivity
** of the backfill to a uniform distribution to coincide
** with a natural backfill base case
**constant
uniform
ThermalConductivityOfBackfill[W/(m-C)]
0.12, 0.45
**0.27
```

The parameters were added to the *tpa.inp* file. **PASSED**

PL - 2 Modification of TPA code to use drift degradation and generate a diameter A(top) and a diameter B(sides) for natural backfill as a function of time

Verify that the code generates a diameter A(top) and a diameter B(sides) of natural backfill as a function of time.

A. No Disruptive Events

This text came from *tpa.out*. It was generated by tpa5 x version of the code for a scenario with no Disruptive events.

```
exec: calling nfenvFl
 Lozano
 Time[yr]                DriftDiaA   DriftDiaB   BFDiaA      BFDiaB
      0.                 5.5         5.5         0.          0.
     2.3101577559532     5.5         5.5         0.          0.
     4.6743995440580     5.5         5.5         0.          0.
      . . .
     47.564168391772     5.5         5.5         0.          0.
     50.987870019756     5.5         5.5         2.78        2.78
     54.491725303243     5.5         5.5         2.78        2.78
     58.077610751690     5.5         5.5         2.78        2.78
     61.747446806275     5.5         5.5         2.78        2.78
     65.503198868395     5.5         5.5         2.78        2.78
     69.346878352250     5.5         5.5         2.78        2.78
     73.280543762065     5.5         5.5         2.78        2.78
     77.306301794538     5.5         5.5         2.78        2.78
      . . .
     9107.1641853546     5.5         5.5         2.78        2.78
     9322.6858258942     5.5         5.5         2.78        2.78
     9543.2531302230     5.5         5.5         2.78        2.78
     9768.9842244047     5.5         5.5         2.78        2.78
    10000.0000000000     5.5         5.5         2.78        2.78
```

Diameter A and diameter B = 2.78 m - **PASSED**

B. Mechanical Degradation - Partial Wedge

```
(FractionAllowedToDegrade[]= 0.25
CircumferentialFractionNotCoveredByFloor[]=.75)
```

The results of a TPA run are found in *equiv.rlt*. The diameters are calculated as BackDiameterA (Top) and BackDiameterB(Sides). These numbers are compared with those calculated an Excel spreadsheet using the same formulas as the code. The results are tabulated in Appendix A - Comparison of Backfill Diameters - Partial Wedge as determined by codes with the same formulas in an Excel Spreadsheet. .

The numbers matched; therefore, this test **PASSED**

C. Mechanical Degradation - Full Wedge

```
(FractionAllowedToDegrade[]= CircumferentialFractionNotCoveredByFloor[]=.75)
```

The results of a TPA run are found in *equiv.rlt*. The diameters are calculated as BackDiameterA (Top) and BackDiameterB(Sides). These numbers are compared with those calculated an Excel spreadsheet using the same formulas as the code. The results are tabulated in Appendix B - Comparison of Backfill Diameters - Full Wedge as determined by codes with the same formulas in an Excel Spreadsheet. .

The numbers matched; therefore, this test **PASSED**

D. Emplacement with fixed thickness

```
(EmplacementBackfillThickness[m]> 0.0)
```

Time	Drift Dia A	Drift Dia B	BF Dia A	BF Dia B
0.00000E+00	5.50000E+00	5.50000E+00	0.00000E+00	0.00000E+00
2.31016E+00	5.50000E+00	5.50000E+00	0.00000E+00	0.00000E+00
...				
4.75642E+01	5.50000E+00	5.50000E+00	0.00000E+00	0.00000E+00
5.09879E+01	5.50000E+00	5.50000E+00	3.78000E+00	3.78000E+00
5.44917E+01	5.50000E+00	5.50000E+00	3.78000E+00	3.78000E+00
5.80776E+01	5.50000E+00	5.50000E+00	3.78000E+00	3.78000E+00
6.17474E+01	5.50000E+00	5.50000E+00	3.78000E+00	3.78000E+00
6.55032E+01	5.50000E+00	5.50000E+00	3.78000E+00	3.78000E+00

Diameter A and diameter B = 3.78 m - **PASSED**

PL - 3 Thermal Models Support Accumulation of Rubble Over Drip Shield

During the software development phase, several spreadsheets were developed to assure that the code correctly implemented the thermal models. The spreadsheets and results of these experiments are found in subdirectory `\TPATest\SpreadSheets\FromGeroge\handcalculations`. Appendix C shows the portion of the code that calculates the temperatures taking account the accumulation of the rubble over the drip shield. The following results compare the spreadsheet and TPA run results at specific time steps.

nfenvIterative - Result summary

Case 1: Prior to closure (2.5694E+01 years)

Calculation for Waste Package Temperature			
kr1	8.635021	8.635000	0.0002%
kcv1	0.758380	0.758370	0.0013%
calculated Temperature WP	363.889673	363.831000	0.0161%
Calculation for Thermal Loading			
gcond	4.636427911	4.64E+00	0.0006%
gbelow	0	0	
gequiv	4.636427911	4.64E+00	0.0006%
Thermal Load Below	22.87613531	2.29E+01	0.0050%
Calculated Thermal Load Above	1432.523865	1.43E+03	0.0017%

Case 2: After Closure, No Backfill

Calculation for Drip Shield Outer Temperature		**Comparison to Test Run**	**Percentage Difference**
kcv2	0.480463	0.480600	-0.0286%
kr2	9.471241	9.471400	-0.0017%
Calculated TemperatureDSO	424.073446	424.070000	0.0008%
Calculation for Drip Shield Inner Temperature			
Calculated TemperatureDSI	424.0928843	424.100000	-0.0017%
Calculation for Waste Package Temperature			
kr1	5.178234	5.18E+00	0.0026%
kcv1	0.271445	2.71E-01	0.0019%
calculated Temperature WP	428.559810	428.560000	0.0000%
Calculation for Thermal Loading			
gcond	4.636427911	4.636400	0.0006%
gbelow	0		
gequiv	4.636427911	4.636400	0.0006%
Thermal Load Below	34.72684506		
Calculated Thermal Load Above	1689.773155	1689.800000	-0.0016%

Case 3a: After Closure, Incompletely Backfilled

Calculation for Outer Backfill Temperature		**Comparison to Test Run**	**Percentage Difference**

kcv2	0.252422	0.252430	-0.0031%
kr2	8.918337	8.918100	0.0027%
Calculated TemperatureBFO	420.270173	420.270000	0.0000%

Calculation for Drip Shield Outer Temperature

phi_bar	-8.228819E+00	-8.228819E+00	0.0000%
sigma_phi	-7.314506E+00	-7.314506E+00	0.0000%
dp_bar	3.698817E-26	3.698817E-26	0.0000%
sigma_dp	1.412130E-20	1.412130E-20	0.0000%
CDp	3.817787E+05	3.817787E+05	0.0000%
e3 (partial skewness calculation)	1.566963E-43	1.566963E-43	0.0000%
skewness {gama}	5.564614E+16	5.564614E+16	0.0000%
perm (m^2)	4.095483E-16	4.095483E-16	0.0000%
rari	9.243869E-08	9.244027E-08	-0.0017%
qc1	2.313416E+02	2.313492E+02	-0.0033%
Nu	3.658409E-05	3.658375E-05	0.0009%
q1	8.463423E-03		
keff(only consider conduction since Nu is less than 1)	2.700000E-01	2.700000E-01	0.0000%
Calculated TemperatureDSO	484.552148	484.550000	0.0004%

Calculation for Drip Shield Inner Temperature

Calculated TemperatureDSI	484.5692346	484.570000	-0.0002%

Calculation for Waste Package Temperature

kr1	7.664231	7.66E+00	-0.0009%
kcv1	0.236730	2.37E-01	-0.0549%
calculated Temperature WP	487.155545	487.150000	0.0011%

Calculation for Thermal Loading

gcond	4.636427911	4.636400	0.0006%
gbelow	115.4173604	115.420000	-0.0023%
gequiv	4.457370973	4.457400	-0.0007%
Thermal Load Below	304.2155689		
Calculated Thermal Load Above	1420.284431	1.42E+03	-0.0011%

Case 3b: After Closure, Completely Backfilled
Calculation for Outer Backfill Temperature

		Comparison to Test Run	Percentage Difference
Calculated TemperatureBFO	421.070000	421.070000	0.0000%

Calculation for Drip Shield Outer Temperature

phi_bar	-8.228819E+00	-8.228819E+00	0.0000%
sigma_phi	-7.314506E+00	-7.314506E+00	0.0000%
dp_bar	3.698817E-26	3.698817E-26	0.0000%
sigma_dp	1.412130E-20	1.412130E-20	0.0000%
CDp	3.817787E+05	3.817787E+05	0.0000%
e3 (partial skewness calculation)	1.566963E-43	1.566963E-43	0.0000%
skewness {gama}	5.564614E+16	5.564614E+16	0.0000%

perm (m^2)	4.095483E-16	4.095483E-16	0.0000%
rari	1.239035E-07	1.239074E-07	-0.0032%
qc1	2.142278E+02	2.142344E+02	-0.0031%
Nu	6.399700E-05	6.399802E-05	-0.0016%
q1	1.370993E-02		
keff(only consider conduction since Nu is less than 1)	2.700000E-01	2.700000E-01	0.0000%
Calculated TemperatureDSO	507.230846	507.230000	0.0002%
Calculation for Drip Shield Inner Temperature			
Calculated TemperatureDSI	507.2478112	507.250000	-0.0004%
Calculation for Waste Package Temperature			
kr1	8.775952	8.776000	-0.0005%
kcv1	0.224855	0.224900	-0.0198%
calculated Temperature WP	509.351659	509.350000	0.0003%
Calculation for Thermal Loading			
gcond	4.636427911	4.636400	0.0006%
gbelow	0	0.000000	
gequiv	4.636427911	4.636400	0.0006%
Thermal Load Below	409.303856		
Calculated Thermal Load Above	1315.196144	1315.200000	-0.0003%

Case 3a: After Closure, Incompletely Backfilled

Calculation for Outer Backfill Temperature		**Comparison to Test Run**	**Percentage Difference**
kcv2	0.261997	0.262010	-0.0049%
kr2	8.925361	8.925200	0.0018%
Calculated TemperatureBFO	420.490431	420.490000	0.0001%
Calculation for Drip Shield Outer Temperature			
perm (m^2)	9.281081E-05	9.281081E-05	0.0000%
rari	3.447918E+03	3.447857E+03	0.0018%
qc1	3.807708E+01	3.807699E+01	0.0002%
Nu	7.065516E+00	7.065326E+00	0.0027%
q1	2.690342E+02	2.690264E+02	0.0029%
keff	1.907689E+00	1.907638E+00	0.0027%
Calculated TemperatureDSO	431.069650	431.070000	-0.0001%
Calculation for Drip Shield Inner Temperature			
Calculated TemperatureDSI	431.092367	431.090000	0.0005%
Calculation for Waste Package Temperature			
kr1	5.431656	5.431700	-0.0008%
kcv1	0.266921	0.266900	0.0078%
calculated Temperature WP	435.258602	435.260000	-0.0003%
Calculation for Thermal Loading			

gcond	4.636427911	4.636400	0.0006%
gbelow	115.4173604	115.420000	-0.0023%
gequiv	4.457370973	4.457400	-0.0007%
Thermal Load Below	72.92258912		
Calculated Thermal Load Above	1651.577411	1.65E+03	-0.0014%

nfenvLinear

Case 1: Prior to closure

Temperatures	
Temperature WP (calculated)	[illegible]
Temperature WP (code generated)	[illegible]

Case 2: After closure but no backfill present

Temperatures	
Temperature WP (calculated)	[illegible]
Temperature WP (code generated)	[illegible]
Temperature DS (calculated)	[illegible]
Temperature DS (code generated)	[illegible]

Case 3: After Closure, Backfill present but not completely backfilled

Temperatures	
Temperature WP (calculated)	[illegible]
Temperature WP (code generated)	[illegible]
Temperature DS (calculated)	[illegible]
Temperature DS (code generated)	[illegible]
Temperature BF (calculated)	[illegible]
Temperature BF (code generated)	[illegible]

Case 3: After Closure, Completely Backfilled

Temperatures	
Temperature WP (calculated)	[illegible]
Temperature WP (code generated)	[illegible]
Temperature DS (calculated)	[illegible]
Temperature DS (code generated)	[illegible]
Temperature BF (calculated)	[illegible]
Temperature BF (code generated)	[illegible]

nfenvWedge

Case 1: Prior to closure no backfill in sections A or B

Temperatures	
Temperature WP (calculated)	92.3148
Temperature WP (code generated)	92.3140

Case 2: After closure backfill is not present in section A or section B

Temperatures	
Temperature WP (calculated)	157.2556
Temperature WP (code generated)	[illegible]
Temperature DS A(calculated)	151.7805
Temperature DS A(code generated)	151.7800
Temperature DS B(calculated)	151.7805
Temperature DS B(code generated)	151.7800

Case 2: After closure backfill is not present in section A but is present in section B

Temperatures	
Temperature WP (calculated)	166.6906

Temperature WP (code generated)	156.8900
Temperature DS A(calculated)	152.1878
Temperature DS A(code generated)	152.1700
Temperature DS B(calculated)	165.7420
Temperature DS B(code generated)	165.7400

Case 3: Both sections contain backfill natural degradation

Temperatures	
Temperature WP (calculated)	[illegible]
Temperature WP (code generated)	[illegible]
Temperature DS A(calculated)	[illegible]
Temperature DS A(code generated)	[illegible]
Temperature DS B(calculated)	[illegible]
Temperature DS B(code generated)	[illegible]
Temperature BF A(calculated)	[illegible]
Temperature BF A(code generated)	[illegible]
Temperature BF B(calculated)	[illegible]
Temperature BF B(code generated)	[illegible]

Case 3: Both sections contain backfill emplaced to the rock wall (1.36 m of backfill)

Temperatures	
Temperature WP (calculated)	[illegible]
Temperature WP (code generated)	[illegible]
Temperature DS A(calculated)	[illegible]
Temperature DS A(code generated)	[illegible]
Temperature DS B(calculated)	[illegible]
Temperature DS B(code generated)	[illegible]
Temperature BF A(calculated)	[illegible]
Temperature BF A(code generated)	[illegible]
Temperature BF B(calculated)	[illegible]
Temperature BF B(code generated)	[illegible]

Case 3: Both sections contain emplaced backfill but not to the rock wall (0.5 m of backfill)

Temperatures	
Temperature WP (calculated)	190.6810
Temperature WP (code generated)	190.6800
Temperature DS A(calculated)	189.8392
Temperature DS A(code generated)	189.8400
Temperature DS B(calculated)	189.8392
Temperature DS B(code generated)	189.8400
Temperature BF A(calculated)	142.9572
Temperature BF A(code generated)	142.9600
Temperature BF B(calculated)	142.9572
Temperature BF B(code generated)	142.9600

The numbers from the code and the spreadsheet agree; therefore, the test **PASSED**.

System Level (SL) Tests

No System Level Tests were performed.

Appendix A

Comparison of Backfill Diameters - Partial Wedge as determined by codes with the same formulas in an Excel Spreadsheet.

Input file tpa.inp as supplied with TPA Version 5.0x Code.

Test SCR 481 Max Normal Stress.

TPA 5.0x, Job started: Mon Aug 23 17:00:58 2004
EQVDIA Results

with the output mode specified in "tpa.inp"

REALIZATION 12

Equivalent diameters due to degradation of the drift

Equivalent Diameters, Subarea Analysis: Subarea 5

These columns are from TPATEST/ TPA50XNew1RealTPAINP/eqvdia.rlt			*These columns are from the spreadsheet, EquivalentRadiusDriftArea.xls*	
Time	BF Dia A	BF Dia B	BF Dia A	BF Dia B
0.00000E+00	0.00000E+00	0.00000E+00	0.0	0.0
2.31016E+00	0.00000E+00	0.00000E+00	0.0	0.0
4.67440E+00	0.00000E+00	0.00000E+00	0.0	0.0
7.09399E+00	0.00000E+00	0.00000E+00	0.0	0.0
9.57023E+00	0.00000E+00	0.00000E+00	0.0	0.0
1.21044E+01	0.00000E+00	0.00000E+00	0.0	0.0
1.46980E+01	0.00000E+00	0.00000E+00	0.0	0.0
1.73522E+01	0.00000E+00	0.00000E+00	0.0	0.0
2.00686E+01	0.00000E+00	0.00000E+00	0.0	0.0
2.28486E+01	0.00000E+00	0.00000E+00	0.0	0.0
2.56937E+01	0.00000E+00	0.00000E+00	0.0	0.0
2.86054E+01	0.00000E+00	0.00000E+00	0.0	0.0
3.15852E+01	0.00000E+00	0.00000E+00	0.0	0.0
3.46349E+01	0.00000E+00	0.00000E+00	0.0	0.0
3.77559E+01	0.00000E+00	0.00000E+00	0.0	0.0
4.09499E+01	0.00000E+00	0.00000E+00	0.0	0.0
4.42188E+01	0.00000E+00	0.00000E+00	0.0	0.0
4.75642E+01	0.00000E+00	0.00000E+00	0.0	0.0
5.09879E+01	2.78000E+00	2.83970E+00	2.78	2.839708493
5.44917E+01	2.78000E+00	3.04200E+00	2.78	3.041985192
5.80776E+01	2.78000E+00	3.23597E+00	2.78	3.235949711
6.17474E+01	2.78000E+00	3.42311E+00	2.78	3.423132037
6.55032E+01	2.78000E+00	3.60460E+00	2.78	3.604612881
6.93469E+01	2.78000E+00	3.78132E+00	2.78	3.781340008
7.32805E+01	2.78000E+00	3.95402E+00	2.78	3.954022426
7.73063E+01	2.78000E+00	4.12327E+00	2.78	4.123284587
8.14263E+01	2.78000E+00	4.28958E+00	2.78	4.289570164
8.56428E+01	2.78000E+00	4.45335E+00	2.78	4.453346396
8.99579E+01	2.78000E+00	4.61494E+00	2.78	4.614959048
9.43741E+01	2.78000E+00	4.77466E+00	2.78	4.774679387
9.88937E+01	2.78000E+00	4.93277E+00	2.78	4.932772199
1.03519E+02	2.78000E+00	5.08949E+00	2.78	5.089491813
1.08253E+02	2.78000E+00	5.24504E+00	2.78	5.245052694

1.13097E+02	2.78000E+00	5.39959E+00	2.78	5.399585795
1.18055E+02	2.98445E+00	5.50000E+00	2.984508234	5.5
1.23129E+02	3.51470E+00	5.50000E+00	3.514720802	5.5
1.28322E+02	3.98496E+00	5.50000E+00	3.985002853	5.5
1.33636E+02	4.41467E+00	5.50000E+00	4.414677457	5.5
1.39075E+02	4.81490E+00	5.50000E+00	4.814927386	5.5
1.44641E+02	5.19265E+00	5.50000E+00	5.192656212	5.5
1.50338E+02	5.55270E+00	5.50000E+00	5.552707839	5.5
1.56167E+02	5.89847E+00	5.50000E+00	5.898482866	5.5
1.62134E+02	6.23251E+00	5.50000E+00	6.232488238	5.5
1.68240E+02	6.55676E+00	5.50000E+00	6.556766571	5.5
1.74489E+02	6.87279E+00	5.50000E+00	6.872789758	5.5
1.80884E+02	7.18183E+00	5.50000E+00	7.181847862	5.5
1.87429E+02	7.48491E+00	5.50000E+00	7.484923744	5.5
1.94127E+02	7.78288E+00	5.50000E+00	7.782889944	5.5
2.00982E+02	8.07644E+00	5.50000E+00	8.076443037	5.5
2.07997E+02	8.36622E+00	5.50000E+00	8.366247294	5.5
2.15177E+02	8.65274E+00	5.50000E+00	8.652764761	5.5
2.22524E+02	8.93646E+00	5.50000E+00	8.936482146	5.5
2.30044E+02	9.21779E+00	5.50000E+00	9.217788703	5.5
2.37740E+02	9.49708E+00	5.50000E+00	9.497075979	5.5
2.45616E+02	9.77464E+00	5.50000E+00	9.774656655	5.5
2.53676E+02	1.00508E+01	5.50000E+00	10.05080059	5.5
2.61926E+02	1.03257E+01	5.50000E+00	10.32573263	5.5
2.70368E+02	1.05997E+01	5.50000E+00	10.59975808	5.5
2.79008E+02	1.08730E+01	5.50000E+00	10.87303483	5.5
2.87850E+02	1.11458E+01	5.50000E+00	11.14583952	5.5
2.96899E+02	1.14181E+01	5.50000E+00	11.41819662	5.5
3.06160E+02	1.16903E+01	5.50000E+00	11.69031503	5.5
3.15638E+02	1.19625E+01	5.50000E+00	11.96257949	5.5
3.25337E+02	1.22347E+01	5.50000E+00	12.23476902	5.5
3.35264E+02	1.25072E+01	5.50000E+00	12.50725365	5.5
3.45423E+02	1.27801E+01	5.50000E+00	12.78020202	5.5
3.55820E+02	1.30534E+01	5.50000E+00	13.05347992	5.5
3.66461E+02	1.33274E+01	5.50000E+00	13.32742668	5.5
3.77350E+02	1.36020E+01	5.50000E+00	13.60200189	5.5
3.88495E+02	1.38775E+01	5.50000E+00	13.8775664	5.5
3.99900E+02	1.41538E+01	5.50000E+00	14.153846	5.5
4.11572E+02	1.44311E+01	5.50000E+00	14.4311317	5.5
4.23518E+02	1.47096E+01	5.50000E+00	14.70963365	5.5
4.35743E+02	1.49891E+01	5.50000E+00	14.98907966	5.5
4.48255E+02	1.52700E+01	5.50000E+00	15.27003702	5.5
4.61059E+02	1.55521E+01	5.50000E+00	15.55212409	5.5
4.74163E+02	1.58357E+01	5.50000E+00	15.83573033	5.5
4.87574E+02	1.61207E+01	5.50000E+00	16.12082918	5.5
5.01299E+02	1.64073E+01	5.50000E+00	16.40720078	5.5
5.15346E+02	1.66955E+01	5.50000E+00	16.69553726	5.5
5.29721E+02	1.69853E+01	5.50000E+00	16.98537009	5.5
5.44432E+02	1.72770E+01	5.50000E+00	17.27690136	5.5
5.59488E+02	1.75704E+01	5.50000E+00	17.57045191	5.5
5.74897E+02	1.78657E+01	5.50000E+00	17.86575075	5.5
5.90666E+02	1.81630E+01	5.50000E+00	18.16297645	5.5
6.06805E+02	1.84623E+01	5.50000E+00	18.46224872	5.5
6.23321E+02	1.87636E+01	5.50000E+00	18.76368597	5.5
6.40224E+02	1.90671E+01	5.50000E+00	19.06706329	5.5
6.57523E+02	1.93727E+01	5.50000E+00	19.37273969	5.5
6.75226E+02	1.96650E+01	5.50000E+00	19.66504005	5.5
6.93345E+02	1.97619E+01	5.50000E+00	19.76196347	5.5
7.11887E+02	1.97823E+01	5.50000E+00	19.78226984	5.5
7.30863E+02	1.98031E+01	5.50000E+00	19.80305532	5.5
7.50284E+02	1.98243E+01	5.50000E+00	19.8243184	5.5
7.70159E+02	1.98461E+01	5.50000E+00	19.84605754	5.5
7.90500E+02	1.98683E+01	5.50000E+00	19.86827119	5.5
8.11317E+02	1.98910E+01	5.50000E+00	19.89101305	5.5

8.32621E+02	1.99142E+01	5.50000E+00	19.91422607	5.5
8.54424E+02	1.99379E+01	5.50000E+00	19.93790862	5.5
8.76738E+02	1.99444E+01	5.50000E+00	19.94441777	5.5
8.99573E+02	1.99444E+01	5.50000E+00	19.94441777	5.5
9.22944E+02	1.99444E+01	5.50000E+00	19.94441777	5.5
9.46861E+02	1.99444E+01	5.50000E+00	19.94441777	5.5

Appendix B

Comparison of Backfill Diameters - Full Wedge as determined by codes with the same formulas in an Excel Spreadsheet.

Input file tpa.inp as supplied with TPA Version 5.0x Code.

Test SCR 481 Max Normal Stress.

TPA 5.0x, Job started: Mon Aug 23 17:00:58 2004
EQVDIA Results

with the output mode specified in "tpa.inp"

REALIZATION 12

Equivalent diameters due to degradation of the drift

Equivalent Diameters, Subarea Analysis: Subarea 5

These columns are from TPATEST/ TPA50XNew1RealTPAINP/eqvdia.rlt			*These columns are from the spreadsheet, EquivalentRadiusDriftArea.xls*	
Time	BF Dia A	BF Dia B	BF Dia A	BF Dia B
0.00000E+00	0.00000E+00	0.00000E+00	0.0	0.0
2.31016E+00	0.00000E+00	0.00000E+00	0.0	0.0
4.67440E+00	0.00000E+00	0.00000E+00	0.0	0.0
7.09399E+00	0.00000E+00	0.00000E+00	0.0	0.0
9.57023E+00	0.00000E+00	0.00000E+00	0.0	0.0
1.21044E+01	0.00000E+00	0.00000E+00	0.0	0.0
1.46980E+01	0.00000E+00	0.00000E+00	0.0	0.0
1.73522E+01	0.00000E+00	0.00000E+00	0.0	0.0
2.00686E+01	0.00000E+00	0.00000E+00	0.0	0.0
2.28486E+01	0.00000E+00	0.00000E+00	0.0	0.0
2.56937E+01	0.00000E+00	0.00000E+00	0.0	0.0
2.86054E+01	0.00000E+00	0.00000E+00	0.0	0.0
3.15852E+01	0.00000E+00	0.00000E+00	0.0	0.0
3.46349E+01	0.00000E+00	0.00000E+00	0.0	0.0
3.77559E+01	0.00000E+00	0.00000E+00	0.0	0.0
4.09499E+01	0.00000E+00	0.00000E+00	0.0	0.0
4.42188E+01	0.00000E+00	0.00000E+00	0.0	0.0
4.75642E+01	0.00000E+00	0.00000E+00	0.0	0.0
5.09879E+01	2.81994E+00	0.00000E+00	2.78	2.839708493
5.44917E+01	2.95724E+00	0.00000E+00	2.78	3.041985192
5.80776E+01	3.09146E+00	0.00000E+00	2.78	3.235949711
6.17474E+01	3.22303E+00	0.00000E+00	2.78	3.423132037
6.55032E+01	3.35235E+00	0.00000E+00	2.78	3.604612881
6.93469E+01	3.47971E+00	0.00000E+00	2.78	3.781340008
7.32805E+01	3.60541E+00	0.00000E+00	2.78	3.954022426
7.73063E+01	3.72966E+00	0.00000E+00	2.78	4.123284587
8.14263E+01	3.85267E+00	0.00000E+00	2.78	4.289570164
8.56428E+01	2.78000E+00	0.00000E+00	2.78	4.453346396
8.99579E+01	2.78000E+00	0.00000E+00	2.78	4.614959048
9.43741E+01	2.78000E+00	0.00000E+00	2.78	4.774679387
9.88937E+01	2.78000E+00	0.00000E+00	2.78	4.932772199
1.03519E+02	2.78000E+00	0.00000E+00	2.78	5.089491813
1.08253E+02	2.78000E+00	0.00000E+00	2.78	5.245052694

1.13097E+02	2.78000E+00	0.00000E+00	2.78	5.399585795
1.18055E+02	2.98445E+00	0.00000E+00	2.984508234	5.5
1.23129E+02	3.51470E+00	0.00000E+00	3.514720802	5.5
1.28322E+02	3.98496E+00	0.00000E+00	3.985002853	5.5
1.33636E+02	4.41467E+00	0.00000E+00	4.414677457	5.5
1.39075E+02	4.81490E+00	0.00000E+00	4.814927386	5.5
1.44641E+02	5.19265E+00	0.00000E+00	5.192656212	5.5
1.50338E+02	5.55270E+00	0.00000E+00	5.552707839	5.5
1.56167E+02	5.89847E+00	0.00000E+00	5.898482866	5.5
1.62134E+02	6.23251E+00	0.00000E+00	6.232488238	5.5
1.68240E+02	6.55676E+00	0.00000E+00	6.556766571	5.5
1.74489E+02	6.87279E+00	0.00000E+00	6.872789758	5.5
1.80884E+02	7.18183E+00	0.00000E+00	7.181847862	5.5
1.87429E+02	7.48491E+00	0.00000E+00	7.484923744	5.5
1.94127E+02	7.78288E+00	0.00000E+00	7.782889944	5.5
2.00982E+02	8.07644E+00	0.00000E+00	8.076443037	5.5
2.07997E+02	8.36622E+00	0.00000E+00	8.366247294	5.5
2.15177E+02	8.65274E+00	0.00000E+00	8.652764761	5.5
2.22524E+02	8.93646E+00	0.00000E+00	8.936482146	5.5
2.30044E+02	9.21779E+00	0.00000E+00	9.217788703	5.5
2.37740E+02	9.49708E+00	0.00000E+00	9.497075979	5.5
2.45616E+02	9.77464E+00	0.00000E+00	9.774656655	5.5
2.53676E+02	1.00508E+01	0.00000E+00	10.05080059	5.5
2.61926E+02	1.03257E+01	0.00000E+00	10.32573263	5.5
2.70368E+02	1.05997E+01	0.00000E+00	10.59975808	5.5
2.79008E+02	1.08730E+01	0.00000E+00	10.87303483	5.5
2.87850E+02	1.11458E+01	0.00000E+00	11.14583952	5.5
2.96899E+02	1.14181E+01	0.00000E+00	11.41819662	5.5
3.06160E+02	1.16903E+01	0.00000E+00	11.69031503	5.5
3.15638E+02	1.19625E+01	0.00000E+00	11.96257949	5.5
3.25337E+02	1.22347E+01	0.00000E+00	12.23476902	5.5
3.35264E+02	1.25072E+01	0.00000E+00	12.50725365	5.5
3.45423E+02	1.27801E+01	0.00000E+00	12.78020202	5.5
3.55820E+02	1.30534E+01	0.00000E+00	13.05347992	5.5
3.66461E+02	1.33274E+01	0.00000E+00	13.32742668	5.5
3.77350E+02	1.36020E+01	0.00000E+00	13.60200189	5.5
3.88495E+02	1.38775E+01	0.00000E+00	13.8775664	5.5
3.99900E+02	1.41538E+01	0.00000E+00	14.153846	5.5
4.11572E+02	1.44311E+01	0.00000E+00	14.4311317	5.5
4.23518E+02	1.47096E+01	0.00000E+00	14.70963365	5.5
4.35743E+02	1.49891E+01	0.00000E+00	14.98907966	5.5
4.48255E+02	1.52700E+01	0.00000E+00	15.27003702	5.5
4.61059E+02	1.55521E+01	0.00000E+00	15.55212409	5.5
4.74163E+02	1.58357E+01	0.00000E+00	15.83573033	5.5
4.87574E+02	1.61207E+01	0.00000E+00	16.12082918	5.5
5.01299E+02	1.64073E+01	0.00000E+00	16.40720078	5.5
5.15346E+02	1.66955E+01	0.00000E+00	16.69553726	5.5
5.29721E+02	1.69853E+01	0.00000E+00	16.98537009	5.5
5.44432E+02	1.72770E+01	0.00000E+00	17.27690136	5.5
5.59488E+02	1.75704E+01	0.00000E+00	17.57045191	5.5
5.74897E+02	1.78657E+01	0.00000E+00	17.86575075	5.5
5.90666E+02	1.81630E+01	0.00000E+00	18.16297645	5.5
6.06805E+02	1.84623E+01	0.00000E+00	18.46224872	5.5
6.23321E+02	1.87636E+01	0.00000E+00	18.76368597	5.5
6.40224E+02	1.90671E+01	0.00000E+00	19.06706329	5.5
6.57523E+02	1.93727E+01	0.00000E+00	19.37273969	5.5
6.75226E+02	1.96650E+01	0.00000E+00	19.66504005	5.5
6.93345E+02	1.97619E+01	0.00000E+00	19.76196347	5.5
7.11887E+02	1.97823E+01	0.00000E+00	19.78226984	5.5
7.30863E+02	1.98031E+01	0.00000E+00	19.80305532	5.5
7.50284E+02	1.98243E+01	0.00000E+00	19.8243184	5.5
7.70159E+02	1.98461E+01	0.00000E+00	19.84605754	5.5
7.90500E+02	1.98683E+01	0.00000E+00	19.86827119	5.5
8.11317E+02	1.98910E+01	0.00000E+00	19.89101305	5.5

8.32621E+02	1.99142E+01	0.00000E+00	19.91422607	5.5
8.54424E+02	1.99379E+01	0.00000E+00	19.93790862	5.5
8.76738E+02	1.99444E+01	0.00000E+00	19.94441777	5.5
8.99573E+02	1.99444E+01	0.00000E+00	19.94441777	5.5
9.22944E+02	1.99444E+01	0.00000E+00	19.94441777	5.5
9.46861E+02	1.99444E+01	0.00000E+00	19.94441777	5.5

Appendix C

Portion of nfenv.f that shows that the Backfill Diameters A & B are used in the thermal calculations.

```
c       GADAMS PA-SCR-480 7-17-04: Generate the thermal factors to a
c       file for analysis
       open (ithermal, file='thermal.dat',status='UNKNOWN')


       write(ithermal, FMT = '(46a12)') 'Time', 'Case', 'Case B',
     &    'Drift_Dia', 'Drift_DiaB',
     &    'BF_Out_Dia', 'BF_Out_DiaB',
     &    'tempwp', 'tempdsiA', 'tempdsiB', 'tempdsoA', 'tempdsoB',
     &    'tempbfoA', 'tempbfoB', 'temprw',
     &    'gcond_keq', 'gcond_kip', 'gcond_k', 'gcond_B',
     &    'gconv_c1', 'gconv_c1_B','grad_r1', 'grad_r1_B', 'gconv_2pd',
     &    'gconv_2pd_B','grad_2pd', 'grad_2pd_B','gconv_2dw',
     &    'gconv_2dw_B', 'grad_2dw',
     &    'grad_2dw_B','gconv_3pd', 'gconv_3pd_B', 'grad_3pd',
     &    'grad_3pd_B',
     &    'gcond_bf3', 'gcond_bf3_B', 'gconv_3bw', 'gconv_3bw_B',
     &    'grad_3bw', 'grad_3bw_B', 'gtot', 'qwp',
     &    'qwp_i', 'qwp_dA', 'qwp_dB'

c   Intitialize the relative humidity transition point
c   to the time of backfill emplaced.
        rh_transition_point = timeofbackfill

        do it = 1, ntim

c          Initialize time-varying parameters in the common
         D_RWDia = eqDriftDiaA(it)
         D_BFDia = eqBFDiaA(it)
         D_RWDia_B = eqDriftDiaB(it)
         D_BFDia_B = eqBFDiaB(it)


          I_case = 0
          I_case_B = 0
          D_gcond_keq = 0.0d0
          D_gcond_kip = 0.0d0
          D_gcond_k = 0.0d0
          D_gcond_B = 0.0d0
          D_gconv_c1 = 0.0d0
          D_gconv_c1_B = 0.0d0
          D_grad_r1 = 0.0d0
          D_grad_r1_B = 0.0d0
          D_gconv_2pd = 0.0d0
          D_gconv_2pd_B = 0.0d0
          D_grad_2pd = 0.0d0
          D_grad_2pd_B = 0.0d0
          D_gconv_2dw = 0.0d0
          D_gconv_2dw_B = 0.0d0
          D_grad_2dw = 0.0d0
          D_grad_2dw_B = 0.0d0
          D_gconv_3pd = 0.0d0
          D_gconv_3pd_B = 0.0d0
          D_grad_3pd = 0.0d0
          D_grad_3pd_B = 0.0d0
          D_gcond_bf3 = 0.0d0
          D_gcond_bf3_B = 0.0d0
```

```
          D_gconv_3bw = 0.0d0
          D_gconv_3bw_B = 0.0d0
          D_grad_3bw = 0.0d0
          D_grad_3bw_B = 0.0d0
          D_gtot = 0.0d0

c           if(it .eq. 41) then
c             B_Debug = .true.
c           else
            B_Debug = .false.
c           endif

c          GADAMS PA-SCR-480 7-17-04: Moved calculation of radiation
c          terms to subroutine
c           grad_pre = 4.0d0 *sbolt *((temprep(it)+273.0d0)**3) /
c     &     ( (1.0d0-emisswp)/ (emisswp*wparea) +
c     &             1.0d0 / (aviewfactor*wparea) +
c     &       (1.0d0-emissrw)/ (emissrw*driftarea*wpspace) )
c
c           grad_post = 4.0d0 *sbolt *((temprep(it)+273.0d0)**3) /
c     &     ( (1.0d0-emisswp)/ (emisswp*wparea) +
c     &             1.0d0 / (aviewfactor*wparea) +
c     &       (1.0d0-emissds)/ (emissds*shieldarea*wpspace) )
c          GADAMS PA-SCR-480 7-17-04: End of change

c          GADAMS PA-SCR-480 7-17-04: Moved calculations for
c          conductivity and heat flux to subroutine
c           if( tim(it) .lt. timeofbackfill ) then
c              qwp = qpermtu( tim(it) ) * wppayload * (1.d0-hloss_fact)
c              gtot = frac_inv*(grad_pre +gconv_pre) +(1.0d0-frac_inv)*
c     &               gcond
c           else
c              qwp = qpermtu( tim(it) ) * wppayload
c              gtot = frac_inv*(grad_post +gconv_post +gcond_post)
c     &               +(1.0d0-frac_inv)*gcond
c           endif
c          GADAMS PA-SCR-480 7-17-04: End of change

c          GADAMS PA-SCR-480 7-17-04: Moved calculation for temperature
c          of the waste package to the subroutine
c           tempwp(it) = temprep(it) + qwp / gtot

c          GADAMS PA-SCR-480 7-17-04: Calculate temperatures
          if(ithermalmodel .eq. 1) then
            call calcTempsLinear(tim(it), timeofbackfill,
     &        tempwp(it), tempdsiA(it), tempdsiB(it),
     &        tempdsoA(it), tempdsoB(it),
     &        tempbfoA(it), tempbfoB(it),
     &        temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
          else
            call calcTempsIterative(tim(it), timeofbackfill,
     &        temprep(it), tempbfoA(it),
     &        tempdsoA(it), tempdsiA(it),
     &        tempwp(it), qwp, qwp_dA, qwp_i)
            qwp_dB = 0.0d0
          endif


c          GADAMS PA-SCR-480 7-17-04: Generate thermal output values
          write(ithermal, FMT = '((1pe12.4), 2i12, 43(1pe12.4))')
     &      tim(it),  I_case, I_case_B, D_RWDia, D_RWDIA_B, D_BFDia,
     &      D_BFDia_B,
     &      tempwp(it), tempdsiA(it), tempdsiB(it), tempdsoA(it),
     &      tempdsoB(it), tempbfoA(it), tempbfoB(it),
```

```
     &        temprep(it),
     &        D_gcond_keq, D_gcond_kip, D_gcond_k, D_gcond_B,
     &        D_gconv_c1, D_gconv_c1_B, D_grad_r1, D_grad_r1_B,
     &        D_gconv_2pd, D_gconv_2pd_B, D_grad_2pd, D_grad_2pd_B,
     &        D_gconv_2dw, D_gconv_2dw_B,
     &        D_grad_2dw, D_grad_2dw_B, D_gconv_3pd, D_gconv_3pd_B,
     &        D_grad_3pd, D_grad_3pd_B,
     &        D_gcond_bf3, D_gcond_bf3_B, D_gconv_3bw, D_gconv_3bw_B,
     &        D_grad_3bw, D_grad_3bw_B, D_gtot, qwp,
     &        qwp_i, qwp_dA, qwp_dB

          tempin     = tempwp(it) + qwp / (gshell * alengthwp )
          tempsf(it) = tempin + qwp / (gint*alengthwp )

c    The relative humidity at the drift wall is the relative humidity for
c    ventilated air during the preclosure period and just after (one time
c    step past) the preclosure period. After this time, the relative humidity
c    at the drift wall ramps up to 1.0.
          if(tim(it) .lt. timeofbackfill) then
            rh_drift_wall = rh_ventilated_air
          elseif(it .gt. 1 .and.
     &      (tim(it-1) .lt. timeofbackfill)) then
            rh_drift_wall = rh_ventilated_air
            rh_transition_point = tim(it)
          elseif(tim(it) .le.
     &      (rh_transition_point + rh_transition_time)) then
            if(rh_transition_time .gt. 0.0d0) then
              rh_drift_wall = rh_ventilated_air +
     &          ((1.0 - rh_ventilated_air) / rh_transition_time) *
     &          (tim(it) - rh_transition_point)
            else
              rh_drift_wall = 1.0d0
            endif
          else
            rh_drift_wall = 1.0d0
          end if
          relhumwp(it) =  rh_drift_wall *
     &      pvap( dmin1( temprep(it), tboil ) ) / pvap( tempwp(it) )

        enddo
```

Appendix C (continued)

Changes to seismo.f file related to SCRs 480 & 481

```
WVer
      SUBROUTINE SEISMO (numTime, maxNumTime, time, numSeismicEvents,
     &                   timeSeismicEvents, typeSeismicEvents,
     &                   dsThickness, dsFailureTime, numSubareas,
     &                   idSubarea, accumWPFailure,
     &                   accumDSFailure, fractionDriftCollapse,
     &                   dsBuckling, dsPlate, dsBulkHead,
     &                   wpTop, wpBottom, sccTop, sccBottom,
     &                   indicatorCorrosion)

XVer
c
c     GADAMS PA-SCR-480 7-23-04: Added this subroutine to calculate
c     the equivalent diameter of the rock wall and backfill.  These
c     drift height calculations are also performed in mechfail.f.
c     If changes are made in this routine, make sure that the drift
c     heights displayed in files eqdiam.rlt and seismo.rlt agree.
      subroutine eqvdia(numTime, time,
     &                   numSeismicEvents,timeSeismicEvents,
     &                   typeSeismicEvents, numSubareas, iSubarea,
     &                   eqDriftDiaA, eqDriftDiaB, eqBFDiaA,
     &                   eqBFDiaB, driftHeight)
c=====================================================================
c     NAME: eqvdia
c
c     PURPOSE:  Calculates the equivalent diameters for the drift and
c               the backfill
c
c     METHOD:
c
c     INPUT:  integer, numTime
c             double precision array, time
c             integer, numSeismicEvents
c             double precision array, timeSeismicEvents
c             double precision array, typeSeismicEvents
c             integer, numSubareas
c             integer, iSubarea
c
c     OUTPUT: double precision array, eqDriftDiaA
c             double precision array, eqDriftDiaB
c             double precision array, eqBFDiaA
c             double precision array, eqBFDiaB
c             double precision array, driftHeight
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      implicit none

      include 'maxntime.i'

c     Parameter declarations
      integer numTime
      integer numSeismicEvents
      integer numSubareas
      integer iSubarea
```

```
      double precision time(numTime)
      double precision timeSeismicEvents(numSeismicEvents)
      double precision typeSeismicEvents(numSeismicEvents)
      double precision eqDriftDiaA(numTime)
      double precision eqDriftDiaB(numTime)
      double precision eqBFDiaA(numTime)
      double precision eqBFDiaB(numTime)
      double precision driftHeight(numTime)

c     Local variable declarations

      character * 60 ch_tpa_name

      double precision area_fallen(maxntime)

      double precision backfill_time
      double precision backfill_thickness
      double precision drift_diameter
      double precision ds_idia
      double precision ds_thick
      double precision circum_frac
      double precision frac_wedge

c     Static variable declarations
      logical flag_initialize
      DATA flag_initialize /.true./
      SAVE flag_initialize

      integer i_backfill_time
      integer i_backfill_thickness
      integer i_drift_diameter
      integer i_ds_idia
      integer i_ds_thick
      integer i_circum_frac
      integer i_frac_wedge
      integer i_thermal_model

      save i_backfill_time
      save i_backfill_thickness
      save i_drift_diameter
      save i_ds_idia
      save i_ds_thick
      save i_circum_frac
      save i_frac_wedge
      save i_thermal_model


c     Function declarations
      integer ispquery
      double precision valuesp
      integer ivaluesp

c     Retrieve tpa.inp parameters
      if(flag_initialize) then
        flag_initialize = .false.

        call clearchar(60, ch_tpa_name)
        ch_tpa_name = 'SelectThermalModel(1,2)'
        i_thermal_model = ivaluesp(ispquery(ch_tpa_name))
```

```
      if(i_thermal_model .lt. 1 .or. i_thermal_model .gt. 2) then
        PRINT *, ' ***>>> Error in NFENV <<<*** '
        PRINT *, ' Invalid thermal model selected '
        print *, ' requires a 1 or a 2 '
        print *, ' Model selected: ', i_thermal_model
        STOP
      endif

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'TimeOfBackfillEmplaced[yr]'
      i_backfill_time = ispquery(ch_tpa_name)

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'EmplacementBackfillThickness[m]'
      i_backfill_thickness = ispquery(ch_tpa_name)

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'EmplacementDriftDiameter[m]'
      i_drift_diameter = ispquery(ch_tpa_name)

      call clearchar( 60, ch_tpa_name)
      ch_tpa_name = 'DripShieldEqvIntDia[m]'
      i_ds_idia = ispquery(ch_tpa_name)

      call clearchar( 60, ch_tpa_name)
      ch_tpa_name = 'DripShieldThickness[m]'
      i_ds_thick = ispquery(ch_tpa_name)

      call clearchar( 60, ch_tpa_name)
      ch_tpa_name = 'CircumferentialFractionNotCoveredByFloor[]'
      i_circum_frac = ispquery(ch_tpa_name)

      call clearchar(60, ch_tpa_name)
      ch_tpa_name = 'FractionAllowedToDegrade[]'
      i_frac_wedge = ispquery(ch_tpa_name)

    endif

c   Assign values to tpa input parameters
    backfill_time = valuesp(i_backfill_time)
    backfill_thickness = valuesp(i_backfill_thickness)
    drift_diameter = valuesp(i_drift_diameter)
    ds_idia = valuesp(i_ds_idia)
    ds_thick = valuesp(i_ds_thick)
    circum_frac = valuesp(i_circum_frac)
    frac_wedge = valuesp(i_frac_wedge)

c   Verify that the fraction allowed to degrade does not exceed
c   the fraction not covered by the floor.
    if(frac_wedge .gt. circum_frac) then
      print *, 'Invalid values from circumferential fractions.'
      print *, 'Fraction allowed to degrade cannot exceed'
      print *, '  the fraction not covered by the floor.'
      print *, 'Fraction to degrade: ', frac_wedge
      print *, 'Fraction not covered by floor: ', circum_frac
      stop
    end if


c   Calculate the drift height and the area of fallen rock
```

```
      call calculateDriftBFParameters(numTime, time,
     &                    numSeismicEvents,timeSeismicEvents,
     &                    typeSeismicEvents, numSubareas, iSubarea,
     &                    driftHeight, area_fallen)
c     Convert the drift height and area of fallen rock into
c     equivalent diameters for the drift and backfill
      call getEquivalentDiameters(numTime, time, backfill_time,
     &  backfill_thickness, drift_diameter/2.0d0,
     &  (ds_idia/2.0d0 + ds_thick), circum_frac,
     &  driftHeight, area_fallen, eqDriftDiaA, eqDriftDiaB,
     &  eqBFDiaA, eqBFDiaB, frac_wedge, i_thermal_model)


      return
      end

C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
      subroutine calculateDriftBFParameters(numTime, time,
     &  numSeismicEvents, timeSeismicEvents, typeSeismicEvents,
     &  numSubareas, iSubarea,
     &  driftHeight, areaFallen)
c=====================================================================
c     NAME: calculateDriftBFParameters
c
c     PURPOSE:  Calculates the drift height and area of fallen rock used
c               to calculate the equivalent diameters of the drift and
c               backfill
c
c     METHOD:
c
c     INPUT:  integer, numTime
c             double precision array, time
c             integer, numSeismicEvents
c             double precision array, timeSeismicEvents
c             double precision array, typeSeismicEvents
c             integer, numSubareas
c             integer, iSubarea
c
c     OUTPUT: double precision array, driftHeight
c             double precision array, areaFallen
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      implicit none

      INCLUDE 'maxnsuba.i'

c     Parameter declarations
      integer numTime
      integer numSeismicEvents
      integer numSubareas
      integer iSubarea

      double precision time(numTime)
      double precision timeSeismicEvents(numSeismicEvents)
      double precision typeSeismicEvents(numSeismicEvents)
      double precision driftHeight(numTime)
      double precision areaFallen(numTime)

c     Local variable declarations
      character * 60 ch_tpa_name
```

```
      logical evaluate_event

      integer index1
      integer index2
      integer index3
      integer NUM_GRID_PER_SUBAREA
      parameter(NUM_GRID_PER_SUBAREA = 2)

      double precision start_processing_time
      double precision time_last
      double precision TIME_INITIAL
      parameter(TIME_INITIAL = 0.0d0)
      double precision PI
      parameter(PI = 3.14159d0)
      double precision delta_time
      double precision rock_fraction

      double precision backfill_time
      double precision fraction_rock_type1
      double precision drift_diameter
      double precision drift_radius
      double precision ds_crown_height
      double precision ds_side_height
      double precision ds_crown_radius
      double precision ds_height
      double precision ds_width
      double precision invert_height
      double precision drift_void_area
      double precision backfill_thickness

c     Grid element parameters
      logical drift_failure_flag(NUM_GRID_PER_SUBAREA)

      double precision bulking_factor(NUM_GRID_PER_SUBAREA)
      double precision drift_height(NUM_GRID_PER_SUBAREA)
      double precision grnd_accel_init(NUM_GRID_PER_SUBAREA)
      double precision grnd_accel_max(NUM_GRID_PER_SUBAREA)
      double precision degrad_time(NUM_GRID_PER_SUBAREA)
      double precision drift_height_max(NUM_GRID_PER_SUBAREA)

c     Static variable declarations
      logical flag_initialize
      DATA flag_initialize /.true./
      SAVE flag_initialize

      integer i_backfill_time
      integer i_fraction_rock_type1(maxnsubarea)
      integer i_bf_rock(NUM_GRID_PER_SUBAREA, maxnsubarea)
      integer i_drift_diameter
      integer i_grnd_accel_init(NUM_GRID_PER_SUBAREA, maxnsubarea)
      integer i_grnd_accel_max(NUM_GRID_PER_SUBAREA, maxnsubarea)
      integer i_degrad_time(NUM_GRID_PER_SUBAREA, maxnsubarea)
      integer i_ds_crown_radius
      integer i_ds_height
      integer i_ds_width
      integer i_invert_height
      integer i_backfill_thickness
      integer i_seismicity_flag
      integer i_value_seismicity_flag
```

```
      integer i_degrad_flag
      integer i_value_degrad_flag

      save i_backfill_time
      save i_fraction_rock_type1
      save i_bf_rock
      save i_drift_diameter
      save i_grnd_accel_init
      save i_grnd_accel_max
      save i_degrad_time
      save i_ds_crown_radius
      save i_ds_height
      save i_ds_width
      save i_invert_height
      save i_backfill_thickness
      save i_value_seismicity_flag
      save i_value_degrad_flag

c     Function declarations
      integer ispquery
      integer isconstant
      integer ivaluesp
      double precision valuesp


c     Retrieve tpa.inp parameters
      if(flag_initialize) then
        flag_initialize = .false.


c   Retrieve control flags

        CALL clearchar(60, ch_tpa_name)
        ch_tpa_name = 'SeismicDisruptiveScenarioFlag(yes=1,no=0)'
        i_seismicity_flag = ispquery(ch_tpa_name)

        IF(isconstant(i_seismicity_flag) .NE. 1) THEN
          PRINT *, ' ***>>> Error in SEISMO <<<*** '
          PRINT *, ' problem with : '
          PRINT *, '     SeismicDisruptiveScenarioFlag(yes=1,no=0)'
          PRINT *, ' not specified as iflag '
          PRINT *, ' needs to be iflag PDF'
          STOP
        ENDIF

        i_value_seismicity_flag = ivaluesp(i_seismicity_flag)

        IF((i_value_seismicity_flag .lt. 0) .or.
     &    (i_value_seismicity_flag .gt. 1) ) THEN
          PRINT *, ' ***>>> Error in SEISMO <<<*** '
          PRINT *, ' problem with : '
          PRINT *, '     SeismicDisruptiveScenarioFlag(yes=1,no=0)'
          PRINT *, ' needs to be either a 0 or a 1'
          STOP
        ENDIF

        CALL clearchar(60, ch_tpa_name)
        ch_tpa_name = 'DriftDegradationScenarioFlag(yes=1,no=0)'
        i_degrad_flag = ispquery(ch_tpa_name)
```

```
      IF(isconstant(i_degrad_flag) .NE. 1) THEN
        PRINT *, ' ***>>> Error in SEISMO <<<*** '
        PRINT *, ' problem with : '
        PRINT *, '     DriftDegradationScenarioFlag(yes=1,no=0)'
        PRINT *, ' not specified as iflag '
        PRINT *, ' needs to be iflag PDF'
        STOP
      ENDIF

      i_value_degrad_flag = ivaluesp(i_degrad_flag)

      IF((i_value_degrad_flag .LT. 0) .OR.
     &   (i_value_degrad_flag .GT. 1) ) THEN
        PRINT *, ' ***>>> Error in SEISMO <<<*** '
        PRINT *, ' problem with : '
        PRINT *, '     DriftDegradationScenarioFlag(yes=1,no=0)'
        PRINT *, ' needs to be either a 0 or a 1'
        STOP
      ENDIF


      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'TimeOfBackfillEmplaced[yr]'
      i_backfill_time = ispquery(ch_tpa_name)

      do index1 = 1, numSubareas
        CALL buildCharacterString(ch_tpa_name, 60,
     &    'FractionRockTypeOneInSubarea_', index1,
     &    '[]')
        i_fraction_rock_type1(index1) = ispquery(ch_tpa_name)

        CALL buildCharacterString(ch_tpa_name, 60,
     &    'BulkingFactorRockTypeOneSubarea_', index1,
     &    '[]')
        i_bf_rock(1, index1) = ispquery(ch_tpa_name)

        CALL buildCharacterString(ch_tpa_name, 60,
     &    'BulkingFactorRockTypeTwoSubarea_', index1,
     &    '[]')
        i_bf_rock(2, index1) = ispquery(ch_tpa_name)

        CALL buildCharacterString(ch_tpa_name, 60,
     &    'GroundAccelerationInitialRockTypeOneSubarea_', index1,
     &    '[pga]')
        i_grnd_accel_init(1, index1) = ispquery(ch_tpa_name)

        CALL buildCharacterString(ch_tpa_name, 60,
     &    'GroundAccelerationInitialRockTypeTwoSubarea_', index1,
     &    '[pga]')
        i_grnd_accel_init(2, index1) = ispquery(ch_tpa_name)


        CALL buildCharacterString(ch_tpa_name, 60,
     &    'GroundAccelerationMaximumRockTypeOneSubarea_', index1,
     &    '[pga]')
        i_grnd_accel_max(1, index1) = ispquery(ch_tpa_name)

        CALL buildCharacterString(ch_tpa_name, 60,
     &    'GroundAccelerationMaximumRockTypeTwoSubarea_', index1,
     &    '[pga]')
```

```
        i_grnd_accel_max(2, index1) = ispquery(ch_tpa_name)

        CALL buildCharacterString(ch_tpa_name, 60,
     &    'DegradationTimeRockTypeOneSubarea_', index1,
     &    '[yr]')
        i_degrad_time(1, index1) = ispquery(ch_tpa_name)

        CALL buildCharacterString(ch_tpa_name, 60,
     &    'DegradationTimeRockTypeTwoSubarea_', index1,
     &    '[yr]')
        i_degrad_time(2, index1) = ispquery(ch_tpa_name)

      enddo

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'EmplacementDriftDiameter[m]'
      i_drift_diameter = ispquery(ch_tpa_name)

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'DripShieldCrownRadius[m]'
      i_ds_crown_radius = ispquery(ch_tpa_name)

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'DripShieldHeight[m]'
      i_ds_height = ispquery(ch_tpa_name)

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'DripShieldWidth[m]'
      i_ds_width = ispquery(ch_tpa_name)

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'InvertHeight[m]'
      i_invert_height = ispquery(ch_tpa_name)

      CALL clearchar(60, ch_tpa_name)
      ch_tpa_name = 'EmplacementBackfillThickness[m]'
      i_backfill_thickness = ispquery(ch_tpa_name)


    endif

c   Assign values to tpa input parameters
    backfill_time = valuesp(i_backfill_time)
    fraction_rock_type1 = valuesp(i_fraction_rock_type1(iSubarea))
    bulking_factor(1) = valuesp(i_bf_rock(1, iSubarea))
    bulking_factor(2) = valuesp(i_bf_rock(2, iSubarea))
    drift_diameter = valuesp(i_drift_diameter)
    drift_radius = drift_diameter / 2.0d0
    grnd_accel_init(1) = valuesp(i_grnd_accel_init(1, iSubarea))
    grnd_accel_init(2) = valuesp(i_grnd_accel_init(2, iSubarea))
    grnd_accel_max(1) = valuesp(i_grnd_accel_max(1, iSubarea))
    grnd_accel_max(2) = valuesp(i_grnd_accel_max(2, iSubarea))
    degrad_time(1) = valuesp(i_degrad_time(1, iSubarea))
    degrad_time(2) = valuesp(i_degrad_time(2, iSubarea))
    ds_crown_radius = valuesp(i_ds_crown_radius)
    ds_height = valuesp(i_ds_height)
    ds_width = valuesp(i_ds_width)
    invert_height = valuesp(i_invert_height)
    backfill_thickness = valuesp(i_backfill_thickness)
```

```
c     Calculate one-time parameters

c     Drip shield crown height
      ds_crown_height = ds_crown_radius - 0.5D0 *
     &  (4.0D0 * ds_crown_radius**2 - ds_width**2)**0.5

c     Drip shield side height
      ds_side_height = ds_height - ds_crown_height

c     Drift void area
      drift_void_area = PI * drift_radius**2 -
     &  (
     &  drift_radius**2 *
     &  DACOS((drift_radius - invert_height) / drift_radius) -
     &  (drift_radius - invert_height) *
     &  ((2.0D0 * drift_radius * invert_height - invert_height**2)**0.5)
     &  ) -
     &  (
     &  ds_crown_radius**2 *
     &  DACOS((ds_crown_radius - ds_crown_height) / ds_crown_radius) -
     &  (ds_crown_radius - ds_crown_height) *
     &  ((2.0D0 * ds_crown_radius * ds_crown_height -
     &  ds_crown_height**2)**0.5)
     &  ) - ds_side_height * ds_width

c      print *, 'Drift void area: ', drift_void_area


c     Initialize parameters across all grid elements
      DO index1 = 1, NUM_GRID_PER_SUBAREA
c       Initialize the failed drift height to the original drift
c       cross_section radius
        drift_height(index1) = drift_radius

c       Drift failure flag
        drift_failure_flag(index1) = .false.

c       Maximum drift failure height
        drift_height_max(index1) =
     &    (2.0D0 * drift_void_area +
     &    (drift_radius ** 2) * (bulking_factor(index1) - 1))
     &    / (PI * drift_radius * (bulking_factor(index1) - 1))

c        print *, 'Bulking factor: ', bulking_factor(index1)
c        print *, drift_height_max(index1)
      enddo



c     Note: The end of the operational period is currently set to
c     the time of backfill emplacement.
      start_processing_time = MAX(TIME_INITIAL, backfill_time)
      time_last = start_processing_time

c     Find the index of the first seismic event after the operational
c     period.
      index2 = 1
      evaluate_event = .TRUE.
      DO WHILE((index2 .LE. numSeismicEvents) .AND.
```

```
     &  (evaluate_event))
        IF(timeSeismicEvents(index2) .LT. start_processing_time) THEN
c         Increment the seismic event index so that seismic
c         events are evaluated after the operational period.
          index2 = index2 + 1
        ELSE
          evaluate_event = .FALSE.
        ENDIF
      ENDDO


      DO index1 = 1, numTime

c      Skip any time increments during the operational period.
       if(time(index1) .lt. start_processing_time) then

         driftHeight(index1) = drift_radius
         areaFallen(index1) = 0.0d0

       else

        IF(index2 .LE. numSeismicEvents) THEN
          IF(timeSeismicEvents(index2) .GT. time(index1)) THEN
            evaluate_event = .FALSE.
          ELSE
            evaluate_event = .TRUE.
          ENDIF
        ELSE
          evaluate_event = .FALSE.
        ENDIF

        DO WHILE(evaluate_event)
c         Determine the delta time.  This time is not only dependent on
c         the given TPA time step but also the time that a seismic event
c         occurred.
          delta_time = timeSeismicEvents(index2) - time_last
          time_last = timeSeismicEvents(index2)


c         Process each grid element at this delta time
c         This time increment has a seismic event
          DO index3 = 1,  NUM_GRID_PER_SUBAREA
            CALL processDriftHeight(timeSeismicEvents(index2),
     &        delta_time,
     &        drift_failure_flag(index3),
     &        drift_height(index3), drift_radius,
     &        drift_height_max(index3), degrad_time(index3),
     &        grnd_accel_init(index3), grnd_accel_max(index3),
     &        typeSeismicEvents(index2), backfill_thickness,
     &        backfill_time, i_value_degrad_flag,
     &        i_value_seismicity_flag)
          ENDDO

c         Increment the index to the next seismic event
          index2 = index2 + 1
          IF(index2 .LE. numSeismicEvents) THEN
            IF(timeSeismicEvents(index2) .GT. time(index1)) THEN
              evaluate_event = .FALSE.
            ELSE
              evaluate_event = .TRUE.
```

```
            ENDIF
          ELSE
            evaluate_event = .FALSE.
          ENDIF

        ENDDO  ! End evaluation of seismic events in this increment

        delta_time = time(index1) - time_last
        time_last = time(index1)

c       It's possible that the delta time will be zero if a seismic
c       event occurred at the TPA time step.  Therefore, check for
c       this condition before proceeding.
        IF(delta_time .GT. 0.0D0) THEN

          DO index3 = 1, NUM_GRID_PER_SUBAREA
c           Process each grid element at this delta time
c           This time increment does not have a seismic event
            CALL processDriftHeight(time(index1), delta_time,
     &        drift_failure_flag(index3),
     &        drift_height(index3), drift_radius,
     &        drift_height_max(index3), degrad_time(index3),
     &        grnd_accel_init(index3), grnd_accel_max(index3),
     &        0.0d0, backfill_thickness,
     &        backfill_time, i_value_degrad_flag,
     &        i_value_seismicity_flag)

C ??????? Indents appear to be wrong Albert Lozano

          ENDDO
        ENDIF
      ENDIF ! Processing after the operational period

        driftHeight(index1) = 0.0D0
        areaFallen(index1) = 0.0D0

c       Each subarea has a fractional ground coverage that is
c       accounted for in fraction_grid.  In addition, each subarea
c       is divided into two grid elements with a fractional rock
c       coverage for rock type 1 assigned to the subarea in
c       fraction_type.

        DO index3 = 1, NUM_GRID_PER_SUBAREA

          IF(((index3 / 2) * 2) .EQ. index3) THEN
c           Rock type 2
            rock_fraction = 1.0D0 - fraction_rock_type1
          ELSE
c           Rock type 1
            rock_fraction = fraction_rock_type1
          ENDIF

          driftHeight(index1) = driftHeight(index1) +
     &      (2.0D0 / DBLE(NUM_GRID_PER_SUBAREA)) * rock_fraction *
     &      drift_height(index3)
          areaFallen(index1) = areaFallen(index1) +
     &      (2.0D0 / DBLE(NUM_GRID_PER_SUBAREA)) * rock_fraction *
     &      bulking_factor(index3) *
     &      (
     &        ((PI / 2.0D0) * drift_height(index3) * drift_radius) -
```

```
     &        ((PI / 2.0D0) * (drift_radius**2))
     &       )
        ENDDO

      ENDDO

      return
      end

C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
      subroutine processDriftHeight(analysisTime, deltaTime,
     &        driftFailureFlag, driftHeight, driftRadius,
     &        driftHeightMax, degradationTime, groundAccelInitial,
     &        groundAccelMax, peakGroundAcceleration, backfillThickness,
     &        backfillTime, iDriftDegradFlag, iSeismicityFlag)
c=======================================================================
c     NAME: processDriftHeight
c
c     PURPOSE:  Calculates the drift height for a grid element
c
c     METHOD:
c
c     INPUT:  integer iDriftDegradFlag
c             integer iSeismicityFlag
c             double precision, analysisTime
c             double precision, deltaTime
c             double precision, driftRadius
c             double precision, driftHeightMax
c             double precision, degradationTime
c             double precision, groundAccelInitial
c             double precision, groundAccelMax
c             double precision, peakGroundAcceleration
c             double precision, backfillThickness
c             double precision, backfillTime
c
c     OUTPUT: double precision, driftHeight
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      implicit none

c     Parameter Declarations
      logical driftFailureFlag

      integer iDriftDegradFlag
      integer iSeismicityFlag

      double precision analysisTime
      double precision deltaTime
      double precision driftHeight
      double precision driftRadius
      double precision driftHeightMax
      double precision degradationTime
      double precision groundAccelInitial
      double precision groundAccelMax
      double precision peakGroundAcceleration
      double precision backfillThickness
      double precision backfillTime

c     Local variable declarations
      logical engineered_backfill_flag
```

```
      double precision delta_height_seismic
      double precision slope_line
      double precision degradation_rate

      if((backfillThickness .gt. 0.0D0) .AND.
     &  (backfillTime .le. analysisTime)) then
        engineered_backfill_flag = .TRUE.
      else
        engineered_backfill_flag = .FALSE.
      endif

      if(
     &    (.NOT. engineered_backfill_flag) .AND.
     &    (iDriftDegradFlag .EQ. 1)
     &  ) then
c       Fixed degradation is only determined if backfill has not yet
c       taken place
c       Current fixed degradation rate
        degradation_rate = (driftHeightMax - driftRadius) /
     &    degradationTime

c       IF the drift has already failed, then the drift height based
c       on the fixed degradation rate will equal the maximum drift
c       failure height.
        IF(driftFailureFlag) THEN
          driftHeight = driftHeightMax
        ELSE
c         Calculate the failed drift height for this time increment
c         based on the fixed degradation rate of the emplacement drift
          driftHeight = driftHeight + degradation_rate * deltaTime
          IF(driftHeight .GE. driftHeightMax) THEN
            driftHeight = driftHeightMax
            driftFailureFlag = .TRUE.
          ENDIF
        ENDIF
      endif

      IF((ISeismicityFlag .EQ. 1) .AND.
     &  (peakGroundAcceleration .GT. 0.0D0) .and.
     &  (.NOT. engineered_backfill_flag)) THEN

c       The two heights and accelerations are used to build a curve from
c       which a new seismic height will be generated.
        IF(groundAccelMax .LE. groundAccelInitial) THEN
          PRINT *, 'Error in SEISMO2:seismicDriftHeight'
          PRINT *, 'Maximum ground acceleration less than or equal ' //
     &      'to initial'
          STOP
        ENDIF

        slope_line = (driftHeightMax - driftHeight) /
     &    (groundAccelMax - groundAccelInitial)

        delta_height_seismic = slope_line *
     &    (peakGroundAcceleration - groundAccelInitial)

        if(delta_height_seismic .LT. 0.0D0) then
          delta_height_seismic = 0.0D0
        endif
```

```
        driftHeight = driftHeight + delta_height_seismic
        if(driftHeight .GE. driftHeightMax) then
          driftHeight = driftHeightMax
          driftFailureFlag = .TRUE.
        endif
      endif


      return
      end

C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
c     GADAMS PA-SCR-480 7-23-04: Added driftheight to parameter list
c      SUBROUTINE SEISMO (numTime, maxNumTime, time, numSeismicEvents,
c     &                   timeSeismicEvents, typeSeismicEvents,
c     &                   dsThickness, dsFailureTime, numSubareas,
c     &                   idSubarea, accumWPFailure,
c     &                   accumDSFailure, fractionDriftCollapse,
c     &                   dsBuckling, dsPlate, dsBulkHead,
c     &                   wpTop, wpBottom, sccTop, sccBottom,
c     &                   indicatorCorrosion)
      SUBROUTINE MECHDRIVER (numTime, maxNumTime, time,
     &                   numSeismicEvents,
     &                   timeSeismicEvents, typeSeismicEvents,
     &                   dsThickness, dsFailureTime, numSubareas,
     &                   idSubarea, accumWPFailure,
     &                   accumDSFailure, fractionDriftCollapse,
     &                   dsBuckling, dsPlate, dsBulkHead,
     &                   wpTop, wpBottom, sccTop, sccBottom,
     &                   indicatorCorrosion, driftHeight)
c     GADAMS PA-SCR-480 7-23-04: End of change

C   Albert Lozano - This section shows the addition of driftHeight to
C   the double precision variables( Seismo WVer, MechDriver XVer)
      DOUBLE PRECISION time(maxNumTime),
     & timeSeismicEvents(numSeismicEvents),
     & typeSeismicEvents(numSeismicEvents), dsThickness(maxNumTime),
     & dsFailureTime, accumWPFailure(maxNumTime),
     & accumDSFailure(maxNumTime), fractionDriftCollapse(maxNumTime),
     & dsBuckling(maxNumTime), dsPlate(maxNumTime),
     & dsBulkHead(maxNumTime), wpTop(maxNumTime),
     & wpBottom(maxNumTime), sccTop(maxNumTime),
     & sccBottom(maxNumTime)

c     GADAMS PA-SCR-480 7-23-04: Added seismic drift height
      double precision driftHeight(maxNumTime)

C   Albert Lozano - This section shows the addition of additional
C   integer variables( Seismo WVer, MechDriver XVer)

      INTEGER InFile, OutFile, IBackfillThickness,
     & IBackfillTime,
     & INumBlockSizePoints, IEmplacementDriftDiameter,
     & IDSHeight, IDSWidth, IHeightInvert, IDSWPClearance,
     & IDSCrownRadius, IDSPlateCreepFactor, IDSBulkHeadCreepFactor,
     & IDSPlateYieldStress, IDSBulkHeadYieldStress, IDSPlateCreepCoeff,
     & IDSBulkHeadCreepCoeff, IDSPlateCreepExp, IDSBulkHeadCreepExp,
     & IDSPlateFlogStrain, IDSBulkHeadFlogStrain, IWPOuterYieldStress,
     & IWPOuterFlogStrain, IRockMassDensity1, IRockMassDensity2,
```

```
     &  IStartBlock1(maxnsubarea), IStartBlock2(maxnsubarea),
     &  IFractionType(maxnsubarea),
     &  IBulkingFactor1(maxnsubarea),
     &  IBulkingFactor2(maxnsubarea),
     &  IDegradationTime1(maxnsubarea),
     &  IDegradationTime2(maxnsubarea),
     &  IGroundAccelerationInit1(maxnsubarea),
     &  IGroundAccelerationInit2(maxnsubarea),
     &  IGroundAccelerationMax1(maxnsubarea),
     &  IGroundAccelerationMAx2(maxnsubarea),
     &  IDSBucklingLoad(maxnsubarea), IRubbleThickness

c     GADAMS PA-SCR-481 6-7-2004: Added Drip Shield impact parameters
      INTEGER IContactAngle, IDeflectionDepth, IBHThickness,
     &        IWPDiameter, IWPUltimateTensileStrength

C   Albert Lozano - This section shows that the additional
C   integer variables were declared with SAVE ( Seismo WVer, MechDriver XVer)

c     GADAMS PA-SCR-481 6-4-2004: Added Drip Shield impact parameters
      SAVE IContactAngle, IDeflectionDepth, IBHThickness, IWPDiameter,
     &     IWPUltimateTensileStrength

C   Albert Lozano - This section shows that the new double precision variables
C   were created in a new common block ( Seismo WVer, MechDriver XVer)

c     GADAMS PA-SCR-481 6-7-2004: Added Drip Shield impact parameters
      DOUBLE PRECISION ContactAngle, DeflectionDepth, BHThickness,
     &  WPDiameter, WPUltimateTensileStrength

      COMMON /mechdrv3/ ContactAngle, DeflectionDepth, BHThickness,
     &  WPDiameter, WPUltimateTensileStrength
c     GADAMS PA-SCR-481 6-7-2004: End of change

C   Albert Lozano - This section shows that the new integer variables( Indexes
??)
C   are initialized from the tpa input file ( Seismo WVer, MechDriver XVer)

c       GADAMS PA-SCR-481 6-7-2004: Added drip shield impact
c       parameters
        CALL clearchar(60, ch_tpa_name)
        ch_tpa_name = 'ContactAngle[degrees]'
        IContactAngle = ispquery(ch_tpa_name)

        CALL clearchar(60, ch_tpa_name)
        ch_tpa_name = 'DeflectionDepth[m]'
        IDeflectionDepth = ispquery(ch_tpa_name)

        CALL clearchar(60, ch_tpa_name)
        ch_tpa_name = 'BulkheadThickness[m]'
        IBHThickness = ispquery(ch_tpa_name)

        CALL clearchar(60, ch_tpa_name)
        ch_tpa_name = 'WPDiameter[m]'
        IWPDiameter = ispquery(ch_tpa_name)

        CALL clearchar(60, ch_tpa_name)
        ch_tpa_name =
     &    'WastePackageOuterBarrierUltimateTensileStrength[MPa]'
        IWPUltimateTensileStrength = ispquery(ch_tpa_name)
```

```
c       GADAMS PA-SCR-481 6-7-2004: End of change

C   Albert Lozano - This section shows that the new double precision variables
C   are initialized from the integer variables ( Seismo WVer, MechDriver XVer)

c   Retrieve TPA input parameters

c     GADAMS PA-SCR-481 6-7-2004: Added drip shield impact parameters
      ContactAngle = valuesp(IContactAngle)
      DeflectionDepth = valuesp(IDeflectionDepth)
      BHThickness = valuesp(IBHThickness)
      WPDiameter = valuesp(IWPDiameter)
      WPUltimateTensileStrength = valuesp(IWPUltimateTensileStrength)
c     GADAMS PA-SCR-481 6-7-2004: End of change

C   Albert Lozano - This section reads 1 line from mechfail.dat file after
mechfail.e
C   terminates. Note that drift height has been added. ( Seismo WVer,
MechDriver XVer)

WVer
        CALL getRealArray(InFile, 11, value_fail, 'Failure Data',
     &    .FALSE.)
XVer
c       GADAMS PA-SCR-480 7-23-04: Added drift height
c        CALL getRealArray(InFile, 11, value_fail, 'Failure Data',
c     &    .FALSE.)
        CALL getRealArray(InFile, 12, value_fail, 'Failure Data',
     &    .FALSE.)
c       GADAMS PA-SCR-480 7-23-04: End of change

C   Albert Lozano - This section updates the driftHeight array element from
the value
C   obtained from mechfail.dat. ( Seismo WVer, MechDriver XVer)

c       GADAMS PA-SCR-480 7-23-04: Added drift height
        driftHeight(index1) = value_fail(12)
```

```
C   Albert Lozano - This section shows the changes made to the
buildMechfailInputFile
C   to write the new information to the mechfail.inp file.
(buildMechfailInputFile)

C   Albert Lozano - The information was optained from tpa.inp and placed in a
common
C   block.  This routine takes the information from the common block and
writes it
C   to mechfail.inp

c     GADAMS PA-SCR-481 6-7-2004: Added Drip Shield impact parameters
      DOUBLE PRECISION ContactAngle, DeflectionDepth, BHThickness,
     &  WPDiameter, WPUltimateTensileStrength

      COMMON /mechdrv3/ ContactAngle, DeflectionDepth, BHThickness,
     &  WPDiameter, WPUltimateTensileStrength
c     GADAMS PA-SCR-481 6-7-2004: End of change

c     GADAMS PA-SCR-481 6-7-2004: Added Drip Shield impact parameters
```

```
      CALL setRealValue(outfile, ContactAngle,
     &  'Contact angle[degrees] {ContactAngle[degrees]}')

      CALL setRealValue(outfile, DeflectionDepth,
     &  'Deflection depth[m]' //
     &  ' {DeflectionDepth[m]}')

      CALL setRealValue(outfile, BHThickness,
     &  'Bulkhead thickness[m] {BulkheadThickness[m]}')

      CALL setRealValue(outfile, WPDiameter / 2.0d0,
     &  'Waste package radius[m] {WPDiameter[m] / 2}')

      CALL setRealValue(outfile, WPUltimateTensileStrength,
     &  'Waste package UTS {WPUltimateTensileStrength[MPa]}')
c     GADAMS PA-SCR-481 6-7-2004: End of change
```

```
C   Albert Lozano - This section shows the code for a new subroutine to
calculate
C   equivalent diameters. (getEquivalentDiameters)

c=====================================================================
      subroutine getEquivalentDiameters(numTime, Time, bfTime, bfThick,
     &  driftRadius, dsoRadius,
     &  fracAbove, driftHeight, areaFallen, equivDiaRWA, equivDiaRWB,
     &  equivDiaBFA, equivDiaBFB, fracWedge, iModel)
c=====================================================================
c     NAME: getEquivalentDiameters
c
c     PURPOSE:  Calculates the equivalent diameter for the drift and
c               backfill given the drift height and area of fallen rock
c
c     METHOD:
c
c     INPUT:  integer numTime
c             double precision array, Time
c             double precision, bfTime
c             double precision, bfThick
c             double precision, driftRadius
c             double precision, dsoRadius
c             double precision, fracAbove
c             double precision array, driftHeight
c             double precision array, areaFallen
c             double precision fracWedge
c             integer iModel
c
c     OUTPUT: double precision array, equivDiaRWA
c             double precision array, equivDiaRWB
c             double precision array, equivDiaBFA
c             double precision array, equivDiaBFB
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

      implicit none

      integer numTime

      integer iModel
```

```
      double precision Time(numTime)
      double precision bfTime
      double precision bfThick
      double precision driftRadius
      double precision dsoRadius
      double precision fracAbove
      double precision equivDiaBFA(numTime)
      double precision equivDiaBFB(numTime)
      double precision equivDiaRWA(numTime)
      double precision equivDiaRWB(numTime)
      double precision driftHeight(numTime)
      double precision areaFallen(numTime)
      double precision fracWedge
      double precision area_max_b

c     local variables
      integer index_value
      integer MAX_VALUES
      parameter (MAX_VALUES = 1000)
      double precision area_change
      double precision PI
      parameter(PI = 3.14159d0)
      double precision test_diameter


c     Convert the drift height and area of fallen rock to equivalent
c     diameters for the drift and the backfill
c     If the fraction of the wedge is zero, then the entire drift
c     is allowed to degrade
      if((fracWedge .ge. fracAbove) .or. (iModel .ne. 1)) then
        do index_value = 1, numTime
c         Calculate the area change for the upper portion of the drift
          area_change = ((PI/2.0d0) * driftHeight(index_value) *
     &      driftRadius) - ((PI/2.0d0) * driftRadius**2)
c         Calculate the equivalent diameter of the rock wall
          equivDiaRWA(index_value) = 2.0d0 *
     &      DSQRT((area_change/fracAbove + PI * driftRadius**2) / PI)
          equivDiaRWB(index_value) = 0.0d0
c         Calculate the equivalent diameter of the outer backfill material
          if(Time(index_value) .lt. bfTime) then
            equivDiaBFA(index_value) = 0.0d0
            equivDiaBFB(index_value) = 0.0d0
          else
c           If engineered backfill is present, then set the
c           equivalent diameter of the backfill to the engineered backfill
c           outer diameter; otherwise, calculate the outer diameter for
c           natural backfill
            if(bfThick .GT. 0.0D0) then
              equivDiaBFA(index_value) = 2.0d0 * dsoRadius +
     &          2.0d0 * bfThick
              equivDiaBFB(index_value) = 0.0d0
            else
              equivDiaBFA(index_value) = 2.0d0 *
     &          DSQRT((areaFallen(index_value)/
     &          fracAbove + PI * dsoRadius**2)/ PI)
              equivDiaBFB(index_value) = 0.0d0
            endif
          endif

        enddo
```

```
      else

         area_max_b = (fracAbove - fracWedge) *
     &     (PI * driftRadius**2 -
     &      PI * dsoRadius**2)

c        Calculate the equivalent diameter for the drift and backfill
c        for a wedge shaped geometry
         do index_value = 1, numTime
c          Calculate the area change for the upper portion of the drift
           area_change = ((PI/2.0d0) * driftHeight(index_value) *
     &       driftRadius) - ((PI/2.0d0) * driftRadius**2)
c          Calculate the equivalent diameter of the rock wall
           equivDiaRWA(index_value) = 2.0d0 *
     &       DSQRT((area_change/fracWedge + PI * driftRadius**2) / PI)
           equivDiaRWB(index_value) = 2.0d0 * driftRadius
c          Calculate the equivalent diameter of the outer backfill material
           if(Time(index_value) .lt. bfTime) then
             equivDiaBFA(index_value) = 0.0d0
             equivDiaBFB(index_value) = 0.0d0
           else
c            If engineered backfill is present, then set the
c            equivalent diameter of the backfill to the engineered backfill
c            outer diameter; otherwise, calculate the outer diameter for
c            natural backfill
             if(bfThick .GT. 0.0D0) then
               equivDiaBFA(index_value) = 2.0d0 * dsoRadius +
     &           2.0d0 * bfThick
               equivDiaBFB(index_value) = 2.0d0 * dsoRadius +
     &           2.0d0 * bfThick
             else

c              The calculation of backfill outer diameter involves two steps.
c              First, up to the point that the backfill goes to the original
c              diameter of the drift in section b, the equivalent diameter of
c              the backfill in section a will be zero and in section b will
c              increase out to the original diameter of the rock wall.  Past
c              this point; however, secton b reaches its maximum since the
c              drift does not degrade in this section but the backfill begins
c              to accumulate in section a.  Therefore the maximum area in
section
c              b is subtracted from the area of fallen rock to determine the
c              equivalent radius for section a.

c              First assume the drift wall has not been reached in section b.
               test_diameter = 2.0d0 *
     &           (
     &             DSQRT(
     &               ((areaFallen(index_value)/(fracAbove - fracWedge))
     &               + PI * dsoRadius**2) / PI
     &             )
     &           )

               if(test_diameter .le. (driftRadius * 2.0d0)) then
c                Section b area has not been exceeded.
                 equivDiaBFA(index_value) = dsoRadius * 2.0d0
                 equivDiaBFB(index_value) = test_diameter
               else
c                Section b area has been exceeded.
                 equivDiaBFB(index_value) = driftRadius * 2.0d0
```

```
                equivDiaBFA(index_value) = 2.0d0 *
     &            (
     &              DSQRT(
     &                (((areaFallen(index_value) - area_max_b) /
     &                fracWedge) +
     &                PI * dsoRadius**2) / PI
     &              )
     &            )
              endif

            endif
          endif

c         Limit the equivalent diameter of the backfill to the
c         equivalent diameter of the rock wall
          equivDiaBFA(index_value) = min(equivDiaBFA(index_value),
     &      equivDiaRWA(index_value))
          equivDiaBFB(index_value) = min(equivDiaBFB(index_value),
     &      equivDiaRWB(index_value))

        enddo

      endif
      return

      end
```

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-481	2. Software Title and Version: TPA 5.0w	3. Project No: 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): *seismo2.f, mechfail.f, tpa.inp, mechfail.def*

The current TPA code does assess the mechanical failure of the drip shield; however, it does not evaluate the potential effects of interactions between the drip shield and waste package under sustained accumulated rockfall rubble loads. Interactions between the drip shield and waste package could occur if the drip shield should buckle or experience creep failure when subjected to accumulated rockfall rubble loads. The bulkheads and support beams of the drip shield provide the structural support of the load. Once the drip shield buckles, the load path changes such that the load is transferred from the bulkhead to the waste package. This potential waste package failure mechanism is to be incorporated as a new model into the TPA code. This new model is described in the*Risk Analysis for Risk Insights Progress Report*, July 31, 2004.

5. Change Requested by: D. Gute Date: 4-14-2004	6. Change Authorized by (*Software Developer*): R. Janetzke Date:4-15-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See Attachment A.

8. Implemented by: G. Adams	Date: 7-27-2004

9. Description of Acceptance Tests:

See Attachment B, 9A Test Plan for SCR481

See Attachment C, 9B Test Results for SCR481

10. Tested by: Albert Lozano	Date: August 24, 2004

UPDATE REQUIREMENTS for TPA.INP

SCR481

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)	Distribution	Range	Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)
Add	SEISMO	ContactAngle[degrees]	Relative orientation of the drip shield bulk head and waste package outer surface. This orientation is characterized in terms of the angle between the surface normals of these two surfaces at the contact location.	normal	0.0, 45.0	Engineering Judgement; The current bounds are based on the drip shield design documented in the ""Design Analysis for the Ex-Container Components""; The bounds of this PDF will have to be updated when the abstractions for the drip sheild design documented in ""Drip Shield Structural Response to Rock Fall"" are implemented.	DG

Add	SEISMO	DeflectionDepth[m]	The deflection depth defines the reduction in the waste package outer barrier thickness that should be used when calculating the drip shield and waste package contact area.	constant	0.004	Engineering Judgement; Note that this parameter will no longer be used after the revised drip shield and waste package abstractions are updated to reflect the results obtained from detailed process-level modeling efforts.	DG
Add	SEISMO	BulkheadThickness[m]	Drip shield bulk head thiickness	constant	0.038	DOE/NRC KTI Agreement Response to CLST.02.01. Based on design drawings provided in the ""Design Analyses for the Ex-Container components"" report; This parameter will have to be updated when the abstractions for the drip shields design documented in ""Drip Shield Structural Response to rock Fall"" are implemented.	DG
Add	SEISMO	WastePackageOuterBarrierUltimateTensileStrength[Mpa]	Ultimate tensile strength of Alloy 22 at 150 °°C [300 °°F]	constant	679.134	True Stress Value at 150 °°C, Derived in ""Assessment of Mechanical Response of Drip Shields Under Repository Environment - Progress Report 2" CNWRA report.	DG

Attachment A

7.0 Description of Change(s) or Problem Resolution

tpa.inp:
Added the following parameters:
1) ContactAngle[degrees] : distributed normally between 0 and 45 degrees
2) DeflectionDepth[m]: constant value of 0.004 m
3) BulkheadThickness[m]: constant value of 0.038 m
4) WastePackageOuterBarrierUltimateTensileStrength[MPa]: constant value of 679.134 Mpa

Seismo2.f: Modified to retrieve the additional *tpa.inp* parameters and pass them to standalone module mechfail

Mechfail.f: Modified to retrieve the additional *tpa.inp* parameters and perform the following calculations: First, the contact area between the drip shield bulkhead and the waste package outer barrier is calculated. This contact area is a function of the contact angle sampled parameter and the assigned allowable deflection/penetration depth. Next, the maximum normal stress for the waste package outer barrier is calculated as follows:

$$\text{maximum normal stress} = \frac{\text{static load acting on the drip shield}}{\text{contact area}}$$

Afterwards, the maximum normal stress is compared to 90 percent of the ultimate tensile strength of the waste package outer barrier. If the maximum normal stress reaches or exceeds this threshold, then the waste package has failed due to mechanical failure for that grid element within that subarea. The failure across all grid elements in all subareas is then accumulated for further analysis.

Equations for calculating the contact area are documented in Appendix A of the Risk Analysis for Risk Insights Progress Report, July 31, 2004.

Attachment B

9A - Test Plan for TPA SCR#481

Test Plan Name: Failed Drip Shield Interaction Test
Tested By: Albert S. Lozano Date: August 24,2004
Host Machine: Spock Host OS: Solaris
Baseline Version: tpa50w Test Version: tpa50x

Process Level (PL) Tests
Create a directory containing the baseline (previously tested) source code.
Create a directory containing the baseline runtime and related files.
Create a directory containing the modified source code.
Create a directory containing the modified runtime and related files.

Create Environment Variables:
TPA_TEST
TPA_DATA

PL1 - Seismo2 Input File Creation Test
Special input files or modifications to input files required : None
Special diagnostic code modifications required : None
Program modes to be used (append flags, scenario/model switches, etc.): None
Utility scripts needed to perform the test: None
Utility codes needed in the analysis of the test data: Text Editor

Test description:
- objective
As described in SCR 481, four new TPA parameters were added to the *tpa.inp* file. They are ContactAngle[degrees], DeflectionDepth[m], BulkheadThickness[m], and WastePackageOuterBarrierUltimateTensileStrength[MPa].

Verify that Seismo2 reads these four parameters from *tpa.inp* and generates an input file , *mechfail.inp*, for the standalone program *mechfail.e* that contains the four new parameters.
- assumptions None
- constraints None
- output files to compare or examine *tpa.inp* and *mechfail.inp* for tpa5.0 x version
- step by step test procedure to be used
Run the tpa5.0 version x code and then use a text editor to determine whether the four new parameters have been added to the *tpa.inp* file and that they appear in *mechfail.inp*
- pass fail criteria
If the parameters are found in the *tpa.inp* file and *mechfail.inp* then this test passes.

PL2 - *Mechfail.e* Test
Special input files or modifications to input files required :
The maximum normal stress calculation will require a new *tpa.inp* file.

Special diagnostic code modifications required : None
Program modes to be used (append flags, scenario/model switches, etc.): None
Utility scripts needed to perform the test: None
Utility codes needed in the analysis of the test data: Text Editor and Excel Spreadsheet
Test description:
- objective
Verify that the four new input parameters are correctly read into *mechfail.e*.

Verify that the implementation of the contact area calculation and the maximum normal stress calculation are correct as per Chapter 2 of the Risk Analysis for Risk Insights Progress Report, July 31, 2004, and also verify that the waste package failure is correctly determined when the maximum normal stress is greater than 90% of the WastePackageOuterBarrierUltimateTensileStrength[MPa].

Verify that the waste package failure is correctly determined when the maximum normal stress is greater than 90% of the WastePackageOuterBarrierUltimateTensileStrength[MPa].

- assumptions: None
- constraints: None
- output files to compare or examine:
The contact area verification will require the *mechfail.out* files created by George Adams.
The maximum normal stress calculation will require the *mechfail.out* file generated from the new tpa5.0 run version x using the new *tpa.inp* file.

- step by step test procedure to be used:
Examination of *mechfail.out* will reveal whether the four new input parameters are correctly read by *mechfail.e* .

A spreadsheet will be used to determine if the contact area calculations and the maximum normal stress calculations are performed correctly by *mechfail.e* using data in several previously stored *mechfail.out* files.

A special print line will appear in *mechfail.out* when a waste package failure occurs.

Pass/Fail criteria: If the calculations are correct, the test passes.

PL3 - Contact Angle Distribution Test
Special input files or modifications to input files required :
tpa.inp file is set up to run one realization starting at realization 12
Special diagnostic code modifications required : None
Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None
Utility codes needed in the analysis of the test data: Text Editor
Test description:
- objective
Verify that the contact angle value in *mechfail.inp* is the same as the 12th realization in *lhs.out*

- assumptions: None
- constraints: None
- output files to compare or examine: *mechfail.inp* and *lhs.out*.
- step by step test procedure to be used:
Examination of *mechfail.inp* and *lhs.out* will show that the right contact angle was selected.

Pass/Fail criteria: If the numbers are the same, the test passes.

System Level (SL) Tests
No special System Level tests were performed.

Notes:

Attachment C

9B - Test Results for TPA SCR#481

Process Level (PL) Tests

The following directories were created on "spock" for the tpa50w and tpa50x versions.
`/home/alozano/tpa5/tpa50w`
`/home/alozano/tpa5/tpa50x`

The following environment variables were created on "spock".
`TPA_TEST=/home/alozano/tpa5/tpa50x`
`TPA_DATA=/home/alozano/tpa5/tpa50x`

In addition to these two directories, images of these two directories and other support directories were also created on Adriana for ease of documentation into the word perfect documents.
This directory tree starts at `D:\alozano\tpatest`

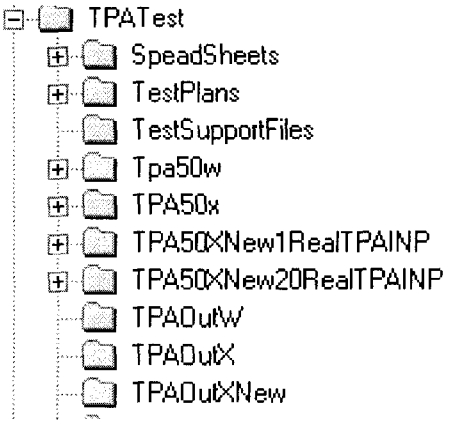


Figure 1. - Directory Tree Structure provided on SCR#481 CD

PL1 - Seismo2 Input File Creation Test

Test Results:

By examination of *tpa.inp* it was determined that four new TPA parameters were added to the *tpa.inp* file. The following was copied from *tpa.inp* file.

```
** GADAMS PA-SCR-481 6-7-04: Added parameters to assess the effect of
** drip shield impact on the waste package
**
normal
ContactAngle[degrees]
```

```
0.0, 45.0
**
constant
DeflectionDepth[m]
0.004
**
constant
BulkheadThickness[m]
0.038
**
constant
WastePackageOuterBarrierUltimateTensileStrength[MPa]
679.134
**
**
** GADAMS PA-SCR-481 6-7-04: End of change
**
```

The four new TPA parameters were added to the *tpa.inp* file. **PASSED**

By examination of *mechfail.inp*, it was verified that Seismo2 read these four parameters from *tpa.inp* and generated an input file, *mechfail.inp*, for the standalone program *mechfail.e* that contains the four new parameters. The following was copied from *mechfail.inp.*

```
:Contact angle[degrees] {ContactAngle[degrees]}
 2.23842E+01       - This value comes from tpa.inp (PASS)
:Deflection depth[m] {DeflectionDepth[m]}
 4.00000E-03       - This value comes from tpa.inp (PASS)
:Bulkhead thickness[m] {BulkheadThickness[m]}
 3.80000E-02       - This value comes from tpa.inp (PASS)
:Waste package radius[m] {WPDiameter[m] / 2}
 7.89500E-01       - WPDiameter[m] = 1.579 from tpa.inp / 2.0 (PASS)
:Waste package UTS {WPUltimateTensileStrength[MPa]}
 6.79134E+02                          - This value comes from tpa.inp
(PASS)
```

Seismo2 read these four parameters from tpa.inp. **PASSED**

PL2 - Mechfail.e Test

Test Results:

The following text came from mechfail.out and demonstrates that the correct values were read into mechfail.e

(These values match the values in mechfail.inp)
Retrieved: 22.384200000000 for parameter: Contact angle
Retrieved: 4.0000000000000D-03 for parameter: Deflection depth
Retrieved: 3.8000000000000D-02 for parameter: Bulkhead thickness
Retrieved: 0.78950000000000 for parameter: Waste package radius
Retrieved: 679.13400000000 for parameter: Waste package ultimate tensile strength

Correct values were read into *mechfail.e.* **PASSED**

Verify that the implementation of the contact area calculation and the maximum normal stress calculation are correct as per Chapter 2 of the Risk Analysis for Risk Insights Progress Report, July 31, 2004. Appendix A shows the code used to implement the equations described in the report.

This verification was performed by George Adams as part of the software development task and I have reviewed his work. A spread sheet was constructed and the equations were programmed into the spread sheet. A table was generated to compute the contact area as a function of the contact angle for a given set of parameters. Several realizations were run and the area values from the TPA runs were compared from the values in the spread sheets. See Figure 2 - Comparison of TPA runs with the spreadsheet.

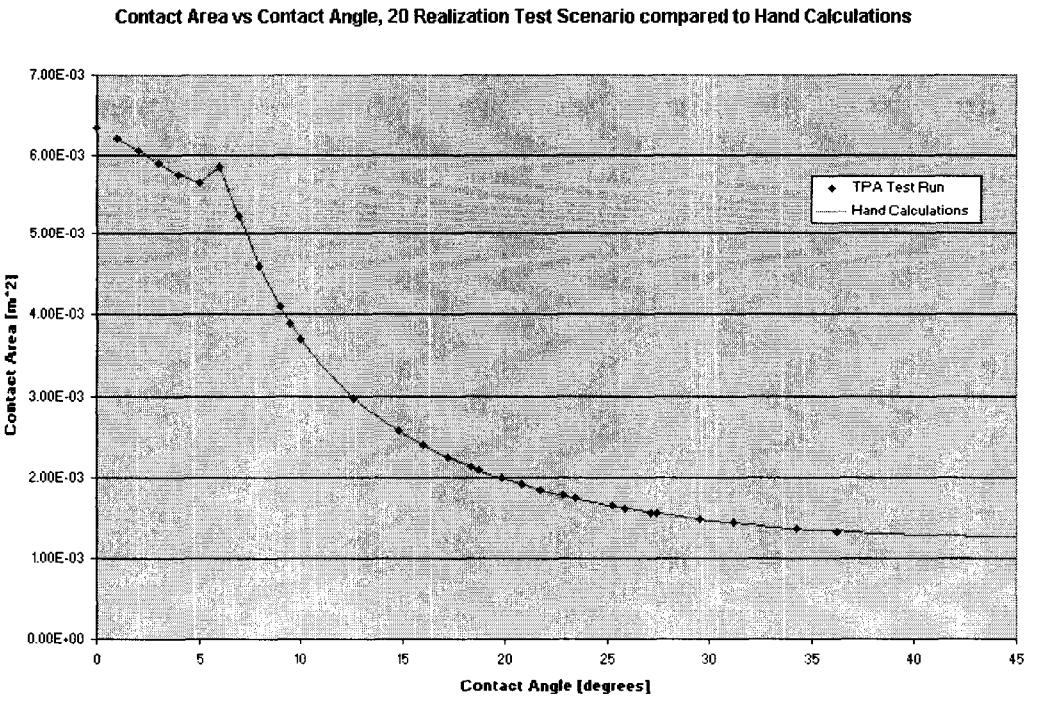


Figure 2. - Comparison of TPA run with spreadsheet for contact area calculation

This graph shows that the TPA test runs and the hand calculations agree. **PASSED**

Verify that the waste package failure is correctly determined when the maximum normal stress is greater than 90% of the WastePackageOuterBarrierUltimateTensileStrength[MPa].

This verification was performed by George Adams as part of the software development task and I have reviewed his work The following text was copied from

...\contactangle\handcalculations.xls

The maximum normal stress is the quotient of the static load acting on the drip shield and the contact area. If the maximum normal stress exceeds 90% of the ultimate tensile strength of the waste package outer barrier, then the waste package is considered to fail by mechanical means.

A special test scenario was setup to provide a test result where the conditions above were met to determine if the calculations were being performed correctly.

For subarea 4, realization 1 of 20, buckling failure of the drip shield is set to occur at 0 years in grid element 1.

The Ultimate Tensile Strength for the waste package outer barrier is 679.134 Mpa. Ninety percent of this value is 611.22 Mpa. At **1.1806E+02** years, the maximum normal stress is the drip shield static load divided by the contact area. This value is 2.9409E+00 metric tonnes / 1.5510E-03 m^2. Converting to MPa, (2.9409/0.001551) * 9.81 * 1e-3 = **18.601 Mpa**

The value generated by the code is **1.8601E+01 MPa** which agrees and is below 90% of the UTS, no waste package failure occurs. However, at **7.6184E+02 years** waste package failure does occur. At this time, the maximum normal stress is (9.7629E+01/1.5510E-03)*9.81*1e-3 = **617.5 Mpa**

.

The output from the code is **6.1749E+02 MPA** which agrees to one decimal place with the hand calculated value. Since 90% of the UTS is exceeded, the waste package is expected to fail at this time and the output file *mechfail.dat* shows that the waste package fails in grid element 1 at **7.70159E+02 years** (the next TPA time step).

The files used to compare results were *mechfail_maxnormalstress.dat* and *mechfail_maxnormalstress.out* .

A second verification was performed by Albert Lozano.

A special test scenario was setup to provide a test result where the conditions above were met to determine if the calculations were being performed correctly.

For subarea 5, realization 12 of 20, buckling failure of the drip shield is set to occur at 5.15346E+02 years in grid element 1.

The Ultimate Tensile Strength for the waste package outer barrier is 679.134 Mpa. Ninety percent of this value is 611.22 Mpa. At **5.15346E+02** years, the maximum normal stress is the drip shield static load divided by the contact area. This value is 7.6601E+01 metric tonnes / 1.4331E-03 m^2. Converting to MPa, (76.601/0.001433) * 9.81 * 1e-3 = **524.39 Mpa**

The value generated by the code is **5.2434E+02 MPa** which agrees and is below 90% of the UTS, no waste package failure occurs. However, at **5.9067E+02** years waste package failure does occur. At this time, the maximum normal stress is (90.154 / 0.001433)*9.81*1e-3 = **617.17Mpa**

.

The output from the code is **6.1711E+02 MPA** which agrees with the hand calculated value. Since 90% of the UTS is exceeded, the waste package is expected to fail at this time and the output file *mechfail.dat* shows that the waste package fails in grid element 1 at **5.9067E+02 years** (the next TPA time step).

The files used to compare results were *mechfail.dat* and *mechfail.out* in directory TPA50XNew1RealTPAINP.

The calculations are correct; therefore, *mechfail.e* **PASSED**.

The files used to compare results were *mechfail.dat* and *mechfail.out* in directory TPA50XNew1RealTPAINP.

PL3 - Contact Angle Distribution Test

Test Results:

lhs.out

```
              12             391
 0.7730297E+01 -0.1815940E+01  0.2434016E+01 -0.9352294E+01  0.3675849E+00
 0.4452197E+00  0.2522581E+01  0.1007705E+01  0.1378474E+00  0.1989910E+01
 0.8838343E+01  0.6493589E-01  0.4240996E-01  0.2945164E-02  0.1014532E+02
 0.7652557E-01  0.9148130E-01  0.1010480E-01  0.6453192E+01  0.2817496E+00
 0.4972406E-01  0.1289272E+00  0.2009633E+02  0.1571558E+01  0.1148365E-05
 0.1566274E-02  0.5303963E+00  0.1933042E-02  0.7664579E+04  0.5405225E+01
 0.3114147E+02  0.1356741E+04  0.2933849E+04  0.3642452E+04  0.2468191E+04
 0.7923755E+04  0.5922131E+04  0.1650298E+04  0.9799559E+03  0.5291482E+04
```

Contact angle from lhs.out = 0.3114147E-02

mechfail.inp

The contact angle from *mechfail.inp*

```
:Contact angle[degrees] {ContactAngle[degrees]}
3.11415E+01
```

The numbers are the same so this test **PASSED**

Additional Information

See Appendix B for an example of the locations of the data used in the waste package failure calculation and Appendix C for an example of a directory containing the run files and spreadsheet used for the contact angle calculations.

Appendix A - Differences in mechfail.f version w and version x

Changes to mechfail.f file related to SCRs 481

```
WVer
      COMMON / CMN_MECH1 / Drift_Radius, DS_Height, DS_Width,

XVer
c     GADAMS PA-SCR-481 6-7-2004: Added drip shield and
c     waste package impact parameters: Alpha,
c     Def_Depth, Thick_BH, DS_Crown_Radius, WP_UTS
      COMMON / CMN_MECH1 / Alpha, Def_Depth, Thick_BH,
     &  DS_Crown_Radius, WP_UTS,
     &  Drift_Radius, DS_Height, DS_Width, WP_Radius,
```

XVer Only

```
c     GADAMS PA-SCR-481 6-7-2004: Added drip shield and
c     waste package impact parameters: Alpha, Def_Depth,
c     Thick_BH, WP_Radius, and DS_Crown_Radius, WP_UTS
      double precision Alpha
      double precision Def_Depth
      double precision Thick_BH
      double precision WP_Radius
      double precision DS_Crown_Radius
      double precision WP_UTS
c     GADAMS PA-SCR-481 6-7-2004: End of change
```

```
WVer
     &  TIME_INITIAL, time_last, ds_crown_radius,

XVer
c       GADAMS PA-SCR-481 6-4-2004: Moved ds_crown_radius to
c       common
c     &  TIME_INITIAL, time_last, ds_crown_radius,
     &  TIME_INITIAL, time_last,
```

```
WVer
      PARAMETER(PI = 3.14159, TIME_INITIAL = 0.0D0)

XVer
      PARAMETER(PI = 3.14159d0, TIME_INITIAL = 0.0D0)
```

XVer Only

```
c     GADAMS PA-SCR-481 6-7-2004: Added parameters to assess the
c     affect of drip shield impact on the waste package.
c
c     Contact angle
      call getRealValue(inFile, Alpha, 'Contact angle',
     &  debugFlag)
c     Convert the contact angle to radians
c     Perform checking of the contact angle
      IF(Alpha .LT. 0.0d0) THEN
        Alpha = 0.0d0
      ENDIF
      Alpha = Alpha * (4.0d0 * DATAN(1.0d0)/180.0d0)
c
```

```
c     Deflection depth
      call getRealValue(inFile, Def_Depth, 'Deflection depth',
     &  debugFlag)
c
c     Bulkhead thickness
      call getRealValue(inFile, Thick_BH, 'Bulkhead thickness',
     &  debugFlag)

c     Waste Package radius
      call getRealValue(inFile, WP_Radius, 'Waste package radius',
     &  debugFlag)

c     Waste Package Ultimate Tensile Strength
      call getRealValue(inFile, WP_UTS,
     &  'Waste package ultimate tensile strength',
     &  debugFlag)
c     GADAMS PA-SCR-481 6-7-2004: End of change
```

```
WVer
c     Common declarations
      COMMON / CMN_MECH1 / Drift_Radius, DS_Height, DS_Width,
     &  Height_Invert, DS_WP_Clearance, Drift_Void_Area,
     &  DS_Plate_Creep_Factor, DS_Bulk_Head_Creep_Factor,
     &  DS_Plate_Yield_Stress, DS_Bulk_Head_Yield_Stress,
     &  DS_Plate_Creep_Coeff, DS_Bulk_Head_Creep_Coeff,
     &  DS_Plate_Creep_Exp, DS_Bulk_Head_Creep_Exp,
     &  DS_Plate_Flog_Strain, DS_Bulk_Head_Flog_Strain,
     &  WP_Outer_Yield_Stress, WP_Outer_Flog_Strain,
     &  Backfill_Thickness, Backfill_Time,
     &  ISeismicity_Flag, IDrift_Degradation_Flag

XVer
c     GADAMS PA-SCR-481 6-7-2004: Added drip shield and
c     waste package impact parameters: Alpha,
c     Def_Depth, Thick_BH, DS_Crown_Radius, WP_UTS
      COMMON / CMN_MECH1 / Alpha, Def_Depth, Thick_BH,
     &  DS_Crown_Radius, WP_UTS,
     &  Drift_Radius, DS_Height, DS_Width, WP_Radius,
     &  Height_Invert, DS_WP_Clearance, Drift_Void_Area,
     &  DS_Plate_Creep_Factor, DS_Bulk_Head_Creep_Factor,
     &  DS_Plate_Yield_Stress, DS_Bulk_Head_Yield_Stress,
     &  DS_Plate_Creep_Coeff, DS_Bulk_Head_Creep_Coeff,
     &  DS_Plate_Creep_Exp, DS_Bulk_Head_Creep_Exp,
     &  DS_Plate_Flog_Strain, DS_Bulk_Head_Flog_Strain,
     &  WP_Outer_Yield_Stress, WP_Outer_Flog_Strain,
     &  Backfill_Thickness, Backfill_Time,
     &  ISeismicity_Flag, IDrift_Degradation_Flag
```

```
XVer Only
c     GADAMS PA-SCR-481 6-7-2004: Added drip shield and
c     waste package impact parameters: Alpha, Def_Depth,
c     Thick_BH, WP_Radius, and DS_Crown_Radius, WP_UTS
      double precision Alpha
      double precision Def_Depth
      double precision Thick_BH
      double precision WP_Radius
      double precision DS_Crown_Radius
      double precision WP_UTS
c     GADAMS PA-SCR-481 6-7-2004: End of change
```

```
XVer Only
c     GADAMS PA-SCR-481 6-4-2004: Added flags for identifying
c     impacts to the drip shield and waste package for
c     testing and debugging
      LOGICAL b_impact_ds_wp1
      DATA b_impact_ds_wp1 /.TRUE./
      SAVE b_impact_ds_wp1
      LOGICAL b_impact_ds_wp2
      DATA b_impact_ds_wp2 /.TRUE./
      SAVe b_impact_ds_wp2
c     GADAMS PA-SCR-481 6-4-2004: End of change
```

```
XVer Only
c     GADAMS PA-SCR-481 6-4-2004: Added local parameters for the
c     effect of drip shield impact on waste package
      double precision theta_ds_max
      double precision theta_analysis_ds_max
      double precision area_contact
      double precision depth_analysis
      double precision x_one
      double precision x_two
      double precision x_three
      double precision projection_length
      double precision temp_impact1
      double precision temp_impact2
      double precision temp_impact3
      double precision temp_impact4
      double precision temp_impact5
      double precision temp_impact6
      double precision wp_max_normal_stress
c     GADAMS PA-SCR-481 6-4-2004: End of change
```

```
XVer Only
c     GADAMS PA-SCR-481 6-4-2004: Initialize local parameter for
c     waste package maximum shear stress
      wp_max_normal_stress = 0.0D0
```

```
XVer Only
c         GADAMS PA-SCR-481 6-4-2004: Added effects of drip shield
c         impact on the waste package.  Only calculate these effects if
c         the waste package failure has not already occurred
          IF(.not. wpFailureFlag) then
            theta_ds_max = DACOS(
     &      (
     &      2.0d0 * DS_Crown_Radius * WP_Radius +
     &      2.0d0 * Def_Depth * WP_Radius -
     &      2.0d0 * Def_Depth * DS_Crown_Radius -
     &      Def_Depth**2 -
     &      2.0d0 * DS_Crown_Radius**2
     &      ) /
     &      (
     &      2.0d0 * DS_Crown_Radius * WP_Radius -
     &      2.0d0 * Def_Depth * DS_Crown_Radius -
     &      2.0d0 * DS_Crown_Radius**2
     &      )
     &    )
          projection_length = DS_Crown_Radius * DSIN(theta_ds_max)

c         Initialize variables
          x_one = 0.0d0
          x_two = 0.0d0
```

```
      x_three = 0.0d0

      temp_impact1 = 0.0d0
      temp_impact2 = 0.0d0
      temp_impact3 = 0.0d0
      temp_impact4 = 0.0d0
      temp_impact5 = 0.0d0
      temp_impact6 = 0.0d0

      theta_analysis_ds_max = 0.0d0
      depth_analysis = 0.0d0

      IF(Alpha .gt. DASIN(Def_Depth / Thick_BH)) THEN

        x_one = 0.0d0
        x_two = theta_ds_max

        temp_impact1 = (DSIN(x_two) / 2.0d0) *
     &    DSQRT(
     &          1.0d0 - (DS_Crown_Radius**2/WP_Radius**2)*
     &          (DSIN(x_two))**2
     &         )

        temp_impact2 = (WP_Radius / (2.0d0 * DS_Crown_Radius)) *
     &    DASIN((DS_Crown_Radius/WP_Radius)*DSIN(x_two))


        area_contact =
     &  ((4.0d0 * DS_Crown_Radius / DSIN(2.0d0 * Alpha)) *
     &   (Def_Depth - WP_Radius + DS_Crown_Radius) * DSIN(x_two)
     &  ) -
     &  ((4.0d0 * DS_Crown_Radius**2 / DSIN(2.0d0 * Alpha)) *
     &   (0.5d0*DSIN(x_two)*DCOS(x_two)+x_two/2.0d0)
     &  ) +
     &  ((4.0d0 * DS_Crown_Radius * WP_Radius/DSIN(2.0d0 * Alpha)) *
     &   (temp_impact1 + temp_impact2)
     &  )

      ELSE
c       The contact angle is less than or equal to asin(bo/tbh)
        depth_analysis = Def_Depth - Thick_BH * DSIN(Alpha)

        theta_analysis_ds_max = DACOS(
     &    1.0d0 +
     &    (2.0d0 * depth_analysis * WP_Radius - depth_analysis**2) /
     &      (2.0d0 * DS_Crown_Radius * WP_Radius -
     &       2.0d0 * depth_analysis * DS_Crown_Radius -
     &       2.0d0 * DS_Crown_Radius**2)
     &    )

        x_one = 0.0d0
        x_two = theta_analysis_ds_max
        x_three = theta_ds_max

        temp_impact1 = (DSIN(x_two) / 2.0d0) *
     &    DSQRT(
     &          1.0d0 - (DS_Crown_Radius**2/WP_Radius**2)*
     &          (DSIN(x_two))**2
     &         )

        temp_impact2 = (WP_Radius / (2.0d0 * DS_Crown_Radius)) *
     &    DASIN((DS_Crown_Radius/WP_Radius)*DSIN(x_two))

        temp_impact3 = (DSIN(x_three) / 2.0d0) *
```

```
     &         DSQRT(
     &               1.0d0 - (DS_Crown_Radius**2/WP_Radius**2)*
     &               (DSIN(x_three))**2
     &              )

            temp_impact4 = (WP_Radius / (2.0d0 * DS_Crown_Radius)) *
     &         DASIN((DS_Crown_Radius/WP_Radius)*DSIN(x_three))

            temp_impact5 = (DSIN(x_two) / 2.0d0) *
     &         DSQRT(
     &               1.0d0 - (DS_Crown_Radius**2/WP_Radius**2)*
     &               (DSIN(x_two))**2
     &              )

            temp_impact6 = (WP_Radius / (2.0d0 * DS_Crown_Radius)) *
     &         DASIN((DS_Crown_Radius/WP_Radius)*DSIN(x_two))

c           Check for Alpha gt. 0
            IF(Alpha .GT. 0.0d0) THEN

            area_contact =
     &      2.0d0 * Thick_BH * DCOS(Alpha) * DSIN(x_two)
     &      + 2.0d0 * (Def_Depth - WP_Radius + DS_Crown_Radius) *
     &      DTAN(Alpha) * DSIN(x_two)
     &      -
     &      ((2.0d0 * DS_Crown_Radius * DTAN(Alpha)) *
     &      (0.5d0*DSIN(x_two)*DCOS(x_two)+x_two/2.0d0)
     &      ) +
     &      2.0d0 * WP_Radius * DTAN(Alpha) *
     &      (temp_impact1 + temp_impact2) +
     &      (4.0d0 * DS_Crown_Radius / DSIN(2.0d0 * Alpha)) *
     &      (Def_Depth - WP_Radius + DS_Crown_Radius) *
     &      (DSIN(x_three) - DSIN(x_two)) -
     &      (4.0d0 * DS_Crown_Radius**2 / DSIN(2.0d0 * Alpha)) *
     &      (0.5d0*DSIN(x_three)*DCOS(x_three) + x_three/2.0d0 -
     &      0.5d0*DSIN(x_two)*DCOS(x_two) - x_two/2.0d0) +
     &      (4.0d0 * DS_Crown_Radius * WP_Radius / DSIN(2.0d0*Alpha)) *
     &      (temp_impact3 + temp_impact4 - temp_impact5 - temp_impact6)

            ELSE

            area_contact =
     &      2.0d0 * Thick_BH * DCOS(Alpha) * DSIN(x_two)
     &      + 2.0d0 * (Def_Depth - WP_Radius + DS_Crown_Radius) *
     &      DTAN(Alpha) * DSIN(x_two)
     &      -
     &      ((2.0d0 * DS_Crown_Radius * DTAN(Alpha)) *
     &       (0.5d0*DSIN(x_two)*DCOS(x_two)+x_two/2.0d0)
    &      ) +
     &      2.0d0 * WP_Radius * DTAN(Alpha) *
     &      (temp_impact1 + temp_impact2)

            ENDIF

          ENDIF

c         Calculate the maximum normal stress in MPa
          wp_max_normal_stress = ds_static_load / area_contact

c         Convert the normal stress from metric tonnes / m^2 to MPa
c         1000 kg/tonne * 9.81 m/sec^2 * 1d-6MPa/Pa
          wp_max_normal_stress = wp_max_normal_stress * 1.0d-3 * 9.81

c         If the waste package maximum shear stress is at or higher than
```

```
c         90% of the ultimate tensile strength, then mark the waste
c         package as failed.
          IF(wp_max_normal_stress .ge. (0.9d0 * WP_UTS)) THEN
            wpFailureFlag = .TRUE.
            wpTopFailureFlag = .TRUE.
          ENDIF

          IF((debugFlag .and. wpFailureFlag) .OR.
     &      (debugFlag .and. b_impact_ds_wp1 .and. idRock .eq. 1) .OR.
     &      (debugFlag .and. b_impact_ds_wp2 .and. idRock .eq. 2)) THEN
            IF(idRock .eq. 1) THEN
              b_impact_ds_wp1 = .FALSE.
            ENDIF
            IF(idRock .eq. 2) THEN
              b_impact_ds_wp2 = .FALSE.
            ENDIF
            WRITE(*, *)
     &        '<<<Start-Drip Shield Impact on Waste Package >>>'
            WRITE(*, FMT = '(1x, a6, i2)') 'Rock: ', idRock
            WRITE(*, FMT = '(18(2x, a20))') 'Theta DS Max',
     &        'Theta Star DS', 'Projection Length',
     &        'x_one', 'x_two', 'x_three', 'Def_Depth',
     &        'Depth Star', 'Thick_BH',
     &        'temp1', 'temp2', 'temp3', 'temp4', 'temp5', 'temp6',
     &        'alpha', 'area', 'max_normal'
            WRITE(*, FMT = '(18(2x, 1pe20.4))') theta_ds_max,
     &        theta_analysis_ds_max,
     &        projection_length, x_one, x_two, x_three, Def_Depth,
     &        depth_analysis,
     &        Thick_BH, temp_impact1, temp_impact2, temp_impact3,
     &        temp_impact4, temp_impact5, temp_impact6, Alpha,
     &        area_contact, wp_max_normal_stress
            WRITE(*, *) '<<<END-Drip Shield Impact on Waste Package >>>'
          ENDIF

          ENDIF ! Waste Package contact angle
```

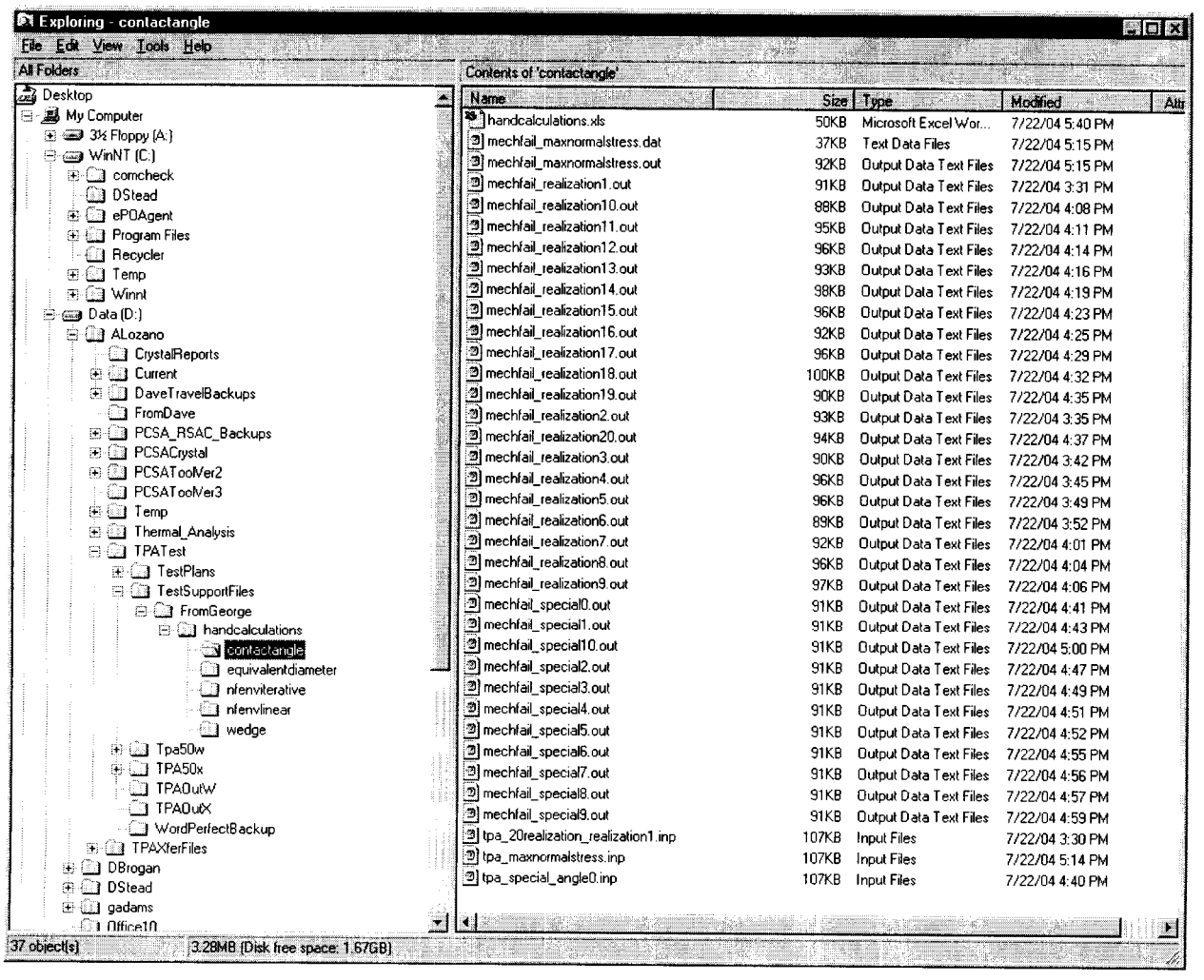
Appendix B - Portion of file showing the numbers used in waste package failure calculation

The following information was extracted from the mechfail.dat and mechfail.out files. The values that were used in the calculations are in bold characters.

```
TITLE - mechfail.dat
DATE/Time: Mon Aug 23 17:01:13 2004
:
:Mechanical Failure Data versus Time
:  Fraction Failed - Subarea Analysis
:Subarea    5
:          Time          Drift   Drip Shield   DS Buckling     Waste Pkg
    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
 .....

    5.01299E+02   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
DS Buckling occurred
    5.15346E+02   0.00000E+00   7.50000E-01   7.50000E-01   0.00000E+00
    5.29721E+02   0.00000E+00   7.50000E-01   7.50000E-01   0.00000E+00
    5.44432E+02   0.00000E+00   7.50000E-01   7.50000E-01   0.00000E+00
    5.59488E+02   0.00000E+00   7.50000E-01   7.50000E-01   0.00000E+00
    5.74897E+02   0.00000E+00   7.50000E-01   7.50000E-01   0.00000E+00
Waste Package Failure occurred
    5.90666E+02   0.00000E+00   7.50000E-01   7.50000E-01   7.50000E-01
    6.06805E+02   0.00000E+00   7.50000E-01   7.50000E-01   7.50000E-01

Analysis performed on rock type:         1
        Analysis Time            Delta Time          Drift Height
Static Load Ht.      Static Load
           5.0130E+02            1.3725E+01            1.7158E+01
1.5373E+01            7.4073E+01

<<<Start-Drip Shield Impact on Waste Package >>>
Rock:  1
         Theta DS Max         Theta Star DS     Projection Length
  x_one                 x_two                x_three              Def_Depth
     Depth Star              Thick_BH                 temp1
temp2                 temp3                 temp4                 temp5
        temp6                 alpha                 area
max_normal
           8.3740E-02            0.0000E+00            1.1869E-01
0.0000E+00            8.3740E-02            0.0000E+00            4.0000E-03
        0.0000E+00            3.8000E-02            4.1346E-02
4.1980E-02            0.0000E+00            0.0000E+00            0.0000E+00
        0.0000E+00            5.4352E-01            1.4331E-03
5.2434E+02
<<<END-Drip Shield Impact on Waste Package >>>
           5.1535E+02            1.4047E+01            1.7606E+01
1.5898E+01            7.6601E+01

           5.2972E+02            1.4375E+01            1.8065E+01
1.6435E+01            7.9187E+01

           5.4443E+02            1.4711E+01            1.8535E+01
1.6984E+01            8.1834E+01

           5.5949E+02            1.5056E+01            1.9015E+01
1.7547E+01            8.4544E+01
```

```
          5.7490E+02            1.5409E+01            1.9507E+01
1.8122E+01            8.7316E+01

<<<Start-Drip Shield Impact on Waste Package >>>
Rock:  1
         Theta DS Max         Theta Star DS     Projection Length
  x_one                 x_two                x_three              Def_Depth
     Depth Star              Thick_BH                 temp1
temp2                 temp3                 temp4                 temp5
        temp6                 alpha                  area
max_normal
          8.3740E-02            0.0000E+00            1.1869E-01
0.0000E+00            8.3740E-02            0.0000E+00            4.0000E-03
        0.0000E+00            3.8000E-02            4.1346E-02
4.1980E-02            0.0000E+00            0.0000E+00            0.0000E+00
        0.0000E+00            5.4352E-01            1.4331E-03
6.1711E+02
<<<END-Drip Shield Impact on Waste Package >>>

          5.9067E+02            1.5769E+01            2.0011E+01
1.8711E+01            9.0154E+01
```

Appendix C - Directory Tree for Hand Calculations



SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-482	2. Software Title and Version: TPA 5.0.0a	3. Project No: 20.06002.01.113 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *ashremob.f, ashremob.h, ashrmovo.f, dcags.f, dcags.h, exec.f, tpa.inp, tpanames.dbs, SIZES.INC, leachrate.h,* and *remob_lut.dat.*

Add the ash redistribution model described in Chapter 6 of the Risk Analysis for Risk Insights – Progress Report (April 2005). Attachments A and B contain a pseudo-code and additional relationships for indoor inhalation exposure for facilitating the code modifications.

5. Change Requested by: M. Smith Date: 4-14-2004	6. Change Authorized by (*Software Developer*): R. Janetzke Date:4-15-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Create new module **ashremob** to implement new model. Update **tpa.inp** accordingly for new input parameters. Modify **exec** for changed argument list and to call **ashremob** instead of **ashplumo, ashremovo** and **dcags** when **AshEvolutionMode** is not set to zero.

Modify **ashrmovo** and **dcags** to revert to version 4.2r algorithms. Incorporate subsequent bug fixes and retain the expansion to the five categories for occupancy fraction and airborne mass load.

See Attachments C & D for more detail.

8. Implemented by: D. Sylvester/R. Janetzke	Date: 9-17-2004

9. Description of Acceptance Tests:

See attachment E.

10. Tested by: R. Benke	Date: 5-6-05

CNWRA Form TOP-5 (05/2000)

Attachment A: Pseudo-Code for Calculating the Airborne Concentration of High-Level Waste at the RMEI Location Through Time

When the AshEvolutionMode flag is set to a value of 1, the following loop is executed:

1. Sample one of the n realizations of ASHPLUME_P code [$c_{HLW,i}$, $c_{ash,i}$, $m_{HLW,f}$, $m_{ash,f}$, $a_{ash,f}$, $m_{HLW,e}$, $m_{ash,e}$, $a_{ash,e}$], from Table 6_1. The selection is accepted if the index k of the realization wasn't previously selected ($k = 1, n$).
2. Calculate c_i using eq. 6-4.
3. Get $S_{ash,out-H}$ from TPA Input file .
4. Set $\rho_{ash,i}$ = AshBulkDensity[g/cm^3] parameter of ASHRMOVO.
5. Calculate $T_{B-0} = c_{ash,i} / (\rho_{ash,i} \times 10000)$.
6. Set λ_B = RelativeRateOfBlanketRemoval[yr^{-1}] parameter of ASHRMOVO.
7. Calculate $T_B(t) = T_{B-0} \exp(-\lambda_B(t - t_{event}))$.
8. Get T_R from TPA Input file (parameter name: DepthOfResuspendableLayer[cm]).
9. If $T_B(t) \le T_R$ calculate $f_R(t) = T_B(t) / T_R$, else $f_R(t) = 1$.
10. Get $\lambda_i(t)$ from TPA Input file .
11. Calculate $H_{i-B}(t)$ using eq. 6-2.
12. Get w_i from TPA Input file.
13. Get $S_{ash,out-L}$ from TPA Input file .
14. Calculate $H_{i-L}(t)$ using eq. 6-3.
15. Get $\rho_{ash,f}$ from TPA Input file.
16. Calculate $v_{ash,f}$ using eq. 6-8.
17. Get $Y_{ash,f}$ from TPA Input file.
18. Calculate $n_{deplete}$ using eq. 6-10.
19. Get $Y_{sediment,f}$ from TPA Input file.
20. Get $A_{basin,f}$ from TPA Input file.
21. Calculate $v_{sediment,f}$ using eq. 6-9.
22. Calculate d_f using eq. 6-7.
23. Get T_f from TPA Input file.
24. Calculate c_f using eq. 6-6.
25. Calculate $t_{duration,f}$ using eq. 6-11.
26. Get $S_f(t)$ equal to the AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3] parameter from TPA Input file if $t \le t_{duration,f}$, and zero otherwise.
27. Get w_f from TPA Input file.
28. Calculate $H_f(t)$, $t \in [t_0, t_{max}]$, using eq. 6-5.
29. Get $A_{eolian,e}$ from TPA Input file.

30. Get $\rho_{ash,e}$ from TPA Input file.

31. Calculate d_e using eq. 6-14.

32. Calculate C_e using eq. 6-13.

33. Get w_e from TPA Input file.

34. Set $S_e(t=0)$ equal to the AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3] parameter from TPA Input file .

35. Get λ_e = RateOfReductionOfMassLoadingFactor[1/yr] from TPA Input file.

36. Calculate $S_e(t) = S_e(t=0)\ exp(-\lambda_e\ t)$ for $t \in [t_0\ .\ t_{max}]$.

37. Calculate $H_e(t)$, $t \in [t_0\ .\ t_{max}]$, using eq. 6-12.

38. Get $f_{out\text{-}H}$, $f_{out\text{-}L}$ from TPA Input file.

39. Calculate $H_{RMEI\text{-}outdoor}(t)$, $t \in [t_0\ .\ t_{max}]$, using eq. 6-1.

40. If $t \le t_{duration}$, $S_f(t) = S_{ash,out\text{-}L}$, otherwise $S_f(t) = 0.0$.

41. Calculate $P_{out\text{-}H}(t)$ using eq. 2 .

42. Calculate $p_{i\text{-}H}(t)$, $p_{f\text{-}H}(t)$, and $p_{e\text{-}H}(t)$ using eq. 3 .

43. If $t \le t_{duration}$, $S_f(t) = S_{ash,out\text{-}L}$, otherwise $S_f(t) = 0.0$.

44. Calculate $P_{out\text{-}L}(t)$ using eq. 4

45. Calculate $p_{i\text{-}L}(t)$, $p_{f\text{-}L}(t)$, and $p_{e\text{-}L}(t)$ using eq. 5 .

46. Calculate $p_i(t)$, $p_f(t)$, and $p_e(t)$ using eq. 6 .

47. Get $f_{in\text{-}H}$ and $f_{in\text{-}H}$ from TPA Input file.

48. Calculate $H_{RMEI\text{-}indoor}(t)$, using eq. 7.

49. Get $f_{offsite}$ and $S_{offsite}$ from TPA Input file.

50. Calculate $H_{RMEI\text{-}offsite}(t)$ using eq. 8.

51. Calculate $H_{RMEI}(t)$ using eq. 9.

52. Let $k = 1$ (1-st radionuclide).

53. Get $SA_k(t)(Ci/g_{HLW})$ from the INVENT module.

54. Get $BR \times DCF_k$ from *gs_cb_ad.dat* or *gs_pb_ad.dat* (where BR = breathing rate (m^3/yr), DCF_k = dose conversion factor for inhalation for radionuclide k (rem/Ci))

55. Calculate the inhalation dose for radionuclide k: $DOSE_k(t) = BR \times DCF_k \times H_{RMEI}(t) \times SA_k(t)$

56. Let $k = k+1$.

57. Go to 52. Repeat 52 to 56 until $DOSE_k(t)$ is calculated for all the radionuclides.

58. Calculate the total inhalation dose: $DOSE(t) = \sum DOSE_k(t)$.

59. Go to 1 for a new realization.

NOTES:

I. The first set of parameters sampled at 1. is randomly sampled from the n entries of Table 6_1.

II. If $n > rmax$, ($rmax$ = total number of realizations), the following $rmax\text{-}1$ sets are non-repetitively sampled from Table 6_1.

III. The non-repetitive sampling is ensured by recording for each realization the index value k, and adding it to the list of the previous indices of selected sets of parameters.

IV. If $n < rmax$, after every n executions of loop 1.-36., the record of indices k is cleared, and the executions of 1.-36. resume and continue as described at I, II, III.

V. Equations 6-x refer to " Ash Remobilization Modeling for Extrusive Volcanism", and equations 1 to 9 refer to "Calculation of the Total Airborne Concentration of High-Level Waste for the Ash Remobilization Model Abstraction " (Roland, 08/31/04).

Attachment B: Calculation of the Total Airborne Concentration of High-Level Waste for the Ash Remobilization Model Abstraction

These calculations are used when the AshEvolutionMode flag is set to a value of 1 in the input file for the TPA Version 5.0.1 code. The reader should reference Chapter 6 of the Risk Analysis for Risk Insights Progress Report (April 2005) for variable definitions. Eq. (6-1) of the Risk Analysis for Risk Insights Progress Report presents the outdoor airborne contribution of high-level waste (g/m^3) at the receptor location weighted by the outdoor occupancy fractions during heavy and light disturbance, $H_{RMEI,outdoor}(t)$, as

$$H_{RMEI,outdoor}(t) = f_{out-H} H_{i-H}(t) + f_{out-L} H_{i-L}(t) + \left(f_{out-H} + f_{out-L}\right) H_f(t) + \left(f_{out-H} + f_{out-L}\right) H_e(t) .$$

As described in Chapter 6, the calculations of the indoor airborne particle load use the same proportions from each of the three contributions (i.e., initial deposition at the receptor location, fluvial remobilization, and eolian remobilization) for the total outdoor airborne particle load to which the receptor is exposed. The term proportion is used in these calculations instead of the term fraction to avoid confusion with the occupancy fractions.

During heavy disturbance outdoors, the total airborne particle loading (g/m^3) at the receptor location is calculated as

$$P_{out-H}(t) = S_{ash,out-H} e^{-\lambda_r t} + w_f S_f(t) + w_e S_{ash,out-L} e^{-\lambda_r t} .$$

Heavy disturbance activities are assumed to occur only on the initial deposit at the receptor location. In other words, heavy disturbance activities and outdoor mass loads during heavy disturbance do not apply to the contributions from fluvial and eolian remobilization. For these reasons, a weighting factor is not included in the first term of the right-hand side of the previous equation above.

The proportions of the particle load from the three contributions (i.e., initial deposition at the receptor location, fluvial remobilization, and eolian remobilization) when the receptor is engaged
in heavy disturbance activities outdoors are

$$p_{i-H}(t) = \frac{S_{ash,out-H} \times \exp(-\lambda_r t)}{P_{out-H}(t)}$$

$$p_{f-H}(t) = \frac{w_f \times S_f(t)}{P_{out-H}(t)}$$

$$p_{e-H}(t) = \frac{w_e \times S_{ash,out-L} \times \exp(-\lambda_r t)}{P_{out-H}(t)} .$$

During light disturbance outdoors, the total airborne particle loading (g/m^3) at the receptor location is calculated as

$$P_{out-L}(t) = w_i S_{ash,out-L} e^{-\lambda_r t} + w_f S_f(t) + w_e S_{ash,out-L} e^{-\lambda_r t} .$$

The proportions of the particle load from the three contributions (i.e., initial deposition at the receptor location, fluvial remobilization, and eolian remobilization) when the receptor is engaged in light disturbance activities outdoors are equal to:

$$p_{i-L}(t) = \frac{w_i S_{ash,out-L} e^{-\lambda_r t}}{P_{out-L}(t)}$$

$$p_{f-L}(t) = \frac{w_f S_f(t)}{P_{out-L}(t)}$$

$$p_{e-L}(t) = \frac{w_e S_{ash,out-L} e^{-\lambda_r t}}{P_{out-L}(t)} .$$

The final proportions for the three contributions are calculated as the weighted sum of the proportions and occupancy fractions for heavy and light disturbance divided by the total fraction of time exposed outdoors

$$p_i(t) = \frac{p_{i-H}(t) f_{out-H} + p_{i-L}(t) f_{out-L}}{f_{out-H} + f_{out-L}}$$

$$p_f(t) = \frac{p_{f-H}(t) f_{out-H} + p_{f-L}(t) f_{out-L}}{f_{out-H} + f_{out-L}}$$

$$p_e(t) = \frac{p_{e-H}(t) f_{out-H} + p_{e-L}(t) f_{out-L}}{f_{out-H} + f_{out-L}}$$

These proportions account for the total outdoor particle load to which the receptor is exposed outdoors and are used to calculate the airborne concentration of high-level waste indoors.

The indoor airborne concentration of high-level waste (g/m^3) at the receptor location weighted by the indoor occupancy fractions during heavy and light disturbance, $H_{RMEI,indoor}(t)$, is calculated as

$$H_{RMEI,indoor}(t) = f_{in-H}\left[p_i(t) \times c_i \times f_R(t) + p_f(t) \times c_f \times d_f + p_e(t) \times c_e \times d_e\right] S_{in-H}$$
$$+ f_{in-L}\left[p_i(t) \times c_i \times f_R(t) + p_f(t) \times c_f \times d_f + p_e(t) \times c_e \times d_e\right] S_{in-L}$$

where

S_{in-H} – indoor mass load for dust with heavy disturbance (g/m^3) = AirborneMassLoadInsideHeavyDisturbance[g/m3]
S_{in-L} – indoor mass load for dust with light disturbance (g/m^3) = AirborneMassLoadInsideLightDisturbance[g/m3]
f_{in-H} – fraction of time receptor spends indoors with heavy disturbance = OccupancyFractionInsideHeavyDisturbance[-]
f_{in-L} – fraction of time receptor spends indoors with light disturbance = OccupancyFractionInsideLightDisturbance[-].

The offsite occupancy fraction is included only for completeness. It is intended that the offsite locations are free of contamination. The default offsite airborne mass load is thus set to zero. Although its contribution is intended to be nil, a relationship is still established for the offsite airborne concentration of high-level waste that is similar to the other relationships presented in Chapter 6 of the Risk Analysis for Risk Insights Progress Report. Since unique concentration and dilution factors are not explicitly derived for offsite locations, the concentration and dilution factors for the

eolian contribution are included as proxies in the relationship for the offsite airborne concentration of high-level waste

$$H_{RMEI,offsite}(t) = f_{offsite} \times c_e \times d_e \times S_{offsite} \times e^{-\lambda_r t}$$

where

$S_{offsite}$ – offsite mass load (g/m^3) = AirborneMassLoadOffsite[g/m3]
$f_{offsite}$ – fraction of time receptor spends offsite = OccupancyFractionOffsite[-].

The total airborne concentration of high-level waste available for inhalation by the receptor is calculated as the sum of the outdoor, indoor, and offsite contributions

$$H_{RMEI}(t) = H_{RMEI,outdoor}(t) + H_{RMEI,indoor}(t) + H_{RMEI,offsite}(t) .$$

Attachment C: List of code changes resulting from the acceptance review

1. Delete line
```
double precision partmassloadinit(maxntime)
```

2. Delete lines for the second call of the same variable
```
call clearchar(60, name)
name = 'AshPlumeRealizationIndex[]'
iiashplumerealindex = ispquery(name)
```

3. Delete both duplicate lines and all earlier parameter declarations and calls for this unused variable
```
indoorshielding=valuesp( iindoorshielding )
indoorshielding=valuesp( iindoorshielding )
```

4. Read comment, perform necessary actions, and delete comment after "!" in the line:
```
do n=1,43                    ! TODO dn & sa could be one dim (n)
```

5. Edit line
```
thicknesseolcm  = 1.d2*masshlweol(iashplumerealindex)/
```
to become
```
thicknesseolcm  = 1.d2*massasheol(iashplumerealindex)/
```

6. Edit line
```
abnmassldinth =  massloadoutheavy * reductionfactor
```
to become
```
abnmassldinth =  massloadashheavy * reductionfactor
```

7. Edit lines
```
hlwgpm3intl(it) = wgtfactorinitial * concentfactorinit *
&                          massloadoutlight *
```
to become
```
hlwgpm3intl(it) = wgtfactorinitial * concentfactorinit *
&                          massloadashlight *
```

8. Edit line
```
abnmassldintl = massloadoutlight * reductionfactor
```
to become
```
abnmassldintl = massloadashlight * reductionfactor
```

9. Delete line
```
C TODO Is this stuff needed?
```

10. Delete line
```
partmassloadinit(it) = 0.0d0
```

11. Delete lines
```
c
c   Change the SoilContaminationExposureTime (scet) value from tpa.inp
c   to GroundSurfaceExposureTime (gset) for dcags
c
      gset = ((occupancyoutheavy + occupancyoutlight) +
     &        (indoorshielding * (occupancyinheavy + occupancyinlight)))
     &       * 8766
      call gentpags( irl, gset )
```

12. Modify block by deleting lines for the conditional
```
~~if (thickashm(it) .eq. 0.0d0) then~~
```

```
                    doseinh(it,k) = 0.0d0
                 else
                    doseinh(it,k) = dcfinh(k) * ciperghlw(it,k)
     &                                        * hrmei(it)
                 endif
```

13. Modify block by deleting lines for the conditional

```
                 if (thickashm(it) .eq. 0.0d0) then
                    doseinh(it,k) = 0.0d0
                 else
                    doseinh(it,k) = dcfinh(k) * ciperghlw(it,k)
     &                                        * hrmei(it)
                 endif
```

14. Modify block by deleting lines for the conditional

```
                 if (thickashm(it) .eq. 0.0d0) then
                    doseinh(it,k) = 0.0d0
                 else
c
                    doseinh(it,k) = dcfinh(k) * ciperghlw(it,k)
     &                                        * hrmei(it)

                 endif
```

15. Modify block by deleting lines for the conditional

```
                 if (thickashm(it) .eq. 0.0d0) then
                    doseinh(it,k) = 0.0d0
                 else
c
                    doseinh(it,k) = dcfinh(k) * ciperghlw(it,k)
     &                                        * hrmei(it)

                 endif
```

16. Delete comment lines

```
c        doseinh is dose per gram spent fuel ejected, convert to
c        dose per MTU for total fuel ejected.
```

17. Edit lines by removing comment character from the first line and deleting the second line below

```
c           remperyrpernuclgs(j,k) = doseinh(j,ik)
            remperyrpernuclgs(j,k) = doseinh(j,ik) * 1.0d6 * amtuejected
```

18. Modify the block by deleting one variable and adding the three highlighted variables. Check if these modifications affect other parts of the code.

```
cc test output of intermediate variables.
      write( ioutunit, '(13(1x,'','',1pe14.6))')
     &  (tim(it), partmassloadinit(it), abnmassldinth, abnmassldintl, partmassloadfluv(it),
     &   partmassloadeoli(it), hlwgpm3inth(it),
     &   hlwgpm3intl(it), hlwgpm3fluv(it), hlwgpm3eoli(it),
     &   hlwgmp3toth(it), hlwgmp3totl(it), hremiout(it), hremiin(it),
     &   hremioff(it), hrmei(it), it=1,ntim)
```

19. Generate an output file containing a time history of doses from each radionulcide for each realization & a time history of the total dose for each realization

20. Generate an output file containing radionulcide doses and total dose at the time of peak total dose for each realization (similar to the airpkdos.res file)

Attachment D: UPDATE REQUIREMENTS for TPA.INP
SCR482

Action	Module	Parameter Name	Distribution	Range
Add	ASHREMOB	AshEvolutionMode[0=no_ashremob,1=ashremob]	iconstant	1
Add	ASHREMOB	AshPlumeRealizationIndex[]	iuniform	1, 1024
Add	ASHREMOB	WeightingFactorInitialDeposit[]	constant	0.3334
Add	ASHREMOB	WeightingFactorFluvial[]	constant	0.3333
Add	ASHREMOB	AmbientSedimentYieldVolumeFromBasin[m/event]	uniform	3.0e-06, 3.3e-05
Add	ASHREMOB	AreaDrainageBasinFluvial[m2]	constant	8.15e+08
Add	ASHREMOB	TimeBetweenFlowEvents[yr]	constant	10.0
Add	ASHREMOB	PostEruptionYieldVolumeFluvialAsh[m/event]	uniform	1.0e-05, 1.0e-04
Add	ASHREMOB	WeightingFactorEolian[]	constant	0.3333
Add	ASHREMOB	DensityOfDistalAsh[g/m3]	constant	8.0e-05
Add	ASHREMOB	AreaEolianSourceRegion[m2]	constant	2.1e+09

Attachment E

Note: Code runs were performed in the PC environment. Because similar results have been obtained recently from the TPA code execution on both the UNIX and PC platforms, the code runs were not duplicated for the second platform.

Test 9-1. Review **ashremob.f** source code and compare the coded calculations with the intended relationships. Examine **ashremob.f** for the type of outputs generated. The **ashremob.f** file from Version 5.0.0m was examined and is archived in the \Test 9-1\ folder. Numerous code changes were identified. See Attachment C for a list of changes to be incorporated into SCR-568 for resolution.
Result for Test 9-1: **FAIL**

Test 9-2. Check that the **dcags** and **ashremovo** modules do not calculate or pass "amassash" variable by inspecting the source code. Check that the **dcags** module contains the five categories for occupancy fraction and airborne mass load by inspecting the source code. This test was performed with the latest version at the time of testing (i.e., Version 5.0.0v). The source code for the **dcags** and **ashremovo** modules is archived in the \Test 9-2\ folder.
Result for Test 9-2: **PASS**

Test 9-3. Verify that the new input parameters, listed in Attachment D, and data file (remob_lut.dat) have been added by inspecting the tpa.inp file and locating the remob_lut.dat file. This test was performed with the latest version at the time of testing (i.e., Version 5.0.0v). The tpa.inp and remob_lut.dat files were located and are archived in the \Test 9-3\ folder.
Result for Test 9-3: **PASS**

Test 9-4. Verify selection of **AshEvolutionMode** invokes the intended module(s). This test was performed with the by executing the TPA Version 5.0.0t code in the PC environment. The tpa.inp file was prepared for this test by setting
`VolcanismDisruptiveScenarioFlag(yes=1,no=0)` equal to `1`,
`DirectReleaseOnlyFlag(yes=1,no=0)` equal to `1`, and
`NumberOfRealizations` equal to `100`.
Runs were performed with the `AshEvolutionMode[0=no_ashremob,1=ashremob]` flag set to 1 and 0. In addition to tpa.inp files for each run, screen captures indicating the modules being called were saved, under the filename tpa.out for both cases, in the
\Test 9-4\ ashevolutionmode1\ and \Test 9-4\ ashevolutionmode0\ folders, respectively.
Result for Test 9-4: **PASS**

Test 9-5. Perform single realization runs with `AshEvolutionMode` set to 0 to invoke the DCAGS module and perform checks on the dose calculations for the inhalation pathway. Compare TPA code results for different input selections with expected behavior (i.e., *Case 1.* dose from ash resuspension decreases with time after event mainly due to mass load reduction and *Case 2.* dose from soil resuspension decreases slowly with time after event due to radioactive decay). This test was performed with the by executing the TPA Version 5.0.0t code in the PC environment. The tpa.inp file was prepared by setting
`VolcanismDisruptiveScenarioFlag(yes=1,no=0)` equal to 1,

`DirectReleaseOnlyFlag(yes=1,no=0)` equal to 1, and `TimeOfNextVolcanicEventinRegionOfInterest[yr]` to a constant at 1000.0 years, and `OutputMode(0=None,1=All,2=UserDefined)` equal to 1. To force all non-inhalation pathway contributions to zero, the `ggenii.def` data file was modified by changing the soil concentrations for all radionuclides from 1.0. to 0.0. Files for the two test cases were saved in the \Test 9-5\ash_only\ and \Test 9-5\soil_only\ directories, respectively for the two cases.

Case 1: For the case focusing only on the resuspension of contaminated ash outdoors, `AirborneMassLoadInsideHeavyDisturbance[g/m3]` was set to a constant at 0.0 and `AirborneMassLoadInsideLightDisturbance[g/m3]` was set to a constant at 0.0 in the tpa.inp file. The results from `dcags.rlt` output file were checked for a couple of radionuclides (Pu-239 and Am-241). Acknowledging that additional losses due to radioactive decay and erosion over a 106.21-year period after the event are not considered, inhalation doses should decrease by at least a factor of 1/Exp[- 0.07/yr *106.21 yr] = 1.7E+03 solely for the reduction in mass load of ash with time. The time difference of 106.21 years is based on actual TPA time steps of the event at `9.9639E+02` years and a following time step at `1.1026E+03` years. For Pu-239 and Am-241 the inhalation dose reduced by factors of 2.2E+03 and 2.4E+03.

Case 2: For the case focusing only on the resuspension of contaminated soil outdoors, `AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]` was set to a constant at 0.0, `AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]` was set to a constant at 0.0, `AirborneMassLoadInsideHeavyDisturbance[g/m3]` was set to a constant at 0.0, `AirborneMassLoadInsideLightDisturbance[g/m3]` was set to a constant at 0.0, `AirborneMassLoadOutsideHeavyDisturbance[g/m3]` was set to a constant at 1.0E-04, and `AirborneMassLoadOutsideLightDisturbance[g/m3]` was set to a constant at 1.0E-04 in the tpa.inp file. The results from `dcags.rlt` output file were checked for a couple of radionuclides (Pu-239 and Am-241). Acknowledging that additional losses due to radioactive decay are not considered, the inhalation doses should decrease by more than a factor of 1.0 solely from a constant mass load of soil with time. The time difference of 106.21 years is based on actual TPA time steps of the event at `9.9639E+02` years and a following time step at `1.1026E+03` years. The inhalation doses for Pu-239 and Am-241 decreased by factors of 1.3 and 1.4.

Result for Test 9-5: **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-483	2. Software Title and Version: TPA 5.0v	3. Project No: 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): exec.f, tpa.inp, invent.f, inventi.i, nuclides.dat, burnup.dat, tpanames.dbs

Update inventory and thermal data in the files *nuclides.dat* and *burnup.dat* with latest DOE values. Also, replace the usage of the **AgeOfWaste** parameter for both inventory and thermal data with two independent values determined from a new parameter **CalendarYearOfEmplacement** and the time applicable to each of the two independent data files.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
O. Povetko Date: 4-14-2004	R. Janetzke Date:4-15-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): Subroutine **setage** was removed from *invent.f.* It was only called by *exec.f.* Input parameter AgeOfWaste was changed to CalendarYearOfEmplacement[A.D.]. Previous versions assumed the SF age to be 26 years for inventory calculations. This was changed in **newinventdb**() to an age determination based on the applicable year in the *nuclides.data* file. Previous versions assumed the SF age to be 16 years for thermal calculations. This was changed in **qpermtu**() to an age determination based on the applicable year in the *burnup.dat* file. Include file *inventi.i* is used to declare new variables **yearofemplacement, yearofburnupdata,** and **yearofnuclidedata**. The applicable year for both new data files is 2033.

8. Implemented by:	Date:
Ron Janetzke	7-24-2004

9. Description of Acceptance Tests:

Duplicated results of previous version using the old data files..
Also, tested the handling of malformed data files burnup.dat and nuclides.dat.
See ATTACHMENT A for details.
Tests passed.

10. Tested by: Zbigniew WOJCIK	Date: Aug 9, 04

CNWRA Form TOP-5 (05/2000

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description** **1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton** **1. site references (journals, sci. notebooks, publishings)** **2. is uncertainty covered by the distribution / range ?** **3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
Delete	nfenv	AgeOfWaste[yr]		constant	26	replaced by less confusing parameter CalendarYearOfEmplacement[A.D.]	
Add	exec	CalendarYearOfEmplacement[A.D.]	Calendar year in which the spent fuel is emplaced in the repository. It must appear before the aqueousnuclides keyword in the tpa.inp file, and be at least one year greater than the date applicable to the burnup.dat and nuclides.dat files.	constant	2034	Use of this parameter removes the coupling between the nuclides.dat file and the burnup.dat file.	

ATTACHMENT A

Test for TPA SCR-483.
TEST NAME: Duplicate results of old version on modified code using old data.
Tested By: Zbigniew Wojcik **Date:** August 9, 2004
Host Machine: PC **Host OS:** Windows XP
(Lahey Fortran compiler v.7.1)
Baseline Version: TPA 5.0v **Test Version: TPA** 5.0w
Disposition and documentation of results: All modified / new source code files, affected old version (before modifications), and all affected input / output files are kept on the CD titled "SCR#483. Test Results. Z. Wojcik" attached. The old version is in the subdirectory tpa50v. The new version is in the subdirectory tpa50w. A separate subdirectory 'test_results' exists keeping only the results of tests. The names of the files keeping the results of tests of the old version have the 3 characters '_v_', and the names of the files keeping the results of tests of the new version are without these 3 characters.

PROCESS LEVEL (PL) Tests:

PL1:
Name: Test logics of invent.f reading data file burnup.dat in new version TPA50w
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat
Program modes to be used: NumberOfRealizations =1.
Description of PL1 Test Plan:
- Objectives: Test if the logics of the new program handles correctly the modifications in the input file burnup.dat
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: burnup.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The test passes if the new program reads the modified file burnup.dat correctly, and the modifications in the Fortran code accommodate to the changes in the input files in question. The correctness of the read-out is tested by visual comparison of the printout of the input file burnup.dat with the print of the contents of the arrays into which burnup.dat is read in the program.

PL1 Test Procedure:
Tested the logics of readout of the file burnup.dat by comparing with that of the former version. The format of the new file burnup.dat was slightly different. Checked, that the new file burnup.dat is read by the new invent.f.
(a) The line starting with word TITLE is skipped as needed; (b) The comments starting with ** are skipped as needed; (c) the yearofburnupdata (time 0) is read as needed; (d) bwrblend (boil water reactor blend) and pwrblend (pressure water reactor blend) are read as needed; (e) header (text) line is skipped; (f) data

values (Time, bwr, pwr) are read in a loop until the end of the file.
Noticed that there are no sufficient checks in the code of invent.f detecting errors in input data file burnup.dat. These checks will be fixed in SCR#516: (a) check in the number of all data records read, and (b) check whether the Time is increasing and each of subsequent values of bwr, pwr are decreasing.
PL1 test Results:

Saved the contents of the arrays bwr() and pwr() in the file scr483_r when burnup.dat is correct. All saved results are in the subdirectory test_results.
Tests passed.

PL2:
Name: See, how input file burnup.dat is read when its data is malformed by removal of one data value.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat malformed by removal of one data value.
Program modes to be used: NumberOfRealizations =1
Description of PL2 Test Plan:
- Objectives: See, how input file burnup.dat is read when data in it is malformed by removal of one data value.
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: burnup.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The test passes if the read-out is robust to data malformed in burnup.dat by removal of one data value.

PL2 Test Procedure and Results:
Tested to see how the data are read when the new input file burnup.dat is formed correctly vs. data in burnup.dat is malformed by removal of one data value.
Made a test bed and compared the print of the tested input file burnup.dat with the print of the contents of the arrays bwr() and pwr() comprising data read from the burnup.dat.
Data file was malformed by removal of one data value from burnup.dat.
Tested outcomes of reading the file burnup.dat when no data was missing vs. one number was erased in the file burnup.dat. When data in the file burnup.dat was corrupted (one value was missing), there was no error message printed to the screen and data in the arrays bwr() and pwr() were incorrect (the number of items was less by 1 for 1 value missing and data were shifted down by 1 from the location of the missing value).
These problems with reading malformed data files will be fixed in SCR#516. After fixing, error message should be printed and the execution stopped in case of malformed data error in data file.
Saved the test bed in invent_r.f. Saved the contents of the arrays bwr() and pwr() in the file scr483_er when burnup.dat is corrupted (one data value was missing). Saved the contents of the arrays bwr() and pwr() in the file scr483_r when burnup.dat is correct.

All saved results are in the subdirectory test_results.
Test failed.

PL3:
Name: See, how input file burnup.dat is read when its data is malformed by inserting extra dot.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat with extra dot inserted.
Program modes to be used: NumberOfRealizations =1
Description of PL3 Test Plan:
- Objectives: See, how input file burnup.dat is read when data in it is malformed by extra dot.
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: burnup.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The test passes if the read-out of burnup.dat is robust to data malformed by extra dot.

PL3 Test Procedure and Results:
Tested to see how the data are read when the new input file burnup.dat is formed correctly vs. data in burnup.dat is malformed.
Used the same test bed and compared visually the print of the tested input file burnup.dat with the print of the contents of the arrays bwr() and pwr() comprising data read from the burnup.dat.
Data file was malformed by inserting extra dot in the middle between data values in burnup.dat.
Program read the dot as value 0.0, subsequent values were shifted right by one column, and the last value in the record was lost. The read out was incorrect, no error message was printed, but the error did not affect the read out of other records.
Problems with reading malformed data files will be fixed in SCR#516. After fixing, error message should be printed and the execution stopped if malformed data error occurs.
The test bed is in file invent_r.f in \scr483\test_results\.
Test failed.

PL4:
Name: See, how input file burnup.dat is read when its data is malformed by inserting an extra non-numerical character.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat malformed by an extra non-numerical character.
Program modes to be used: NumberOfRealizations =1

Description of PL4 Test Plan:
- Objectives: See, how input file burnup.dat is read when data in it is malformed by inserting an extra non-numerical character.
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: burnup.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The test passes if the read-out is robust to data malformed in burnup.dat by inserting an extra non-numerical character

PL4 Test Procedure and Results:
Tested to see how the data are read when the new input file burnup.dat is formed correctly vs. data in burnup.dat is malformed.
Used the same test bed and compared visually the print of the tested input file burnup.dat with the print of the contents of the arrays bwr() and pwr() comprising data read from the burnup.dat.
Data file was malformed by inserting an extra non-numerical character in the middle between data values in burnup.dat. System printed error message, execution was stopped. No fix was needed.
The test bed is in file invent_r.f in \scr483\test_results\.
Test passed.

PL5:
Name: See, how input file burnup.dat is read when its data is malformed by inserting one extra digit.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat
Program modes to be used: NumberOfRealizations =1

Description of PL5 Test Plan:
- Objectives: See, how input file burnup.dat is read when data in it is malformed by inserting one extra digit.
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: burnup.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The test passes if the read-out is robust to data malformed in burnup.dat by inserting one extra digit

PL5 Test Procedure and Results:
Tested to see how the data are read when the new input file burnup.dat is formed correctly vs. data in burnup.dat is malformed.
Used the same test bed and compared visually the print of the tested input file burnup.dat with the print of the contents of the arrays bwr() and pwr() comprising data read from the burnup.dat.
Data file was malformed by inserting one extra digit in the middle between data values in burnup.dat. Program read the extra number, subsequent values were shifted right by one column, and the last value in the record was lost. The read out was incorrect, no error message was printed, but the error did not affect

the read out of other records.

Data formed correctly are read from the files without problems. Any value in a file can be incorrect, what is harder to detect than spotting a missing value. Data files must be carefully tested by hand. It can be seen how the minor tests for robustness failed for the initial code.

The readout method and the structure of burnup.dat in the new version is the same as in the old version, probably robustness of reading data from burnup.dat was not tested before.

Problems with reading malformed data files will be fixed in SCR#516. The modifications remedying the problems with reading malformed data should:

1. Test the number of values recorded in the arrays from the file, because one missing value may change all other input values, vs. one incorrect (e.g. miss-typed) value does not change other input values.
2. Test if the time values read are increasing and all the subsequent values of arrays bwr() and pwr() are decreasing.

Each problem should stop the program execution with a burnup.dat read error message.

Test failed.

PL6:

Name: Test logics of invent.f when reading data file nuclides.dat in new version TPA50w

Path of run directory of initial code: \scr483\tpa50v\

Path of run directory of modified code: \scr483\tpa50w\

Path of results: \scr483\test_results\

Special input files or modifications to input file: nuclides.dat

Program modes to be used: NumberOfRealizations =1

Description of PL6 Test Plan:

- Objectives: (a) See if the logics of the new program handles correctly the modifications in the input file nuclides.dat;
  (b) Check logics of the key changes in the invent.f.
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: nuclides.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The test passes if:

(a) The new program reads the modified file nuclides.dat correctly, and the modifications in the Fortran code accommodate to the changes in the input files in question. The correctness of the read-out should be tested by visual comparison of the printout of the input file nuclides.dat with the print of the contents of the arrays into which the read is made in the program; (b) Logics of the key modifications in the program is correct. The correctness of the logics should be tested by visually.

PL6 Test Procedure:

1. Tested the logics of inputting the modified file nuclides.dat. Compared with the previous file nuclides.dat and noticed differences. A new parameter exists:

yearofinventorydata=2033.

Practically all values in the fields CPMTU and CPMGLASS are now different because of the decay process. The number of nuclides iNuclides=57 is inputted first and then iNuclides records of data are

read. The logic of inputting data from nuclides.dat is correct.
2. Tested the logic of the new three key statements:
storetimeatemplacement = yearofemplacement - yearofinventorydata (1)
time(2) = storetimeatemplacement (2)
tyr = time + yearofemplacement - yearofburnupdata (3)
The yearofemplacement is inputted in invent.f from tpa.inp from under the name CalendarYearOfEmplacement[A.D.]=2034.
The yearofinventorydata=2033 is inputted from the file nuclides.dat.
The time(2) is the storage time at emplacement, now data is different and so time(2) no longer adjusts to the data (by subtracting 10). This adjustment is no longer valid in tpa50w and so is no longer used.
A new valuable check exists printing an error message when yearofburnupdata + time(1) > yearofemplacement (see the next two tests).
PL6 test Results:
(a) The new program reads the modified file nuclides.dat correctly, and the modifications in the Fortran code accommodate to the changes in the input files in question. The correctness of the read-out was tested by visual comparison of the printout of the input file nuclides.dat with the print of the contents of the arrays into which the read is made in the program; (b) Logics of the key modifications in the program is correct as justified above.
Saved the test bed in invent_r.f (together with the test bed for testing the readout of burnup.dat).
All saved results are in the subdirectory test_results.
Test PASSED

PL7:
Name: Test visually and by hand a new module printing an error message when
yearofburnupdata + time(1) > yearofemplacement
in new version TPA50w.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input file: nuclides.dat
Program modes to be used: NumberOfRealizations =1
Description of PL7 Test Plan:
- Objectives: Test printing an error message when yearofburnupdata + time(1) > yearofemplacement in the invent.f in new version TPA50w
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: nuclides.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The test passes if:
(a) Logics of the statement yearofburnupdata + time(1) > yearofemplacement is correct; (b) A test by hand proves that the error message is printed when yearofburnupdata + time(1) > yearofemplacement.
PL7 Test procedure:

1. Checked visually the logics of the module

```
if (yearofburnupdata + times(1) .gt. yearofemplacement) then
      print *, '***>>> Error in newinventdb <<<*** '
      print *, 'First entry in burnup.dat applies to a time'
      print *, 'greater than the emplacement time. '
      End if
```

The yearofburnupdata + time(1) > yearofemplacement is the correction for the difference between the date the waste is placed into repository and the date of the first burn-up data in the file burnup.dat. The yearofemplacement comes from tpa.inp, see the constant name CalendarYearOfEmplacement[A.D.] set to 2034. The yearofburnupdata=2033 is the first number read from the file burnup.dat. The time(1)=1 is the first time [year] read from the file burnup.dat.

2. Tested the statement

yearofburnupdata + time(1) > yearofemplacement by hand.

PL7 test Results:

Inequality: yearofburnupdata + time(1) > yearofemplacement

for: yearofburnupdata=2033, time(1)=1, yearofemplacement=2034, gives:

2033 + 1 >2034 to print the error message for the current setting of data.

Test Passed.

PL8:

Name: Test of a new module printing an error message when yearofburnupdata + time(1) > yearofemplacement in new version TPA50w

Path of run directory of initial code: \scr483\tpa50v\

Path of run directory of modified code: \scr483\tpa50w\

Path of results: \scr483\test_results\

Special input files or modifications to input file: nuclides.dat

Program modes to be used: NumberOfRealizations =1

Description of PL8 Test Plan:

- Objectives: Test printing an error message when yearofemplacement - yearofburnupdata -time(1) <0 in the invent.f in new version TPA50w
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: nuclides.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The test passes if the error message is printed only when yearofburnupdata + time(1) > yearofemplacement.

PL8 Test Procedure:

Made a test bed by changing the CalendarYearOfEmplacement[A.D.] in tpa.inp to 2033.

Got the error message and the program execution stopped as expected :

'First entry in burnup.dat applies to a time grater than the emplacement time.

. . . '

With the correct values of the arguments to yearofburnupdata + time(1) > yearofemplacement no error

message is printed, as required.

PL8 test Results:

Saved the test bed tpa.inp as tpa_er.inp. All saved results are in the subdirectory test_results.

Test passed.

PL9:

Name: Tests of robustness of invent.f when data file nuclides.dat is malformed by deleting one value.

Path of run directory of initial code: \scr483\tpa50v\

Path of run directory of modified code: \scr483\tpa50w\

Path of results: \scr483\test_results\

Special input files or modifications to input file: file nuclides.dat, one data value deleted.

Program modes to be used: NumberOfRealizations =1

Description of PL9 Test Plan:

- Objectives: See if invent.f is robust when reading data from malformed file nuclides.dat.
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: nuclides.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The tests pass if the readout is robust to data malformed by deleting one value.

PL9 Test Procedure and Results:

Tested to see how the data is read when the new input file nuclides.dat is malformed by deleting of one value under column epalim(iNucIndex) in record 4. The malformed file nuclides.dat was saved as nuclides_nr.dat.

Made a test bed (see invent_nr.f) and compared the print of the correct input file nuclides.dat with the print of the index i=iNucIndex and the contents of the arrays epalim(iNucIndex), cipermtuat10yr(iNucIndex), cipermtuat10yrglass(iNucIndex), idecaytype(iNucIndex) comprising the last 4 columns of the data read from the corrupted file nuclides_nr.dat.

No error message was printed and the results of reading were corrupted (see file scr483_nr.tst).

Formatted Fortran read statement took digits only from the strictly predefined fields ignoring even a piece of a number if it belonged to the blank field nx. Positive result was of not corrupting any other records (compare records 5 up to end of the file scr483_nr.tst with the last 4 columns of the initial file nuclides.dat).

Problems with reading malformed data files will be fixed in SCR#516. The modifications remedying the problems with reading malformed data should apply unformatted read. With this fix the program will detect the problem, then print the error message and stop the execution.

Tested also the read of the correct file nuclides.dat using the fixed code. Saved the result of reading in file scr483_n.tst. This time the read was correct (compared the output scr483_n.tst with the initial input file nuclides.dat: the data agreed).

All saved results are in the subdirectory test_results.

Test failed.

PL10:
Name: Tests of robustness of invent.f when data file nuclides.dat was malformed by inserting extra dot.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input file: nuclides.dat with extra dot inserted.
Program modes to be used: NumberOfRealizations =1
Description of PL10 Test Plan:
- Objectives: See if invent.f is robust when reading data from malformed file nuclides.dat with extra dot inserted.
- Assumptions: All code modifications are marked in the new file invent.f by scr 483.
- Input file to test: nuclides.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The tests pass if the readout is robust to data malformed by inserting extra dot.

PL10 Test Procedure and Results: Data file was malformed by inserting extra dot in the middle between data values in nuclides.dat. The malformed file nuclides.dat was saved nuclides_dot.dat.
The initial program did not read the dot, error message was printed.
Also the modified program did not read the dot, error message was printed.
Test passed.

PL11:
Name: Tests of robustness of invent.f when reading data from file nuclides.dat malformed by shifting one number one space left.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input file: nuclides.dat
Program modes to be used: NumberOfRealizations =1
Description of PL11 Test Plan:
- Objectives: See if invent.f is robust when reading data from malformed file nuclides.dat when shifting one number one space left.
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: nuclides.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The tests pass if the readout is robust to data malformed by shifting one number one space left.

PL11 Test Procedure and Results:
Data file was malformed by shifting one number left by one space in nuclides.dat (see file nuclides_f.dat, data record 4). The initial program (with formatted read statement, see file invent_0.f) has read the extra numbers. The read out was incorrect (see file scr483_f, record i=4), no error

message was printed, but the error did not affect the read out of other records.
Problems with reading malformed data files will be fixed in SCR#516. The modified program should use unformatted read statement, and should read the shifted number correctly.
Test failed.

PL12:
Name: Tests of robustness of invent.f when reading data from file nuclides.dat malformed by by inserting extra numbers.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input file: nuclides.dat malformed by by inserting extra numbers.
Program modes to be used: NumberOfRealizations =1
Description of PL12 Test Plan:
- Objectives: See if invent.f is robust when reading data from malformed file nuclides.dat by inserting extra numbers.
- Assumptions: All modifications are marked in the new file invent.f by scr 483.
- Input file to test: nuclides.dat.
- Fortran file to test: invent.f
- Pass / fail criteria: The tests pass if the readout is robust to data malformed by shifting one number one space left.

PL12 Test Procedure and Results:
Data file was malformed by inserting extra numbers between data values in nuclides.dat (see file nuclides_0.dat). The initial program (with formatted read statement, see file invent_0.f) has read the extra numbers. The read out was incorrect (see file scr483_0, record i=4), no error message was printed, but the error did not affect the read out of other records. Test failed.
Using the modified version with unformatted read (see file invent_y.f), the read out was incorrect (see file scr483_0m, record i=4), no error message was printed, and the error did not affect the read out of other records.
Problems with reading malformed data files will be fixed in SCR#516. The modified program should read each line as a string and count contiguous sequences of strings or digits.
Any value in a file can be incorrect, what is harder to detect than spotting an extra value. Data files must be carefully tested.
All saved results are in the subdirectory test_results.
Test failed.

PL13:
NAME: Duplicate results of array amolepermtu and the results totdose.res of old version using old data files.

Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat and nuclides.dat.
Program modes to be used: NumberOfRealizations =1.

Description of PL13 Test:

- Objective: See if results of array amolepermtu and the results totdose.res of old version using old data files can be duplicated on the new version test bed.
- Assumptions: All modifications are marked in the new invent.f file by scr 483.
- Output file / array to test: array amolepermtu in subroutine newinventdb().
- Fortran files to test: invent.f
- Pass / fail criteria: The test passes if:
  the results of array amolepermtu and the results totdose.res of old version using old data files can be duplicated on the new version test bed.

PL13 Test Procedure and Test Results:

Tested values in the array amolepermtu, output of subroutine allchain() called in subroutine newinventdb() in file invent.f.

(a) Prepared the test bed on the new version newinventdb() in file invent.f.

(b) Used old data from files burnup.dat and nuclides.dat in the new version tpa50w:

(i) Set yearofburnupdata in burnup.dat to 2008

(ii) Set yearofinventorydata to 2018

(iii) Replaced the new data by the old data, without touching anything above the names of fields of the data.

(c) Collected the results of array amolepermtu in the file scr483.tst of TPA50v and in the file scr483.tst of TPA50w.

Recompiled the TPA50w code. Executed and compared the two files: scr483.tst of TPA50v and scr483.tst of TPA50w.

These two files were the same. The array amolepermtu of old version using old data files can be duplicated on the new version.

(d) Compared the results totdose.res of old version to that of the new version. These two results totdose.res were the same.

Saved the file scr483.tst as scr483_v_a.tst in TPA50v and as scr483_a.tst of TPA50w.

Saved the file invent.f of TPA50v as invent_v_a.f, and file invent.f of TPA50w as invent_a.f. Saved the results totdose.res of the old version as totdose_v_a.res and of the new version as totdose_a.res.

All saved results are in the subdirectory test_results.

Test PASSED.

PL14:

NAME: Duplicate results of array amolepermtuglass of old version using old data files.
Path of run directory of initial code: \scr483\tpa50v\

Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat and nuclides.dat.
Program modes to be used: NumberOfRealizations =1.

Description of PL14 Test:

- Objective: As in the previous test, to see if results of array amolepermtuglass of old version using old data files can be duplicated on new version test bed.
- Assumptions: All modifications are marked in the new invent.f file by scr 483.
- Output file / array to test: array amolepermtuglass in subroutine newinventdb().
- Fortran files to test: invent.f
- Pass / fail criteria: The test passes if:
  the results of array amolepermtuglass of old version using old data files can be duplicated on the new version test bed.

PL14 test procedure and Test Results:

Tested array amolepermtuglass, output from another call to subroutine allchain() in subroutine newinventdb() in file invent.f.
(a) Used the test bed as above.
(b) Used old data from files burnup.dat and nuclides.dat to run the new version tpa50w with yearofburnupdata in burnup.dat set to 2008 and yearofinventorydata in nuclides.dat set to 2018.
Compared the two files: scr483.tst of TPA50v and scr483.tst of TPA50w.
These two files were the same: results of previous version were duplicated by the new version when working on the old data files.
Saved scr483.tst as scr483_v_b.tst in TPA50v and as scr483_b.tst of TPA50w.
Saved invent.f as invent_v_b.f of TPA50v and invent.f as invent_b.f of TPA50w.
All saved results are in the subdirectory test_results.
Test PASSED.

PL15:

NAME: Duplicate results of array amolepermtuat10yr of old version using old data files.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat and nuclides.dat.
Program modes to be used: NumberOfRealizations =1.

Description of PL15 Test Plan:

- Objective: As in the previous tests, to see if results of array amolepermtuat10yr of old version using old data files can be duplicated on new version test bed.
- Assumptions: All modifications are marked in the new invent.f file by scr 483.
- Output file / array to test: array amolepermtuat10yr in subroutine newinventdb().
- Fortran files to test: invent.f

- Pass / fail criteria: The test passes if:
  the results of array amolepermtuat10yr of old version using old data files can be duplicated on the new version test bed.

PL15 Test Procedure and Test Results:

Tested array amolepermtuat10yr filled with data in subroutine newinventdb() in file invent.f:
(a) Used the test bed as above.
(b) Used old data from files burnup.dat and nuclides.dat to run the new version tpa50w as before with yearofburnupdata in burnup.dat set to 2008 and yearofinventorydata in nuclides.dat set to 2018.
(c) Compared the two files: scr483.tst of TPA50v and scr483.tst of TPA50w.
These two files were the same.
Saved scr483.tst as scr483_v_c.tst of TPA50v.
Saved invent.f as invent_v_c.f of TPA50v.
Saved scr483.tst as scr483_c.tst of TPA50w
Saved invent.f as invent_c.f of TPA50w.
All saved results are in the subdirectory test_results.
Test PASSED.

PL16:

NAME: Duplicate results of array amolepermtuat10yrglass of old version using old data files.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat and nuclides.dat.
Program modes to be used: NumberOfRealizations =1.

Description of PL16 Test Plan:

- Objective: As in the previous tests, to see if results of array amolepermtuat10yrglass of old version using old data files can be duplicated on new version test bed.
- Assumptions: All modifications are marked in the new invent.f file by scr 483.
- Output file / array to test: array amolepermtuat10yrglass in subroutine newinventdb().
- Fortran files to test: invent.f
- Pass / fail criteria: The test passes if:
  the results of array amolepermtuat10yrglass of old version using old data files can be duplicated on the new version test bed.

PL16 Test Procedure and Test Results:

Tested the array amolepermtuat10yrglass filled with data in subroutine newinvent in db() file invent.f:
(a) Used the same test bed;
(b) Used old data from files burnup.dat and nuclides.dat to run the new version tpa50w as before with yearofburnupdata in burnup.dat set to 2008 and yearofinventorydata in nuclides.dat set to 2018.
(c) Compared the two files: scr483.tst of TPA50v and scr483.tst of TPA50w
These two files were the same.

Saved scr483.tst as scr483_v_d.tst of TPA50v
Saved invent.f as invent_v_d.f of TPA50v.
Saved scr483.tst as scr483_d.tst of TPA50w
Saved invent.f as invent_d.f of TPA50w.
All saved results are in the subdirectory test_results.
Test PASSED.

PL17:
NAME: Duplicate results of arrays amolepermtuatemplace, cipermtuatemplace and amolepermtuatemplaceglass of old version using old data files.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat and nuclides.dat.
Program modes to be used: NumberOfRealizations =1.
Description of PL17 Test Plan:
- Objective: As in the previous tests, to see if results of arrays amolepermtuatemplace, cipermtuatemplace and amolepermtuatemplaceglass of old version using old data files can be duplicated on new version test bed.
- Assumptions: All modifications are marked in the new invent.f file by scr 483.
- Output file / array to test: arrays amolepermtuatemplace, cipermtuatemplace and amolepermtuatemplaceglass in subroutine newinventdb().
- Fortran files to test: invent.f
- Pass / fail criteria: The test passes if:
  the results of arrays amolepermtuatemplace, cipermtuatemplace and amolepermtuatemplaceglass of old version using old data files can be duplicated on the new version test bed.

PL17 Test Procedure and Test Results:
Tested / verified arrays amolepermtuatemplace, cipermtuatemplace and amolepermtuatemplaceglass.
The arrays amolepermtuatemplace and amolepermtuatemplaceglass are the copies of amolepermtu and amolepermtuglass correspondingly which passed the testes already.
This way actually tested the array cipermtuatemplace in subroutine newinventdb() in file invent.f.
(a) Used test bed as before;.
(b) Used old data from files burnup.dat and nuclides.dat to run tpa50w as before with yearofburnupdata in burnup.dat set to 2008 and yearofinventorydata in nuclides.dat set to 2018.
(c) Compared the two files: scr483.tst of TPA50v and scr483.tst of TPA50w.
These two files were the same.
Saved scr483.tst as scr483_v_e.tst of TPA50v
Saved invent.f as invent_v_e.f of TPA50v.
Saved scr483.tst as scr483_e.tst of TPA50w

Saved invent.f as invent_e.f of TPA50w.
All saved results are in the subdirectory test_results.
Test PASSED.

PL18:
NAME: Duplicate results of function qpermtu() of old version using old data files.
Path of run directory of initial code: \scr483\tpa50v\
Path of run directory of modified code: \scr483\tpa50w\
Path of results: \scr483\test_results\
Special input files or modifications to input files: burnup.dat and nuclides.dat.
Program modes to be used: NumberOfRealizations =1.
Description of PL18 Test Plan:
- Objective: As in the previous tests, to see if results of function qpermtu() of old version using old data files can be duplicated on new version test bed.
- Assumptions: All modifications are marked in the new invent.f file by scr 483.
- Output file / array to test: function qpermtu() in subroutine newinventdb().
- Fortran files to test: invent.f
- Pass / fail criteria: The test passes if:
the results of function qpermtu() of old version using old data files can be duplicated on the new version test bed.
PL18 Test Procedure and Test Results:
Tested output of function qwp=qpermtu() returning thermal output of blended HLW in nfenv.f:
(a) Used the test bed as before.
(b) Used old data from files burnup.dat and nuclides.dat to run tpa50w as before with yearofburnupdata in burnup.dat set to 2008 and yearofinventorydata in nuclides.dat set to 2018.
Placed the write to a file 'ebs_tst.txt' of qwp when calling qwp=qpermtu() in nfenv.f both in old version tpa50v and in new version tpa50w.
Compiled and executed tpa.exe, then saved results in nfenv_tst.txt file, both in tpa50v and in new tpa50w.
(c) Compared these two outcome data files after 1st realization- they were the same.
Saved ebs_tst.txt as ebs_tst_v.txt of tpa50v.
Saved ebs_tst.txt as ebs_tst.txt of tpa50w.
Saved nfenv.f as nfenv_v.f of tpa50v.
Saved nfenv.f as nfenv.f of new tpa50w.
All saved results are in the subdirectory test_results.
Test PASSED.

SYSTEM LEVEL (SL) Tests:

SL1:

NAME: Duplicate repository temperature of old version using old data files on the modified version with the mean input parameters.

Path of run directory of initial code: \scr483\tpa50v\

Path of run directory of modified code: \scr483\tpa50w\

Path of results: \scr483\test_results\

Special input files or modifications to input files: Copied tpameans.out into tpa.inp.

Program modes to be used: NumberOfRealizations =1, OutputMode(...) = 1.

Description of SL1 Test Plan:

- Objective: As in the previous tests, to see if repository temperature of old version using old data files can be duplicated on new version tpa50w.
- Assumptions: none.
- Output file to test: file ebsrel.ech.
- Fortran files to test: all tpa.
- Pass / fail criteria: The test passes if:

the repository temperature of old version using old data files can be duplicated on the modified version.

SL1 Test Procedure and Test Results:

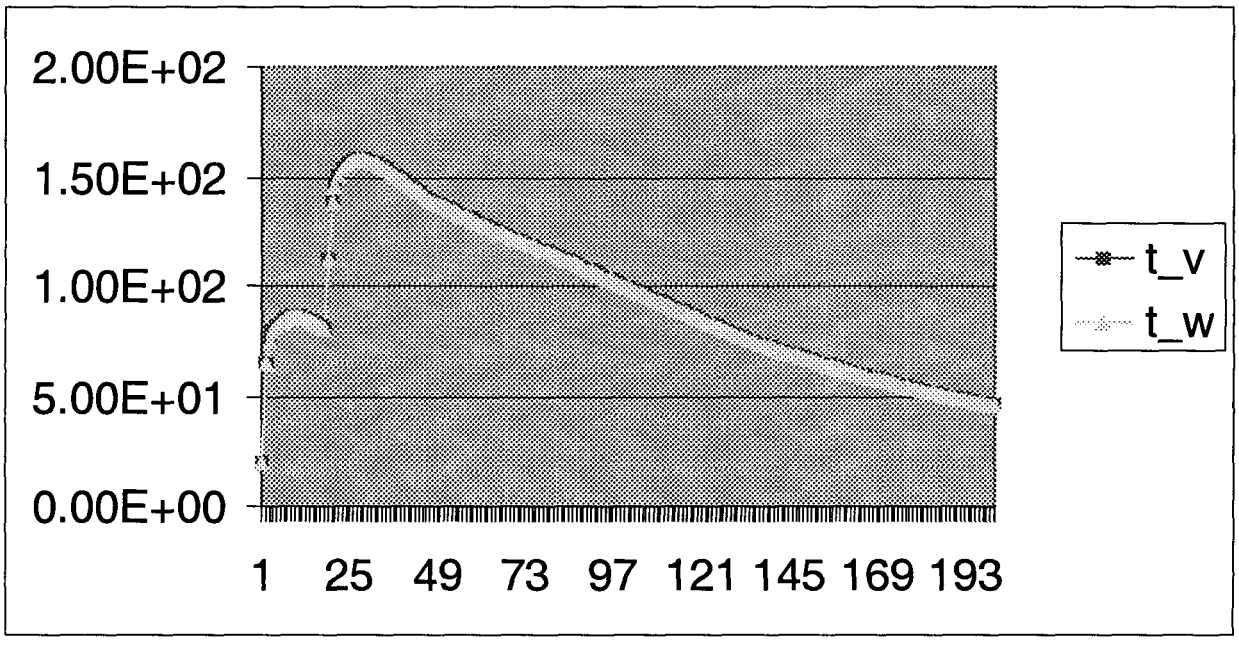
Used old data from files burnup.dat and nuclides.dat to run tpa50w as before with yearofburnupdata in burnup.dat set to 2008 and yearofinventorydata in nuclides.dat set to 2018. Set OutputMode(...) to 1 in tpa.inp in both versions tpa50v and tpa50w.

Copied tpameans.out into tpa.inp after the initial run, then executed for 1 realization, both versions tpa50v and tpa50w with the old data.

Tested output file ebsrel.ech (filled with data by exec()), column temprep for area 7, in version tpa50v and version tpa50w.

Fig. 1. Repository temperature t_v and t_w identical in the tpa50v and tpa50w

Saved ebsrel.ech as ebsrel_w.ech obtained in version tpa50w. Saved ebsrel.ech as ebsrel_v.ech obtained in version tpa50v. Saved area 7 data in temprep_v from version tpa50v, and area 7 data in temprep_w from version tpa50w. Also saved results in temp_v_w.txt file, combining results from both tpa50v and new tpa50w: in temp_v_w.txt column t_v is the repository temperature from tpa50v, and t_w is the repository temperature from tpa50w.
Tested if the temperature column temprep in versions tpa50v and tpa50w is identical.



The column temprep was identical for area 7 in both versions tpa50v and tpa50w with the mean input parameters.
Made the graph (Fig.1) to make sure that they indeed are identical.
Saved tpa.inp obtained from tpameans.out on tpa50v as tpa_v.inp (in test_results subdirectory). Saved tpa.inp obtained from tpameans.out on tpa50w as tpa_w.inp.
Test passed.

SL2:
NAME: Duplicate repository temperature of old version using old data files on the modified version with regular input parameters.

Path of run directory of initial code:	\scr483\tpa50v\
Path of run directory of modified code:	\scr483\tpa50w\
Path of results:	\scr483\test_results\

Special input files or modifications to input files: regular tpa.inp.
Program modes to be used: NumberOfRealizations =1, OutputMode(...) = 1.

Description of SL2 Test Plan:

- Objective: As in the previous tests, to see if repository temperature of old version using old data files can be duplicated on new version tpa50w.
- Assumptions: none.
- Output file to test: file ebsrel.ech.
- Fortran files to test: all tpa
- Pass / fail criteria: The test passes if:

the repository temperature of old version using old data files can be duplicated on the modified version.

SL2 Test Procedure and Test Results:

Used old data from files burnup.dat and nuclides.dat to run tpa50w as before, with yearofburnupdata in burnup.dat set to 2008 and yearofinventorydata in nuclides.dat set to 2018.
Executed for 1 realization, both version tpa50v and version tpa50w with the old data.
Tested output file ebsrel.ech (filled with data by exec()), column temprep for area 7, in version tpa50v and version tpa50w.
The column temprep was identical for area 7 in both versions tpa50v and tpa50w.
Each regular tpa.inp exists already in both versions tpa50v and tpa50w.
Test passed.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-484	**2. Software Title and Version:** TPA 5.0v	**3. Project No:** 20.06002.01.113
4. Affected Software Module(s), Description of Problem(s): *uzft.f, szft.f. nefmks.f, tpa.inp* Change the mechanism for calculating reversible colloids from a separated *tpa.inp* input file to one that can operate with the base case input file. See Attachment A.		
5. Change Requested by: D. Pickett Date: 4-14-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date:4-15-2004 R. Janetzke	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): Code in *szft.f* and *uzft.f* that used the old sampled parameters for Kds and Rds per element per layer was modied to use the new colloid retardation factor for each layer, and a new column for mass load transfer coefficient was added to the ELEMENT PROPERTIES ARRAY printed out to *nefii.inp*. New subroutines were added to *szft.f* and *uzft.f*. Kds and Rds are now modified to simulate the affect of reversibles on release and dose. *Reversibles.inp* is no longer required. *Nefmks.f* was modified to use the new mass load transfer factor in calculations. Parameters were added to and deleted from *tpa.inp*. See Attachment B for details of the code modifications and Attachment C for changes to *tpa.inp*.		
8. Implemented by: S. Painter / C. Scherer Carol S. Scherer	**Date:** 8-6-2004	
9. Description of Acceptance Tests: See attachment D.		
10. Tested by: M. Muller Michael Muller	**Date:** 8-20-2004	

CNWRA Form TOP-5 (05/2000)

Attachment A

COLLOID-FACILITATED TRANSPORT: EQUILIBRIUM SORPTION ON COLLOIDS

For that part of the heterogeneous colloid population with rapid desorption rates relative to the transport time scale, equilibrium partitioning of radionuclides among solution, colloids, and porous matrix is an adequate approximation. The effect of those colloids can be modeled using the single-component advection dispersion equation with appropriately defined transport parameters.

For the alluvium, colloid-facilitated transport has the net effect of reducing the effective retardation factor. Neglecting colloid filtration and defining a new coefficient K_0 for partitioning between colloids and solution, the advection dispersion equation becomes

$$R^{eff}\frac{\partial C}{\partial t} + \mathcal{J}C = -\lambda R^{eff} C \tag{1}$$

where $\mathcal{J}$ is the transport operator and

$$R^{eff} = \frac{R + K_0 R_c}{1 + K_0} \tag{2}$$

is the new effective retardation that takes into account the effects of colloids. Similarly, the equations describing transport in the fractured tuff become

$$R_f\frac{\partial C}{\partial t} + \mathcal{J}C = -\beta_0^{eff}(\omega C - C') - \lambda R_f C \tag{3}$$

$$R_S^{eff}\frac{\partial C'}{\partial t} = \beta_0^{eff}(\omega C - C') - \lambda R_S^{eff} C' \tag{4}$$

where

$$R_S^{eff} = \frac{R_S}{1 + K_0} \tag{5}$$

$$\beta_0^{eff} = \frac{\beta_0}{1 + K_0} \tag{6}$$

and

$$R_f = \frac{1 + R_c K_0}{1 + K_0} \tag{7}$$

Thus, equilibrium partitioning to colloids reduces the mass exchange coefficient and the immobile retardation factor, with the net effect of reducing matrix diffusion. In addition, retardation in the fractures is introduced, with retardation coefficient given by Eq. (7).

Equation 1 is in the form used by NEFTRAN in the fractured alluvium and in each of the fracture and matrix continua in the unsaturated zone. Equations 3 and 4 are in the form used by NEFTRAN in the saturated tuff. The net effect of reversible sorption to colloids is simply to modify the transport parameters.

The parameter K_0 in the equations is a dimensionless partitioning coefficient for radionuclides on colloids. Pickett and Dam (2003) following Contardi et al. (2001) write

$$K_0 = C F K_d \tag{8}$$

where C is the colloid concentration in water, F is a dimensionless factor accounting for surface area differences between matrix and colloid (equal to 590; Contardi et al. 2001), and K_d is the distribution coefficient for radionuclides on the porous matrix.

The required modifications are as follows:

(1) The colloid concentration C and the colloid retardation factor R_c should be made input parameters. Different values for each hydrostatigraphic unit are required. For the unsaturated zone, separate matrix and fracture values are needed.

(2) After the current calculation of the Kd for each unit, the new parameters defined by equations 2 and 5-8 should be calculated. Equation 2 with 8 applies to the alluvium, and to the unsaturated zone. Equations 5-8 applies to the saturated tuff.

(3) The new retardation values should be written to the NEFTRAN input file. R^{eff} defined by Equation 2 simply replaces the current retardation factor written to NEFTRAN. The same is true for the parameters defined in Equations (5) and (7). These are the element- and unit-specific values of retardation used in NEFTRAN.

(4) Element specific values of the mass transfer coefficient are not currently allowed in NEFTRAN. The parameter β_0 should be written to the NEFTRAN as before, and a new element-specific mass-transfer modification factor $\frac{1}{1 + K_0}$ should be written to the NEFTRAN input file. This modification factor is element- and unit-specific. It should be

written as a new field at the end of the input line for the element- and unit-specific retardation factors.

(5) NEFTRAN should be revised to read the new mass-transfer modification factor. The modification factor should be used in the mass-transfer calculation in NEFTRAN.

Colloids with irreversibly attached radionuclides

(6) For the fraction of radionuclides that are attached irreversibly to colloids, the new colloid retardation factor Rc should be used as the retardation factor. The separate input for retardation factors is not needed for these species and can be removed. However, the filtration factors and the irreversible fraction should still be read.

Attachment B

Modifications to Source Code

nefmks.f:

at line 141, add the following:

```
C
C SP            6/28/04 SCR484 Scott Painter
C                       added an element- and leg- dependent multiplier
C                       for the mass transfer coefficient.
C                       new arrays are XFF and AXFF
```

at line 400, add the following:

```
C-SP-6.28.04
     1 AXFF(MXPTH,MXELEM),
     1 RKI(MXPTH,MXMEM),RKIM(MXPTH,MXMEM),XFF(MXPTH,MXMEM)
```

at line 897, modify the code as follows:

```
CSP-4.28.04 SCR484
          READ(2,*) KEL, CSALL(J), LG, AKI(1,J), AKIM(1,J),
     1              AXFF(1,J)
CSP
```

at line 905, make the following modification:

```
            READ(2,*) LG, AKI(I,J), AKIM(I,J), AXFF(I,J)
```

at line 3962, modify the code as follows:

```
C-SP-6.28.04
     1 AXFF(MXPTH,MXELEM),
     1 RKI(MXPTH,MXMEM),RKIM(MXPTH,MXMEM),XFF(MXPTH,MXMEM)
```

at line 4346, modify the code as follows:

```
C-SP-6.28.04
     1 AXFF(MXPTH,MXELEM),
     1 RKI(MXPTH,MXMEM),RKIM(MXPTH,MXMEM),XFF(MXPTH,MXMEM)
```

at line 5013, make the following modifications:

```
csp  SCR484 change 1. to 0. in the error check below
csp         immobile rd less than 1 is acceptable in this model
                  IF(AKIM(M,I) .LT. 0. .AND. INCHN(J) .EQ. 0 .AND.
```

at line 5653, modify the code as follows:

```
C-SP-6.28.04
     1 AXFF(MXPTH,MXELEM),
     1 RKI(MXPTH,MXMEM),RKIM(MXPTH,MXMEM),XFF(MXPTH,MXMEM)
```

at line 5694, make the following modifications:

```
CSP-4.28.04 SCR484
          IF(IMB(K) .NE. 0) XFF(K,I) = AXFF(K,LMTX(J))
CSP
```

at line 7248, modify the code as follows:

```
C-SP-6.28.04
     1 AXFF(MXPTH,MXELEM),
     1 RKI(MXPTH,MXMEM),RKIM(MXPTH,MXMEM),XFF(MXPTH,MXMEM)
```

at line 7510, modify the code as follows:

```
     1  ' Elem.  Solubility  Leg     Mobil    Immobile  x-fer',/,
     2  ' Index   (kg/kg)     #        Rd        Rd     mult.')
CSP-4-28-04  SCR484 added write for x-fer coefficient multiplier
```

at line 7513, modify the code as follows:

```
          WRITE(6,9410) J, CSALL(J), MPATH(1), AKI(1,J),
     1                  AKIM(1,J), AXFF(1,J)
 9410     FORMAT(/,1X,I3,4X,1PE10.3,2X,I2,3X,1PE10.3,
     1             2X,1PE10.3,2X,1PE10.3)
```

at line 7516, modify the code as follows:

```
            WRITE(6,9420) MPATH(I), AKI(I,J), AKIM(I,J), AXFF(I,J)
 9420       FORMAT(20X,I2,3X,1PE10.3,2X,1PE10.3,2X,1PE10.3)
```

at line 7604, modify the code as follows:

```
C-SP-6.28.04
     1 AXFF(MXPTH,MXELEM),
     1 RKI(MXPTH,MXMEM),RKIM(MXPTH,MXMEM),XFF(MXPTH,MXMEM)
C-SP-6.28.04
```

at line 8527, make the following modification:

```
     1 AXFF(MXPTH,MXELEM),
     1 RKI(MXPTH,MXMEM),RKIM(MXPTH,MXMEM),XFF(MXPTH,MXMEM)
```

at line 8555, make the following modification:

```
CSP-4.28.04  SCR484
CSP XFF is a element-dependent modifier
CSP     for the mass transfer coefficient
            PC = XFC(I)*XFF(I,IR)*DT/PM
CSP
```

szft.f:

at line 183, make the following changes:

```
c css 8/13/2004; SCR484:  reverse order of layer names to be
c     consistent with convention used throughout code; in reality,
c     the tuff layer comes before the alluvium layer
cc        salayernam(1) = 'SAV'
cc        salayernam(2) = 'STFF'
        salayernam(1) = 'STFF'
        salayernam(2) = 'SAV'
```

at line 216, make the following changes:

```
        ilayer=2
```

at line 220, make the following changes:

```
           fname= 'AlluviumMatrixRD_'//salayernam(2)(1:3)//'_'//
```

at line 221, make the following changes:

```
           iradelemkown(i,2)= iaddconsmv( fname )
           iradelemkd(i,2)  = imvquery( fname )
           call clearchar( 60, fname )
           fname= 'ImmobileRD_'//salayernam(1)(1:4)//'_'//radelems(i)
```

at line 225, make the following changes:

```
           fname='FractureRD_'//salayernam(1)(1:4)//'_'//radelems(i)
           iradelemfown(i,1)= iaddconsmv( fname )
           iradelemfr(i,1)  = imvquery( fname )
```

at line 255, make the following changes:

```
c css  8/13/2004; SCR484:  use standard TPA convention where
c      layer 1 = tuff (STFF) and layer 2 = alluvium (SAV)
ccc           Set the matrix Rds by layer (1=SAV,2=STFF).
c            Set the matrix Rds by layer (1=STFF,2=SAV).
```

at line 271, modify the code as follows:

```
c
c css  8-13-2004; SCR484:   use standard TPA convention where
c      layer 1 = tuff (STFF) and layer 2= alluvium (SAV)
ccc        Set the fracture Rds by layer(2=STFF).
cc         ilayer   = 2
         ilayer   = 1

comment out the following code at line 232:
c
c css - 7/19/2004; SCR484:  remove code that isn't used
c        call clearchar( 60, fname )
c        fname = 'IrreversibleColloidModel[0=no,1=yes]'
c        i_colloidmodel = ispquery(fname)
c        icollmod = ivaluesp(i_colloidmodel)
c end change: SCR484

at line 608, add the following new variables:
c css - 7/20/2004; SCR484:  allow for reversible colloids
c       declare new variables for mass transfer modification factors
c
      double precision xfermod(maxiso,maxlyr)
```

```
      double precision xfermodmix(maxiso)
c end change:  SCR484
```

at line 848, make the following modification:

```
c css - 7/15/2004; SCR484:  allow for reversibles;
c       remove FractureRD for J-species elements; use
c       ColloidRetardationFactor_ for layer instead
        if (elemnam(1:1) .eq. 'J') then
            spname = 'FractureColloidRetardationFactor_' //
     &         mixsalayernam(1:4) // '[m3/kg]'
         else
            spname='FractureRD_'//mixsalayernam(1:4)//elemnam
         end if
cc      Each spname section must get its own rd value.
c end change:  SCR484
```

at line 858, add the following comment and modify code as follows:

```
c
c css - 7/15/2004; SCR484:  allow for reversibles
c       remove AlluviumMatrix_RDLog10_ and FractureRDLog10_
c       sampled parameters (per element) and replace with
c       ColloidRetardationFactor_SAV & ColloidRetardationFactor_STFF
c       don't need to convert from Log10 anymore
c             spname = 'AlluviumMatrixRDLog10_' // mixsalayernam(1:3) //
c     &                '_' // elemnam
              spname = 'ColloidRetardationFactor_SAV_[m3/kg]'
.
.
.
c             spname='FractureRDLog10_'//mixsalayernam(1:4)//'_'//elemnam
              spname = 'ColloidRetardationFactor_STFF[m3/kg]'
.
.
.
c           rdmix(idelm(nelm)) = 10.d0**rdmix(idelm(nelm))
c end change:  SCR484
```

at line 899, add the following comment and modify code as follows:

```
c
c css - 7/15/2004; SCR484:  allow for reversibles
c       remove AlluviumMatrix_RDLog10_ and FractureRDLog10_
c       sampled parameters (per element) and replace with
c       ColloidRetardationFactor_SAV & ColloidRetardationFactor_STFF
c       don't need to convert from Log10 anymore
.
.
.
c           spname = 'AlluviumMatrixRDLog10_' // szsalayernam(k)(1:3) //
c     &               '_' // elemnam
            spname = 'ColloidRetardationFactor_' // szsalayernam(k)(1:3)
     &               // '_[m3/kg]'
.
.
.
c           spname='FractureRDLog10_'//szsalayernam(k)(1:3)//'_'//elemnam
            spname = 'ColloidRetardationFactor_' // szsalayernam(k)(1:3)
     &               // '_[m3/kg]'
.
.
.
c           spname='FractureRDLog10_'//szsalayernam(k)(1:4)//'_'//elemnam
            spname = 'ColloidRetardationFactor_' // szsalayernam(k)(1:4)
     &              // '[m3/kg]'
.
.
.
c           rd(idelm(nelm),k) = 10.d0**rd(idelm(nelm),k)
```

```
c end change:  SCR484
```

at line 947, modify the code as follows:

```
c css  8/5/2004; SCR484:  modify rds to simulate effect of reversibles
c      ImmobileRDLog10_STFF_Ja, Jc, Jp, and Jt values no longer necessary;
c      sampled parameters deleted from tpa.inp; set to 1.0d0
cc           spname='ImmobileRDLog10_'//szsalayernam(k)(1:4)//'_'//elemnam
cc           rdi(idelm(nelm),k) = valuesp(ispquery( spname ))
           rdi(idelm(nelm),k) = 1.0d0
cc           rdi(idelm(nelm),k) = 10.d0**rdi(idelm(nelm),k)
c end change:  SCR484
```

modify line 1569 as follows:

```
c
c css - 7/15/2004; SCR484:  include irreversibles
c       add column for Mass Transfer Modification Factor
c
```

modify lines 1572,1573 as follows:

```
      write(i3,'(a)') 'ELEM.    SOLUBILITY    LEG   MOBIL RD       ' //
     &                'IMMOBILE RD       ' //
     &                'MASS XFER'
c end change:  SCR484
```

modify lines 1575,1576 as follows:

```
      write(i3,'(a)') 'INDEX      (KG/KG)      #                    ' //
     &                '                  ' //
     &                'MOD FACTOR'

1641,1650d1597

c css - 7/15/2004; SCR484:  allow for reversible colloids
c       call routine to modify rds to approximate the effect of
c          reversible colloids
c       need to modify rd, rdi and rdmix; rdimix values are already
c          set to 1.0d0
c       add column for Mass Transfer Modification Factor
          call mod_rdrdi(elementlist,maxiso,maxlyr,maxnumelem,numelm,
     &                   rd,rdi,rdmix,xfermod,xfermodmix)
```

at line 1603, modify the code as follows:

```
          if (kk .eq. 1) then
             write(i3,'(i5,3x,e10.3,2x,i5,3x,e10.3,5x,e10.3,8x,
     &            e10.3)') ii,0.0, kk, rdmix(ii),rdimix(ii),
     &            xfermodmix(ii)
             write(i3,'(8x,10x,2x,i5,3x,e10.3,5x,e10.3,8x,e10.3)')
     &            kk+1, rd(ii,kk),rdi(ii,kk), xfermod(ii,kk)
          else
             write(i3,'(8x,10x,2x,i5,3x,e10.3,5x,e10.3,8x,e10.3)')
     &            kk+1, rd(ii,kk),rdi(ii,kk), xfermod(ii,kk)
          endif
c end change:  SCR484
```

after line 3034, add the new subroutine mod_rdrdi

add new include file, *mod_rdrdi.h*:

uzft:

add at line 62:

```
c                 subroutine mod_kd
```

at line 1123, add the following:

```
c     rdmod              = holds rd to be modified to allow for
c                          reversible colloids
```

at line 1271, add the following:

```
c css 7/22/2004; SCR484:  allow for reversible colloids;
c     add variable to hold rd to be modified to allow for
c     reversible colloids
      double precision rdmod
c end change:  SCR484
```

at line 1516, modify the code as follows:

```
c css 7/22/2004; SCR484:  allow for reversible colloids;
c     for J-species colloids, use layer-specific colloid
c     retardation factor (Rd) instead of layer-element-specific
c     KD
            if (elemnam(1:1) .eq. 'J') then
               spname = 'MatrixColloidRetardationFactor_' //
     &            salayernam(k)(1:4) // '[m3/kg]'
            else
               if (elemnam(2:2) .eq. ' ') then
                 spname = 'MatrixKD_' // salayernam(k)(1:4) //
     &              elemnam(1:1) // '[m3/kg]'
               else
                 spname = 'MatrixKD_' // salayernam(k)(1:4) //
     &              elemnam // '[m3/kg]'
               endif
            end if
            if (ireflag.ne.0) then
               kd(idelm(nelm),k,1) = valueconsmv(imvquery( spname ))
            else
               kd(idelm(nelm),k,1) = valuesp(ispquery( spname ))
            endif
c end change:  SCR484
```

at line 1534, modify the code as follows:

```
c css 7/22/2004; SCR484:  allow for reversible colloids;
c     for J-species colloids, use layer-specific colloid
c     retardation factor (Rd) instead of layer-element-specific
c     RD
            if (elemnam(1:1) .eq. 'J') then
               spname = 'FractureColloidRetardationFactor_' //
     &            salayernam(k)(1:4) // '[m3/kg]'
            else
               spname='FractureRD_'//salayernam(k)(1:4)//elemnam
            endif
            if (ireflag.ne.0) then
               kd(idelm(nelm),k,2) = valueconsmv(imvquery( spname ))
            else
               kd(idelm(nelm),k,2) = valuesp(ispquery( spname ))
            end if
c end change:  SCR484
```

at line 2128, modify the code as follows:

```
c
c css - 7/12/04; SCR484:  incorporate reversibles; modify kds/rds
c       modify array kd before values are written to nefii.inp
c            DO 505 II=1,numelm
c               IF (media .eq. 1) THEN
c                  BDENSE=GDENSE(LAYUNS,MEDIA)*(1.0 - POR(LAYUNS,MEDIA))
c                  NEFRD(II,INC) = 1.0 + BDENSE*KD(II,LAYUNS,MEDIA)/
c     &                            POR(LAYUNS,MEDIA)
c               ELSE
c                  nefrd(ii,inc) = kd(ii,layuns,media)
c               END IF
c  505       CONTINUE

            DO 505 II=1,numelm
               IF (media .eq. 1) THEN
c convert to Rd if still Kd; J-species colloids are already in Rd form
                  if (elementlist(ii)(1:1) .ne. 'J') then
                     BDENSE = GDENSE(LAYUNS,MEDIA)*(1.0 -
     &                        POR(LAYUNS,MEDIA))
                     rdmod  = 1.0 + BDENSE*KD(II,LAYUNS,MEDIA)/
     &                        POR(LAYUNS,MEDIA)
                  else
                     rdmod = kd(ii,layuns,media)
                  end if
               ELSE
                  rdmod = kd(ii,layuns,media)
               END IF
c J-species colloids (irreversible colloids) are not affected by
c modification for reversible colloids
               if (elementlist(ii)(1:1) .ne. 'J') then
                  call mod_kd(salayernam(layuns), elementlist(ii),
     &               media, kd(ii,layuns,media), rdmod)
               end if
               NEFRD(II,INC) = rdmod
```

at line 2131, modify the code as follows:

```
c convert to Rd if still Kd; J-species colloids are already in Rd form
                  if (elementlist(ii)(1:1) .ne. 'J') then
                     BDENSE = GDENSE(LAYUNS,MEDIA)*(1.0 -
     &                        POR(LAYUNS,MEDIA))
                     rdmod  = 1.0 + BDENSE*KD(II,LAYUNS,MEDIA)/
     &                        POR(LAYUNS,MEDIA)
                  end if
                  BDENSE=GDENSE(LAYUNS,MEDIA)*(1.0 - POR(LAYUNS,MEDIA))
                  NEFRD(II,INC) = 1.0 + BDENSE*KD(II,LAYUNS,MEDIA)/
     &                           POR(LAYUNS,MEDIA)
```

modify line 2135 as follows:

```
                  rdmod = kd(ii,layuns,media)
```

add the following code at line 2136:

```
c J-species colloids (irreversible colloids) are not affected by
c modification for reversible colloids
               if (elementlist(ii)(1:1) .ne. 'J') then
                  call mod_kd(salayernam(layuns), elementlist(ii),
     &               media, kd(ii,layuns,media), rdmod)
               end if
               NEFRD(II,INC) = rdmod
c end change:  SCR484
```

at line 2473, add the following:

```
c
c css - 12/13/04; SCR484:  allow for reversible colloids
c       add extra column to nefii.inp
```

at line 2551, modify the code as follows:

```
     &                 'IMMOBILE RD        ' //
     &                 'MASS XFER'
```

at line 2477, modify the code as follows:

```
      WRITE(i3,'(A)') 'INDEX      (KG/KG)      #                    '//
     &                '                   ' //
     &                'MOD FACTOR'
```

at line 2481, modify the code as follows:

```
         DO 903 KK=1,NEFLEG
            IF (KK .EQ. 1) THEN
               WRITE(i3,'(I5,3X,E10.3,2X,I5,3X,E10.3,5X,E10.3,8X,
     &               E10.3)') II, 0.0,KK, NEFRD(II,KK),0.0, 0.0
               WRITE(i3,'(8X,10X,2X,I5,3X,E10.3,5X,E10.3,8X,E10.3)')
     &               KK+1, NEFRD(II,KK), 0.0, 0.0
            ELSE
                WRITE(i3,'(8X,10X,2X,I5,3X,E10.3,5X,E10.3,8X,E10.3)')
     &                KK+1, NEFRD(II,KK), 0.0, 0.0
            ENDIF
c end change: SCR484
```

after line 3973, add the new subroutine mod_kd

add new include file *mod_kd.h*

Attachment C

UPDATE REQUIREMENTS for *TPA.INP*

Status (Add, Delete, Modify To, Modify From)	**Module**	**Parameter Name**	**Description** **1.** definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)	**Distribution**	**Range**	**Justification** **1.** cite references **2.** is uncertainty covered by distribution/range? **3.** why this range/distribution vs. other possible values/ methods/distributions	**Source** (Initials)
Delete	UZFT	MatrixKD_TSw_Ja[m3/kg]		constant	0.0	replaced by level-specific colloid retardation factors per SCR484	SLP
Delete	UZFT	MatrixKD_CHnvJa[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_CHnzJa[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_PPw_Ja[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_UCF_Ja[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_BFw_Ja[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_UFZ_Ja[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_TSw_Jc[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_CHnvJc[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_CHnzJc[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_PPw_Jc[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_UCF_Jc[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_BFw_Jc[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_UFZ_Jc[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_TSw_Jp[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_CHnvJp[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_CHnzJp[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_PPw_Jp[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_UCF_Jp[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_BFw_Jp[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_UFZ_Jp[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_TSw_Jt[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_CHnvJt[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_CHnzJt[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_PPw_Jt[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_UCF_Jt[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_BFw_Jt[m3/kg]		constant	0.0	"	SLP
Delete	UZFT	MatrixKD_UFZ_Jt[m3/kg]		constant	0.0	"	SLP

Delete	UZFT	FractureRD_TSw_Ja[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_CHnvJa[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_CHnzJa[m3/kg]		constant	1.0	"	PSLP
Delete	UZFT	FractureRD_PPw_Ja[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_UCF_Ja[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_BFw_Ja[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_UFZ_Ja[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_TSw_Jc[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_CHnvJc[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_CHnzJc[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_PPw_Jc[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_UCF_Jc[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_BFw_Jc[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_UFZ_Jc[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_TSw_Jp[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_CHnvJp[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_CHnzJp[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_PPw_Jp[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_UCF_Jp[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_BFw_Jp[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_UFZ_Jp[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_TSw_Jt[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_CHnvJt[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_CHnzJt[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_PPw_Jt[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_UCF_Jt[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_BFw_Jt[m3/kg]		constant	1.0	"	SLP
Delete	UZFT	FractureRD_UFZ_Jt[m3/kg]		constant	1.0	"	SLP
Delete	SZFT	FractureRDLog10_STFF_Ja		usersuppliedpwis ecdf	6 0.025308, 0.0 0.04139, 0.039 0.77815, 0.08125 2.0, 0.2605 2.4472, 0.7605 2.9031, 1.0	"SLP	

Delete	SZFT	FractureRDLog10_STFF_Jc		usersuppliedpwis ecdf	"	"	SLP
Delete	SZFT	FractureRDLog10_STFF_Jp		usersuppliedpwis ecdf	"	"	SLP
Delete	SZFT	FractureRDLog10_STFF_Jt		usersuppliedpwis ecdf	"	"	SLP
Delete	SZFT	AlluviumMatrixRDLog10_S AV_Ja		usersuppliedpwis ecdf	10 0.01, 0.0 0.1273, 0.1933 0.38086, 0.3088 1.3958, 0.5311 2.556, 0.7432 3.013, 0.8244 3.5105, 0.9047 3.9989, 0.9655 4.8795, 0.9978 6.3624, 1.0	"SLP	
Delete	SZFT	AlluviumMatrixRDLog10_S AV_Jc		usersuppliedpwis ecdf	"	"	SLP
Delete	SZFT	AlluviumMatrixRDLog10_S AV_Jp		usersuppliedpwis ecdf	"	"	SLP
Delete	SZFT	AlluviumMatrixRDLog10_S AV_Jt		usersuppliedpwis ecdf	"	"	SLP
Delete	SZFT	ImmobileRDLog10_STFF_Ja		usersuppliedpwis ecdf	6 0.025308, 0.0 0.04139, 0.039 0.77815, 0.08125 2.0, 0.2605 2.4472, 0.7605	removed per SCR484	SLP

					2.9031, 1.0		
Delete	SZFT	ImmobileRDLog10_STFF_Jc		usersuppliedpwis ecdf	"	"	SLP
Delete	SZFT	ImmobileRDLog10_STFF_Jp		usersuppliedpwis ecdf	"	"	SLP
Delete	SZFT	ImmobileRDLog10_STFF_Jt		usersuppliedpwis ecdf	"	"	SLP
Add	UZFT	SurfaceAreaFactor_TSw_[]	Ratio of colloid to formation surface area.	constant	590	added per SCR484 1. Contardi et al. 2001. 2. Parameter is fairly well-constrained. 3. Dervied using site-specific data.	DAP, SLP
Add	UZFT	SurfaceAreaFactor_CHnv[]	"	constant	590	"	DAP,
Add	UZFT	SurfaceAreaFactor_CHnz[]	"	constant	590	"	DAP,
Add	UZFT	SurfaceAreaFactor_PPw_[]	"	constant	590	"	DAP,
Add	UZFT	SurfaceAreaFactor_UCF_[]	"	constant	590	"	DAP,
Add	UZFT	SurfaceAreaFactor_BFw_[]	"	constant	590	"	DAP,
Add	UZFT	SurfaceAreaFactor_UFZ_[]	"	constant	590	"	DAP,
Add	UZFT	FractureColloidRetardationF actor_TSw_[]	Retardation factor for colloids.	usersuppliedpwis ecdf	15 1.0, 0.0 1.01, 0.01 1.5, 0.04 2.0, 0.06 4.0, 0.12 6.0, 0.15 10.23, 0.25 14.86, 0.35 26.00, 0.5 34.35, 0.60 45.39, 0.70 59.98, 0.80 219.0, 0.90 418.6, 0.95 800.0, 1.00	Modified from DOE distribution (ANL-NBS-HS-000031 Rev 1, Table 7) Linearly interpolated in Log space between tabulated values and with DOE truncation removed. Presumes 1% are unretarded.	DAP, SLP
Add	UZFT	FractureColloidRetardationF actor_CHnv[]	"	usersuppliedpwis ecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidRetardationF	"	usersuppliedpwis	"	"	DAP,

		actor_CHnz[]		ecdf			SLP
Add	UZFT	FractureColloidRetardationFactor_PPw_[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidRetardationFactor_UCF_[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidRetardationFactor_BFw_[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidRetardationFactor_UFZ_[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	MatrixColloidRetardationFactor_TSw_[]	"	usersuppliedpwisecdf	20 1.0, 0.0 1.01, 0.01 1.50, 0.07 2.0, 0.12 4.0, 0.22 6.0, 0.29 8.0, 0.33 14.4, 0.4 22.14, 0.45 34.0, 0.5 56.15, 0.55 92.85, 0.6 153.5, 0.65 253.9, 0.7 419.7, 0.75 694.0, 0.8 1148, 0.85 1897, 0.9 3138, 0.95 5188.0, 1.0	Modified from DOE distribution ANL-NBS-HS-000031 Rev 1, Table 8. Linearly interpolated in Log space between tabulated values and with DOE truncation removed. Presumes 1% are unretarded.	DAP, SLP
Add	UZFT	MatrixColloidRetardationFactor_CHnv[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	MatrixColloidRetardationFactor_CHnz[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	MatrixColloidRetardationFactor_PPw_[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	MatrixColloidRetardationFactor_UCF_[]	"	usersuppliedpwisecdf	"	"	DAP, SLP

Add	UZFT	MatrixColloidRetardationFactor_BFw_[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	MatrixColloidRetardationFactor_UFZ_[]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidConcentration_TSw_[kg/m3]	Colloid Concentration	usersuppliedpwisecdf	16 1.0e-6, 0.0 2.51e-6, 0.1 6.31e-6, 0.2 1.58e-5, 0.3 3.98e-5, 0.4 1.0e-4, 0.5 2.51e-4, 0.6 6.31e-4, 0.7 1.0e-3, 0.75 2.15e-3, 0.8 4.64e-3, 0.85 1.0e-2, 0.9 2.24e-2, 0.94 5.0e-2., 0.98 0.1, 0.99 0.2, 1.	MDL-EBS-PA-000004 Rev 0, Table 5, linearly interpolated in log space. Best available information.	DAP, SLP
Add	UZFT	FractureColloidConcentration_CHnv[kg/m3]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidConcentration_Chnz[kg/m3]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidConcentration_PPw_[kg/m3]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidConcentration_UCF_[kg/m3]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidConcentration_BFw_[kg/m3]	"	usersuppliedpwisecdf	"	"	DAP, SLP
Add	UZFT	FractureColloidConcentration_UFZ_[kg/m3]	"	usersuppliedpwisecdf	"	"	DAP, SLP

Add	UZFT	MatrixColloidConcentration_TSw_[kg/m3]	"	usersuppliedpwisecdf	16 1.6e-7, 0.0 3.02e-7, 0.1 1.01e-6, 0.2 2.53e-6, 0.3 6.37e-6, 0.4 1.60e-5, 0.5 4.02e-5, 0.6 1.01e-4, 0.7 1.6e-4, 0.75 3.44e-4, 0.8 7.42e-4, 0.85 1.6e-3, 0.9 3.58e-3, 0.94 8.0e-3, 0.98 0.016, 0.99 0.032, 1.	MDL-EBS-PA-000004 Rev 0, Table 5 after scaling by a filtration factor. See scientific notebook 133, pages 85 to 90	DAP, SLP
Add	UZFT	MatrixColloidConcentration_CHnv[kg/m3]	"	usersuppliedpwisecdf	16 3.1e-7, 0.0 7.78e-7, 0.1 1.96e-6, 0.2 4.99e-6, 0.3 1.23e-5, 0.4 3.1e-5, 0.5 7.78e-5, 0.6 1.96e-4, 0.7 3.1e-4, 0.75 6.66e-4, 0.8 1.44e-4, 0.85 3.1e-3, 0.9 6.94e-3, 0.94 1.55e-2., 0.98 0.031, 0.99 0.062, 1.	"	DAP, SLP

Add	UZFT	MatrixColloidConcentration_ Chnz[kg/m3]	"	usersuppliedpwis ecdf	16 1.1e-7, 0.0 2.768e-7, 0.1 6.94e-7, 0.2 1.74e-6, 0.3 4.38e-6, 0.4 1.1e-5, 0.5 2.76e-5, 0.6 6.94e-5, 0.7 1.1e-4, 0.75 2.37e-4, 0.8 5.10e-4, 0.85 1.1e-3, 0.9 2.46e-3, 0.94 5.5e-3, 0.98	"	DAP, SLP
Add	UZFT	MatrixColloidConcentration_ PPw_[kg/m3]	"	usersuppliedpwis ecdf	16 4.1e-7, 0.0 1.03e-6, 0.1 2.59e-6, 0.2 6.48e-6, 0.3 1.63e-5, 0.4 4.1e-5, 0.5 1.03e-4, 0.6 2.59e-4, 0.7 4.1e-4, 0.75 8.81e-4, 0.8 1.90e-3, 0.85 4.1e-3, 0.9 9.18e-3, 0.94 2.05e-2, 0.98 0.041, 0.99	"	DAP, SLP

Add	UZFT	MatrixColloidConcentration_ UCF_[kg/m3]	"	usersuppliedpwis ecdf	16 3.3e-7, 0.0 8.28e-7, 0.1 2.08e-6, 0.2 5.21e-6, 0.3 1.31e-5, 0.4 3.3e-5, 0.5 8.28e-5, 0.6 2.08e-4, 0.7 3.3e-4, 0.75 7.09e-4, 0.8 1.53e-3, 0.85 3.3e-3, 0.9 7.39e-3, 0.94 0.0165, 0.98 0.033, 0.99 0.066, 1.	"	DAP, SLP
Add	UZFT	MatrixColloidConcentration_ BFw_[kg/m3]	"	usersuppliedpwis ecdf	16 7.1e-8, 0.0 1.78e-7, 0.1 4.48e-7, 0.2 1.122e-6, 0.3 2.82e-6, 0.4 7.1e-6, 0.5 1.78e-5, 0.6 4.48e-5, 0.7 7.1e-5, 0.75 1.53e-4, 0.8 3.29e-4, 0.85 7.1e-4, 0.9 1.59e-3, 0.94 3.55e-3, 0.98	"	DAP, SLP
Add	UZFT	MatrixColloidConcentration_	constant	0	not used in		
Add	SZFT	SurfaceAreaFactor_SAV_[]	Ratio of colloid to formation surface area.	constant	590	added per SCR484 1. Contardi et al. 2001. 2. Parameter is fairly well-constrained. 3. Dervied using site-specific data.	DAP, SLP

Add	SZFT	SurfaceAreaFactor_STFF[]	"	constant	590	added per SCR484 1. Contardi et al. 2001. 2. Parameter is fairly well-constrained. 3. Dervied using site-specific data.	DAP, SLP
Add	SZFT	ColloidRetardationFactor_SAV_[]	Colloid Retardation factor in Alluvium.	usersuppliedpwisecdf	20 1.0, 0.0 1.01, 0.01 1.50, 0.07 2.0, 0.12 4.0, 0.22 6.0, 0.29 8.0, 0.33 14.4, 0.4 22.14, 0.45 34.0, 0.5 56.15, 0.55 92.85, 0.6 153.5, 0.65 253.9, 0.7 419.7, 0.75 694.0, 0.8 1148, 0.85 1897, 0.9 3138, 0.95 5188.0, 1.0	Modified from DOE distribution (ANL-NBS-HS-000031 Rev 1, Table 7) Linearly interpolated in Log space between tabulated values and with DOE truncation removed. Presumes 1% are unretarded.	DAP, SLP

Add	SZFT	ColloidRetardationFactor_STFF[]	Colloid Retardation factor in fractures in the fractured volcanic leg of saturated zone.	usersuppliedpwisecdf	15 1.0, 0.0 1.01, 0.01 1.5, 0.04 2.0, 0.06 4.0, 0.12 6.0, 0.15 10.23, 0.25 14.86, 0.35 26.00, 0.5 34.35, 0.60 45.39, 0.70 59.98, 0.80 219.0, 0.90 418.6, 0.95 800.0, 1.00	odified from DOE distribution ANL-NBS-HS-000031 Rev 1, Table 8. Linearly interpolated in Log space between tabulated values and with DOE truncation removed. Presumes 1% are unretarded.	DAP, SLP
Add	SZFT	ColloidConcentration_SAV_[kg/m3]	Colloid concentration in alluvium.	usersuppliedpwisecdf	16 1.0e-6, 0.0 2.51e-6, 0.1 6.31e-6, 0.2 1.58e-5, 0.3 3.98e-5, 0.4 1.0e-4, 0.5 2.51e-4, 0.6 6.31e-4,	MDL-EBS-PA-000004 Rev 0, Table 5, linearly interpolated in log space. Best available information.	DAP, SLP
Add	SZFT	ColloidConcentration_STFF[kg/m3]	Colloid concentration in fractures the factured volcanic leg of the saturated zone.	usersuppliedpwisecdf	"	"	DAP, SLP

Attachment D

Test Plan for TPA SCR484

Tested By: Michael Muller Date: Aug 20, 2004
Host Machine: spock Host OS: Solaris
Baseline Version: TPA 5.0v Test Version: TPA 5.0v with SCR mods.

Process Level (PL) Tests

PL-1. Name: proclevl1
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/proclevl1
Environment variables: TPA_DATA=. TPA_TEST=.
Special input files or modifications to input files required: none.
Special diagnostic code modifications required: none.
Program modes to be used (append flags, scenario/model switches,etc.):
NumberOfRealizations: 3
Utility scripts needed to perform the test: none
Utility codes needed in the analysis of the test data: none
Test description:
objective: The 'mass-transfer modification factor' (1/1+Ko), by definition, is only used for SZ
and fractured TUFF. Test the code to see that this occurs.
assumptions: This code does not affect UZ so only SZ tested.
constraints: none.
output files to compare/examine: nefiisz.inp
procedure to be used:
note changes to nefmks.f (IMB controls whether or not (1/1+Ko) is used). See the lines:

```
5714:    IF(IMB(K) .NE. 0) XFF(K,I) = AXFF(K,LMTX(J))
```

and unchanged:

```
8582:    IF(IMB(I) .NE. 0) THEN
8588:      PC = XFC(I)*XFF(I,IR)*DT/PM
```

SO: if IMB = 0, then calculations NOT used. If IMB ≠ 0, then calculations are used.
Run tpa50v+scr489 and look at nefiisz.inp. See if IMB number for leg 2 (TUFF) is NOT 0 and
IMB number for leg3 (ALUV) is 0. This is under part: 'MIGRATION PATH PROPERTIES
ARRAY', subheader: DIFFUS
Pass/fail criteria: A successful test has IMB of leg 2 ≠ 0 and IMB of leg 3 = 0.
Overall test status: PASS

PL-2. Name: proclevl2
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/proclevl2
Environment variables: TPA_DATA=. TPA_TEST=.
Special input files or modifications to input files required:
For TPA50v, add 4 dummy sampled parameters.
For TPA50v+scr484, Set colloid concentration (C) to 0 in tpa.inp.
Special diagnostic code modifications required: none
Program modes to be used (append flags, scenario/model switches,etc.):
NumberOfRealizations: 3
Utility scripts needed to perform the test: none
Utility codes needed in the analysis of the test data: none
Test description:
objective: By setting C=0, Ko=(CFKd)=0 and so all factors with Ko are 0
which gives a New Retardation = to the original TPA 5.0v retardation.
assumptions: SCR484 code modifications do not significantly alter retardation factors from
the original TPA 5.0v base.
constraints: Many parameters have been deleted and some have been added
that change the retardation factors. So, one cannot expect
that the factors will remain completely unchanged.
There are 381 sampled parameters in tpa50v and there are 385
in tpa50v+scr484+testtpa.inp. So needed to add 4 dummy params to
tpa50v to get the same same values for sampled parameters for the majority
of the parameters.
output files to compare/examine: nefii.inp
procedure to be used:
Run tpa50v and tpa50v+mods. compare output from nefii.inp files.
Pass/fail criteria: somewhat subjective: For success, values in nefii.inp should be very similar.
Overall test status: PASS

System Level (SL) Tests:

SL-1. syslevl1
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/syslevl1
Environment variables: TPA_DATA=. TPA_TEST=.
Test description:
objective:
Short run to see if program runs to successful completion and final peak mean dose is reasonable.
procedure to be used:
Run TPA50v for 3 realizations to get 'success' and dose from screen output.
Run TPA50v+scr484 for 3 realizations.
Look at end of screen output from both runs.
Pass/fail criteria: For success: 1) Must get line with 'success' at end of program run.
2) Final dose must be within an order of magnitude of TPA50v.

Overall test status: PASS

SL-2. syslevl2
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/syslevl2
Environment variables: TPA_DATA=. TPA_TEST=.
Test description:
procedure to be used:
Run TPA50v+scr484 for 25Kyears and 403 realizations.
objective: To run a long run with many years and realizations to successful completion. The values picked are mostly arbitrary (ie. 50K yrs and 500 realizations could be used just as well but would take longer to run).
assumptions: 25K years is a sufficiently long time and 403 realizations is sufficiently long and is more than 400 parameters to get correlation.
Pass/fail criteria: For success: 1) Must get line with 'success' at end of program run. 2) Final dose must be within an order of magnitude of TPA50v.

Overall test status: FAIL

Retest with: 10Kyears and 403 realizations.: FAIL

Reason: NEFTRAN cannot take the values fed to it. Array size too large.

Comment: SCR 518 was generated from this information.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-485	**2. Software Title and Version:** TPA 5.0s	**3. Project No:** 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): exec.f, releaset.f

A problem occurred while running the tpamin.out and tpamax.out files as tpa.inp. Failed WPs that should have been reported as due to bathtub model were listed as flowthrough in relfrac.out and ebsrel.rlt. Also, some values in wpfillstats.out were listed as NaN. The IEEE Invalid Operation flag was raised during execution and seemed to be related to a divide by zero at line 3538 of exec.f.

5. Change Requested by: C. Scherer Date: 5-6-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 5-6-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

In *exec.f*, an IF check that at least one of the values of wp_filled and tot_wp_filled is greater than 0.0 is added to prevent the divide by zero. In *releaset.f*, the statement at line 859 "IF (waste_package_fill_start.ne.waste_package_fill_stop) THEN" should be modified to use the **bathflow** flag instead of start and stop fill times. See Attachment A.

8. Implemented by: C. Scherer	**Date:** 5-6-2004

9. Description of Acceptance Tests:

The software was tested as presented in Attachment B.
All tests PASSED.

10. Tested by: Zbigniew Wojcik	**Date:** July-2-2004

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ATTACHMENT A

In exec.f, change:

```
         ELSE
           wp_fill_time_average = ((wp_fill_time_average *
     &     tot_wp_filled) + (wp_fill_time * wp_filled)) /
     &     (tot_wp_filled + wp_filled )
           tot_wp_filled = tot_wp_filled + wp_filled
           tot_wp_flowthru = tot_wp_flowthru + wp_flowthru
           IF((wp_fill_time .GT. wp_fill_time_maximum) .AND.
     &        (wp_filled .GT. 0)) THEN
             wp_fill_time_maximum = wp_fill_time
           ENDIF
```

to:

```
         ELSE
c
c         it's possible that no wp will be filled
c         avoid divide by 0; wp_fill_time_average will
c         keep its previous value
c
           if ((tot_wp_filled .gt. 0) .or. (wp_filled .gt. 0)) then
              wp_fill_time_average = ((wp_fill_time_average *
     &        tot_wp_filled) + (wp_fill_time * wp_filled)) /
     &        (tot_wp_filled + wp_filled )
           end if
           tot_wp_filled = tot_wp_filled + wp_filled
           tot_wp_flowthru = tot_wp_flowthru + wp_flowthru
           IF((wp_fill_time .GT. wp_fill_time_maximum) .AND.
     &        (wp_filled .GT. 0)) THEN
             wp_fill_time_maximum = wp_fill_time
           ENDIF
```

In releaset.f, change:

```
         IF ( waste_package_fill_start.ne.waste_package_fill_stop ) THEN
           tot_waste_packages_filled = tot_waste_packages_filled +
     &       numwp
           tot_waste_package_fill_time = tot_waste_package_fill_time +
     &       numwp * (waste_package_fill_stop - waste_package_fill_start)
         ELSE
           tot_waste_packages_flothru =
     &     tot_waste_packages_flothru + numwp
         ENDIF

c     change to check water contact flag
c         IF ( waste_package_fill_start.ne.waste_package_fill_stop ) THEN
         IF (bathflow .eq. 0) THEN
           tot_waste_packages_filled = tot_waste_packages_filled +
     &       numwp
           tot_waste_package_fill_time = tot_waste_package_fill_time +
     &       numwp * (waste_package_fill_stop - waste_package_fill_start)
         ELSE
```

```
      tot_waste_packages_flothru =
&     tot_waste_packages_flothru + numwp
   ENDIF
```

ATTACHMENT B

Test for TPA SCR-485

Test Name: Compare TPA code results before and after modifications to see if values NaN disappeared.

Tested By: Zbigniew Wojcik

Date: July 2, 2004

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8 (4.2 solapps compiler)

Baseline Version: TPA 5.0t

Test Version: TPA 5.0v

PROCESS LEVEL (PL) Test:
None

SYSTEM LEVEL (SL) Tests:

I. SL1:

Name: Compare versions and see if error NaN disappeared
Path of run directory if initial code: /home/zwojcik/scr485/
Path of run directory if modified code: /home/zwojcik/scr485/
Special input files or modifications to input files: tpamin.out used as tpa.inp.
Program modes to be used: NumberOfRealizations =1.

I. Description of SL1 Test Plan:

- Objective: Demonstrate that the old code produces NaN values. Show that modified code runs successfully to completion and the outputs to the file wpfillstats.out are without values NaN. (i.e. that the problem was fixed).

- Assumptions: 1. The system TPA is complete in the run directory /home/zwojcik/scr485/.
2. Files exec.f and releaset.f in tpa5.0v are the modifications of the files exec.f and releaset.f in tpa5.0t prepared to fix the problem.

- Output files to compare: wpfillstats.out generated by original tpa.e with wpfillstats.out generated by modified tpa.e when using tpamin.out as tpa.inp.

- Pass /fail criteria: The test passes if:
1. The modified TPA runs successfully to completion;
2. Screen outputs of the TPA of before and after the modifications are the same when using regular tpa.inp as input (except of the dates of Job Started lines).

3. The output file wpfillstats.out generated by the modified code is free from values NaN when using tpamin.out as tpa.inp

I. Step by step SL1 test procedure:

1. Compile and execute the code before modifications in /home/zwojcik/scr485/ (with version tpa5.0t) on basic inputs:
make
tpa.e > tpa_orig.out

2. Save files in question in the run directory as before modification in /home/zwojcik/scr485/:
cp tpa.e tpa_orig.e
cp tpa.inp tpa_orig.inp
cp tpamin.out tpamin_orig.out
cp tpamax.out tpamax_orig.out
cp wpfillstats.out wpfillstats_orig.out
The wpfillstats.out had no values NaN (because of not minimum inputs only).

3. Execute the code before modifications in /home/zwojcik/scr485/ (with version tpa5.0t) when switching input to tpamin.out. Copy initial input to the modified code tpa50v to be sure that the inputs are the same:
cp tpamin.out tpa.inp
tpa.e>tpa_min_orig.out
cp tpa_orig.inp ./tpa50v/tpa.inp

4. Execute the code before modifications in /home/zwojcik/scr485/ (with version tpa5.0t) when switching input to tpamax.out. Copy screen output to /home/zwojcik/scr485/tpa50v/ for the System Test II:
cp tpamax.out tpa.inp
tpa.e>tpamax_orig.out
cp tpa.e>tpamax_orig.out ./tpa50v/.

5. Save tested results wpfillstats.out in /home/zwojcik/scr485/ (with version tpa5.0t) and see if they have error values NaN :
cp wpfillstats.out wpfillstats_min.out
The results wpfillstats_min.out had the error values NaN (as before the modifications).

Now test the modified code in /home/zwojcik/scr485/tpa50v (with version tpa5.0v):

6. Get the new system tpa5.0v in /home/zwojcik/scr485/tpa50v and compile it:
~janetz/gettpa
make

7. Execute the new (modified) codes on the regular inputs and on the minimum inputs in /home/zwojcik/scr485/tpa50v (with version tpa5.0v):
tpa.e > tpa_485.out
cp tpamin.out tpa.inp
tpa.e > tpa_min_485.out

8. See, if results of execution before and after modifications are the same (in /home/zwojcik/scr485/tpa50v with version tpa5.0v):
diff tpa_485.out tpa_orig.out
The results were the same (except the dates in Job Started lines).
Test PASSED.

9. Save test results wpfillstats.out and see if they have error values NaN (in /home/zwojcik/scr485/tpa50v (with version tpa5.0v):
cp wpfillstats.out wpfillstats_min.out
No error values NaN exist in output wpfillstats_min.out after modifications.
Test PASSED.

II. SL2:

Name: See if any side effects exist in the modified version.
Path of run directory if initial code: /home/zwojcik/scr485/
Path of run directory if modified code: /home/zwojcik/scr485/
Special input files or modifications to input files: tpamax.out used as tpa.inp.
Program modes to be used: NumberOfRealizations =1.

II. Description of SL2 Test Plan:

- Objective: Show that modified code runs to completion on different inputs and the outputs to the file wpfillstats.out are still without any values NaN (i.e. that no unexpected side effect exist).

- Assumptions: 1. The new system TPA is complete in the run directory /home/zwojcik/scr485/tpa50v/.
2. Files exec.f and releaset.f in tpa5.0v are the modifications of the files exec.f and releaset.f in tpa5.0t prepared to fix the problem.

- Output files to compare: wpfillstats.out generated by tpa.e of the new system tpa50v with wpfillstats.out generated by tpa.e of the new system tpa50v when using tpamax.out as tpa.inp. TPA code results printed to the screen for the maximum input values before and after modifications.

Pass /fail criteria: The test passes if:
1. The modified TPA runs successfully to completion;

2. The output file wpfillstats.out generated by the modified code is free from NaN values when using tpamax.out as tpa.inp;
3. The screen output file from the original code and the screen output of the modified code when replacing tpa.inp by tpamax.out are the same (except for time/date stamps).

II. Step by step SL2 test procedure:

1. Execute the code after the modifications when switching input to maximum values tpamax.out in /home/zwojcik/scr485/tpa50v (with version tpa5.0v):
cp tpamax_orig.out tpa.inp
tpa.e > tpa_max.out

2. Save tested results wpfillstats.out and see if they have error values NaN (in /home/zwojcik/scr485/tpa50v with version tpa5.0v):
cp wpfillstats.out wpfillstats_max.out
The results wpfillstats_max.out did not have error values NaN (because input values were at the maximum).
Test PASSED.

3. Compare screen outcomes of the original code (before modifications) with the screen outcomes when replacing tpa.inp by tpamax.out:
diff tpa_max.out tpamax_orig.out
The results were the same (except the time/date stamps in Job Started lines).
Test PASSED.

Overall test status: **PASS.**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-486	**2. Software Title and Version:** TPA 5.0t	**3. Project No:** 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): exec.f

Version 5.0s was reported to produce a step increase in total dose at the last time step of the 10,000 year period.

5. Change Requested by: B. Ibrahim Date: 4-29-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date:4-29-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

This was caused by one section of the code disallowing releases from the SZ prior to the UZ release. The colloid contribution was moved to the parent nuclide before they were screened for SZ release. As a result the screening was based on the time of release of the parent from the UZ rather than on the time of the colloid release.

This behavior had little effect on the peak dose since the last time step is not subject to screening and was calculated correctly in all cases.

8. Implemented by: Ron Janetzke	**Date:** 5-10-2004

9. Description of Acceptance Tests:

The software was tested in accordance with the Test Plan for TPA SCR #486 (see tp_scr486.wpd). The software, test directories, and test results are contained on a CD labeled "TPA SCR #486 - Test Directories." All tests passed.

10. Tested by: Carol Scherer	**Date:** 5-26-2004

06/02/4

Test Plan/Report for TPA SCR #486

Test Plan Name:

Tested By: Carol S. Scherer

Date: May 26, 2004

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0t
(4.2 solapps compiler)

Test Version: TPA 5.0u
(4.2 solapps compiler)

Code Modifications:

The following code modifications were made to **TPA** for SCR #486 (*see scr486.wpd*):

1. in exec.f: In the section of code disallowing releases from the SZ prior to the UZ release, the colloid contributions were moved to the parent nuclides before they were screened for SZ release. As a result, the screening was based on the time of release of the parent from the UZ rather than on the time of the colloid release. The section of code was moved.

Testing Setup:

Directories/paths used for testing:
$HOME = /net/spock/home/cscherer
Path for U run directory: ***$HOME/scr486***
Path for T run directory: ***$HOME/scr486/tpa50t***

Environment variables:

TPA_TEST = $HOME ***/scr486***
TPA_DATA = $HOME ***/scr486***

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 486 - Test Directories*" (attached).

Test preparation instructions:

2. In the directory **$HOME**, create the following subdirectory: ***scr486***.

3. Copy **TPA** version 5.0u to the ***scr486*** directory. Compile *tpa.e* using *Makefile4.2.* Save a copy of the original *tpa.inp* as *tpa_orig.inp*.

4. In the directory ***scr486***, create the following subdirectories: ***tpa50t*** and ***orig300r_run***

5. Copy **TPA** version 5.0t to the ***tpa50t*** subdirectory. Compile *tpa.e* using *Makefile4.2.* Save a copy of the original *tpa.inp* as *tpa_orig.inp*.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

1. Name: Compare Modified Code To Previous Version Of The Code Using Base Case ***tpa.inp*** with 300 Realizations.

   Paths for archives of results: ***$HOME /scr486/orig300r_run***
   $HOME /scr486/tpa50t/orig300r_run

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use base case *tpa.inp* from both the u and t versions of the TPA code; make the following modification to each file:

   Set NumberOfRealizations to 300

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to show that the modified **TPA** code generates the same results as before the code changes except for total dose values

   - assumptions: none

   - constraints: the file *tpa_orig300r.out* does not exist in either run directory.

- output files to compare or examine: *tpa_orig300r.out* and *totdose.res* from each run directory

- step by step test procedure to be used:
  1. —> change directory to <<U run directory>>
  2. use the modified *tpa.inp*
  3. run *tpa.e* using command "***tpa.e > tpa_orig300r.out***"
  4. copy *tpa_orig300r.out* to ***orig300r_run/****tpa_orig300r.out*
  5. copy *totdose.res* to ***orig300r_run/****totdose.res*
  6. create the file *totdose_orig300rVu.xls* (see existing file for format) from *totdose.res*
  7. —> change directory to <<T run directory>>
  8. use the modified *tpa.inp*
  9. run *tpa.e* using command "***tpa.e > tpa_orig300r.out***"
  10. copy *tpa_orig300r.out* to ***orig300r_run/****tpa_orig300r.out*
  11. copy *totdose.res* to ***orig300r_run/****totdose.res*
  12. create the file *totdose_orig300rVt.xls* (see existing file for format) from *totdose.res*
  13. look at output files, *totdose.res* files, and Excel spreadsheets

- pass/fail criteria: the test passes if:

  1. Both versions of the **TPA** code run successfully to completion.

  2. The Peak Mean Dose from the *tpa*.out* files is the same for both versions.

  3. See *totdose_orig300rVu.xls* and *totdose_orig300rVt.xls*. There should be a significant decrease in the percentage of "outliers" (see below) from the **TPA**5.0t run to the **TPA**5.0u run.

     For each TPA run, both version u and version t, *totdose.res* was converted to Excel. The dilution volume (dilutvol) information was deleted, leaving the total effective dose (**tede**) for each time step. The difference in **tede** between the third to last time step and the second to last time step was calculated as was the difference between the second to last time step and the last time step. A heuristic threshold of 2.5 is used. If the difference in **tede** between the last time step and second to last time step was $\leq 2.5 \times$ the difference between the third to last and second to last time step, it was acceptable. Otherwise, it was determined to be an "outlier" (i.e., the value lay outside the acceptable range). If the difference in **tede** between the last time step and second to last time step showed a change of direction (sign) from the difference in **tede** between the third to last and second to last time steps, it was also

deemed to be an "outlier". For the **TPA** 5.0t run, the percentage of "outliers" was 49.67%; for the **TPA** 5.0u run, the percentage was 6%.

4. See *totdose_orig300r_u_t_25.xls*. Graphs of the same realizations, from the two different runs, of the 6% that failed the step test described in 3 above should show that step increase at the last time step has decreased.

   All the realizations that failed the step test from both runs were copied to this spreadsheet. **Tede** data from the same realization from both TPA runs were plotted on the same graph for comparison. The graphs showed that the step increase at the last time step had decreased.

Results of running test:

PASSED.

NOTES:

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-487	2. Software Title and Version: TPA 5.0u	3. Project No: 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): gentpa/chain.f, releaset.f

An invalid operation flag is raised when Volcanism = 1, and Direct Release Only = 1, Number of Realizations = 1000, Start & Stop Realization = 668. This is due to the lack of precision in the GENII data transfer files between envin.e and env.e. This was caused by the sum of the lambda for decay (AL) and the leaching factor (AB) being equal for two consecutive members of a decay chain. In this case it was U232 an Th232 in genv.in chain number 19. A contributing factor is that the variability was severely constrained due to the few significant digits in the data transfer files. The gftrans.dat file uses 2 significant digits for the leaching factor and the env.in file uses 3 significant digits for the LEACHT parameter. The ALT variable comes from the file grmdlib.dat. The (ALT + LEACHT) in env.in for U232 equals the (ALT + LEACHT) for Th232. The module chain.f in env.e takes the difference between these sums and uses it for the denominator when determining A(), one of the coefficients that determine the activity of each nuclide. The resulting divide by the difference of zero caused the error.

The following e-mail from R. Codell is also addressed for releaset:

I found one coding error. The code inadvertently corrects the total radionuclide in the waste for the gap fraction in the glass model. In subroutine liqrel, the loop beginning with "do 410 k=1,nchns" should be bypassed for the glass model (imodel=5). This accounted for a small removal of the radionuclides from the solid glass mass. It had a small effect on the release rate and cumulative release from the waste package.

5. Change Requested by: C. Scherer / R. Codell Date: 6-8-2004	6. Change Authorized by (*Software Developer*): R. Janetzke Date: 6-10-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): chain.f

The third line in the divide by lambda loop was changed to:

```
ABD(IJK) + DBLE (AB(IJK)) + DBLE (AL(IJK))
```

releaset.f

The referenced 'do loop' was bypassed for the glass model by enclosing in an IF block using:

```
if (imodel .ne. 5) then
```

8. Implemented by: Ron Janetzke	Date: 6-11-2004

9. Description of Acceptance Tests:

The software was tested as described in Attachment A.

Report shows, int.al. difference in peak dose and difference in szft release.

Overall test status: **PASS**

10. Tested by: Zbigniew Wojcik	Date: 7-12-2004

CNWRA Form TOP-5 (05/2000)

ATTACHMENT A

Test for TPA SCR-487

Test Name: Compare TPA code results before and after modifications for the two problems (I) the lack of bypassing gapfraction correction for the glass model, and (II) for the division by 0 errors.

Tested By: Zbigniew. Wojcik

Date: July 12, 2004

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8 (4.2 solapps compiler)

Baseline Version: TPA 5.0u

Test Version: TPA 5.0v

Disposition and documentation of results: All modified / new source code files, all ald version (before modifications), all executables used for testing, and all input / output files are kept on the CD ROM titled "TPA SCR#487. Test Results. Z. Wojcik" attached.

PROCESS LEVEL (PL) Test:
None

SYSTEM LEVEL (SL) Tests:

I. SL1 overview:

Name: Compare results from versions before and after modifications and see if problem with not bypassing the glass model disappeared.
Path of run directory if initial code: /home/zwojcik/scr487/tpa50u/
Path of run directory if modified code: /home/zwojcik/scr487/tpa50v/
Special input files or modifications to input files: none.
Program modes to be used:
IModel = 5
OutputMode = 2
SelectAppendFile = 9
NumberOfRealizations = 1

I. Description of SL1 Test Plan:

- Objective: Show that the problem with not bypassing the glass model was fixed in the modified code. Specifically, show that the modified code runs to completion, and detect small increases or decreases in the output szft.rlt after the modifications, as reported by R. Codell in the change request.

- Assumptions: 1. The systems tpa50u and tpa50v are complete in the run directory /home/zwojcik/scr487/.
2. On /home/zwojcik/scr487/, the system tpa50v comprises the modifications with the problem fixed, and tpa50u is the initial version with the problem.

- Output files to compare: 1. szft.rlt generated by tpa.e after the modifications in tpa50v, and szft.rlt generated by tpa.e before the modifications in tpa50u; 2. Screen outputs sent to files.

Pass /fail criteria: The test passes if:
1. The modified TPA runs successfully to completion and their screen outputs are the same, except time stamps;
2. (a) The output szft.rlt generated by tpa.e after the modifications shows small differences as reported by R. Codell in the change request, both increases and decreases; and (b) the outputs displayed on the screen show differences associated with bypassing for the glass model.
3. There are no values NaN in any output when running the version after the modifications.

I. Step by step SL1 test procedure:

1. Copy the newest version tpa50v of the TPA system into /home/zwojcik/scr487/tpa50v.
It comprises the modifications to the problems:
ssh zwojcik@spock
cd scr487
cd tpa50v
~rjanetz/gettpa

2. Copy the version tpa50u before the improvements into /home/zwojcik/scr487/tpa50u:
cp -Rv ./tpa50u/* ~/scr487/tpa50u

3. Set the parameters in tpa.inp at which the problem occurred, in the version /home/zwojcik/scr487/tpa50u before the modifications:
cp tpa.inp tpa_ini.inp
OutputMode = 2
SelectAppendFile = 9
IModel = 5
cp tpa.inp tpa_bypass.inp

4. Set the same input parameters in tpa.inp in tpa50v. Make sure that the input tpa.inp is the same in tpa50v and in tpa50u. In tpa50v:
cp ../tpa50u/ tpa.inp .

5. Execute tpa in tpa50u:
tpa.e > tpa_no_bypass.out

6.. Execute tpa in tpa50v:

tpa.e > tpa_bypass.out

7. Compare their outputs to szft.rlt in tpa50v and save the results of the comparison:
cp ../tpa50u/szft.rlt szft_no_bypass.rlt
diff -i szft_no_bypass.rlt szft.rlt > diff_bypass
cp szft.rlt szft_bypass.rlt
Observed differences indicated by the change *c* character, both increases and decreases. Most differences are at the first place after the decimal point, and there are practically changes in almost each non-zero number.
Test PASSED.

8. Compare their outputs to the screen in tpa50v and save the differences:
cp /home/tpa50u/ tpa_no_bypass.out .
diff -i tpa_bypass.out tpa_no_bypass.out > diff_bypass_screen
The outputs were different, as a result of the bypassing when using IModel = 5. The differences were related to the bypassing when using IModel = 5 and were complementary to the differences detected in the files szft.rlt. The differences were indicated by the change c character.
Test PASSED.

9. Save the input files both in tpa50u and tpa50v:
cp tpa.inp tpa_bypass.inp

10. See if there are error values NaN in any file in tpa50v:
grep NaN *
No NaN values detected. Also the screen did not show any error values NaN. So, neither any file nor screen output generated NaN values.
Test PASSED.

II. SL2:

Name: Verify that the original code produces the error. Compare results from versions before and after modifications and see if problems with division by 0 disappeared.
Path of run directory if initial code: /home/zwojcik/scr487/tpa50u/
Path of run directory if modified code: /home/zwojcik/scr487/tpa50v/
Special input files or modifications to input files: Special parameters set in tpa.inp (see below).
Program modes to be used:
VolcanismDisruptiveScenarioFlag =1
DirectReleaseOnlyFlag =1
NumberOfRealizations=1000
StartAtRealization=668
StopAtRealization=668

II. Description of SL2 Test Plan:

- Objective: Show that the problem was fixed in the modified code.

- Assumptions: 1. The systems tpa50u and tpa50v are complete in the run directory /home/zwojcik/scr487/.
2. The system tpa50v comprises the modifications with the problem fixed, and tpa50u is the initial version with the problem.

- Output files to compare: totdose.res generated by original tpa.e in tpa50u, and totdose.res generated by modified tpa.e in tpa50v.

- Pass /fail criteria: The test passes if:
1. The modified TPA runs successfully to completion;
2. totdose.res generated by modified tpa.e has non-empty dose peak;
3. There are no values NaN in any output when running the version after the modifications.

II. Step by step SL2 test procedure:

1. The newest version of the TPA system with the modifications to the problems is already in /home/zwojcik/scr487/tpa50v.
The version tpa_50u before the improvements is already in /home/zwojcik/scr487/tpa50u.

2. Set the parameters in tpa.inp listed below at which the problem occurred, in the version /home/zwojcik/scr487/tpa50u before the code modifications:
cp tpa_ini.inp tpa.inp
Then using vi-editor, set these parameters in the file tpa.inp:
VolcanismDisruptiveScenarioFlag =1
DirectReleaseOnlyFlag =1
NumberOfRealizations=1000
StartAtRealization=668
StopAtRealization=668

3. Set the same input parameters in tpa.inp in tpa50v. Make sure that the input file tpa.inp is the same in tpa50v and in tpa50u. In tpa50v:
cp /home/tpa50u/ tpa.inp .

4. Execute the code, both in the /home/zwojcik/scr487/tpa50u before the modifications and in the /home/zwojcik/scr487/tpa50v after the modifications:
tpa.e > & tpa_487.out
The /home/zwojcik/scr487/tpa50v after the modifications executed successfully to completion.
Test PASSED.

5. Compare screen outputs in tpa50v, observe if the errors disappeared in the modified version, and save the results of the comparison:
cp /home/tpa50u/tpa_487.out tpa_487_div0.out

diff tpa_487_div0.out tpa_487.out > tpa_487_diff
Error messages 'Invalid Operation" disappeared in the new version in tpa50v.
The new version (in tpa50v) has a non-zero Peak Mean Dose in non-zero year, whereas the pertinent initial version (in tpa50u) has a zero Peak Mean Dose in zero year.
Test PASSED.

6. Observe the results totdose.res both in tpa50u and in tpa50v:
Save totdose.res resulting from initial version in tpa50v.
In the initial version totdose.res has all zero values in the tede column except for three NaN error values.
The modified version has three non-zero values instead of NaN error values.
cp totdose.res totdose_470.res
Test PASSED.

7. See if there are error values NaN in any file in tpa50v:
grep NaN *
The screen did not show any error values NaN in the modified version.
Test PASSED.

Overall test status: **PASS.**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-488	2. Software Title and Version: TPA 5.0x	3. Project No: 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): climato2.dat, nfenv.f, uzflow.f, tpanames.dbs, tpa.inp.
The basis for climato2.dat cannot be supported.
The relative humidity for the pre-closure period is based on repository temperature rather than ground surface temperature.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
R. Fedors Date: 7-20-2004	R. Janetzke Date: 7-21-2004 R. Janetzke

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):
Because the DOE estimates for precipitation with climate change are dramatically greater than those used by the NRC, the climato2.dat file was modified. The DOE analyses (CRWMS M&O, 2000; USGS, 2000) since NRC (1997) was completed suggest the modern climate will persist for 600 years, followed by 1400 years of monsoonal climate with 303 mm/yr precipitation. The remaining years to the performance period of 10,000 years are described as glacial transition with an mean case of 323 mm/yr precipitation. Values used DOE precipitation estimates are based on repository averages from USGS (2000). The climato2.dat file was modified with a smoothly increasing fraction such that the first 10,000 years of the file were similar to fractions used by DOE. After full glacial begins at approximately 40,000 years, the remaining years to 100,000 are left unchanged in the climato2.dat file. Thus, maintaining the NRC (1997) conclusion that 60-80% of the 100,000 year cycle will be glacial climate.

An equation was added to nfenv.f to calculate the relative humidity for the pre-closure period using the ground surface temperature.

8. Implemented by:	Date:
R. Janetzke R. Janetzke	8-21-04

9. Description of Acceptance Tests:
The software was tested in accordance with the Test Plan for TPA SCR #488 (see tp_scr488.wpd). The software, test directories, and test results are contained on a CD labeled "TPA SCR #488 - Test Directories (Code Development)." All tests passed.

10. Tested by:	Date:
C. Scherer Carol S. Scherer	9-13-04

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description** **1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton** **1. site references (journals, sci. notebooks, publishings)** **2. is uncertainty covered by the distribution / range ?** **3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
Add	uzflow nfenv	GroundSurfaceTe mperature[C]	Temperature of the ground surface to be used as the temperature for ventilated air up to the time of backfill, and also as the initial climate temperature.	constant	17.38 C		
Add	uzflow	CurrentAnnualPre cipitation[mm/yr]	Current climate annual precipitation for initial climate conditions.	constant	162.8		

09/17/4

Test Plan/Report for TPA SCR #488

Test Plan Name: New Climato2.dat and Relative Humidity Calculation Based on Ground Surface Temperature

Tested By: Carol S. Scherer

Date: September 16, 2004

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0x
(4.2 solapps compiler)

Test Version: TPA 5.0y
(4.2 solapps compiler)

Testing Setup:

Directories/paths used for testing:
$HOME = /home/cscherer
Path for run directory:***$HOME/scr488***

Environment variables:

TPA_TEST = $HOME ***/scr488***
TPA_DATA = $HOME ***/scr488***

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 488 - Test Directories*" (attached).

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***scr488*** and ***tpa50x***.

2. In the directory ***scr488***, create the following subdirectories: ***slt1***, ***slt2***, ***slt3***, ***slt4***, ***slt5***, and ***slt6***.

3. Copy **TPA** version 5.0x to the ***tpa50x*** directory. Compile *tpa.e* using *Makefile4.2*. Save a copy of the executable as *tpa_x.e*. Save a copy of the original *tpa.inp* as *tpa_orig.inp*. Run *tpa.e*. Copy *tpameans.out* to *tpa_x.inp*. Set OutputMode to 1 in *tpa_x.inp*. Copy *tpa_x.e* and *tpa_x.inp* to the run directory. Copy *burnup.dat* to run/***data*** as *burnup_x.dat*. Copy *climato2.dat* to the run/***data*** directory as *climato2_x.dat*.

4. Copy **TPA** version 5.0y to the run directory. Compile *tpa.e* using *Makefile4.2*. Save a copy of the executable as *tpa_y.e*. Save a copy of the original *tpa.inp* as *tpa_orig.inp*. Run *tpa.e*. Copy *tpameans.out* to *tpa_y.inp*. Set OutputMode to 1 in *tpa_y.inp*. Copy the latest version of *burnup.dat* (see *scr_518.wpd*) to the run***/data*** directory as *burnup-scr518.dat*. Save a copy of *climato2.dat* as *climato2_y.dat* in the run***/data*** directory.

Functional Level Tests:

1. Name: Compare Modified *climato2.dat* to Previous Version of *climato2.dat*.

   Path for archives of results: ***$HOME /scr488/flt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: none.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to show that specified modifications were carried out to the data file.
   - assumptions: none.
   - constraints: none.
   - output files to compare or examine: none
   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>***/data***
     2. compare *climato2_y*.dat with *climato2_x.dat*.
   - pass/fail criteria: the test passes if:
     1. The modified *climato2_y.dat* file contains the changes described in *scr_488.wpd*.

Results of running test:

PASSED.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

NOTE: Changes had to be made to TPA5.0y versions *nuclides.dat* and *burnup.dat* (change year from 2033 to 2008), as well as *tpa.inp* (change CalendarYearOfEmplacement[A.D.] from 2034 to 2033) before test results looked like expected results from a basecase run. More changes were made to *burnup.dat* (see SCR # 518) around the same time as testing was done for SCR # 488. Since the *burnup.dat* changes affected the validity of the output for the SCR # 488 tests, the modified *burnup.dat* was used for these tests.

1. Name: Compare Modified Code To Previous Version Of The Code.

   Paths for archives of results: ***$HOME /scr488/slt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use *tpa_x.inp* and tpa_y.inp

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to show that the modified **TPA** code generates different results and the results differ in the way expected

   - assumptions: all setup instructions have been carried out.

   - constraints: the file *tpa_meanscase_y.out* does not exist in the run directory and *tpa_meanscase.out* does not exist in **$HOME/*tpa50x***.

- output files to compare or examine: *ebsfail.ech & infilper.res* in the run directory and in **$HOME/*tpa50x***.

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. run *tpa.e* using command "***tpa.e > tpa_meanscase_y.out***"
  4. —> change directory to **$HOME/*tpa50x***
  5. copy *tpa_x.e* to *tpa.e*
  6. run *tpa.e* using command "***tpa.e > tpa_meanscase_x.out***"
  7. compare the files *ebsfail.ech* and *infilper.res* from each run (see spreadsheets *ebsfail_ech.xls* and *infilper_res.xls*) for a single subarea (subarea 7 was used for this test report)

- pass/fail criteria: the test passes if:

  1. The modified code runs successfully to completion.

  2. *infilper_res.xls*: Infiltration is higher for TPA5.0y. Reflux and divert start out lower for TPA5.0y than TPA5.0x, then go higher (around 1900 years for subarea 7).

  3. *ebsfail_ech.xls*: Relhumwp, tempwp, and temprep are all higher for TPA5.0y, especially relhumwp in the preclosure period (0 - 50 years).

Results of running test:

PASSED.

2. Name: Run TPA5.0y Using *climato2.dat* from TPA5.0x.

Paths for archives of results: ***$HOME /scr488/slt2***

Special input files or modifications to input files required: *use climato2_x.dat*

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp*

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code and data file do not cause unintended side effects

- assumptions: all setup instructions have been carried out.

- constraints: the file *tpa_50y-clim2x.out* does not exist in the run directory.

- output files to compare or examine: *ebsfail.ech & infilper.res*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. run *tpa.e* using command "***tpa.e > tpa_50y-clim2x.out***"
  4. compare ebsfail.ech and infilper.res files from this run and the TPA5.0y run in slt1 (see spreadsheets ebsfail_ech.xls and infilper_res.xls).

- pass/fail criteria: the test passes if:

  1. The modified code runs successfully to completion.

  2. *infilper_res.xls*: Results are the same for this run as for the TPA5.0x run from slt1.

  3. *ebsfail_ech.xls*: Results are the same for this run as for the TPA5.0x run from slt1 for tempwp, temprep, and postclosure relhumwp. However, for preclosure relhumwp, the results for this run are the same as for the TPA5.0y from slt1.

Results of running test:

PASSED.

3. Name: Vary Ground Surface Temperature from 17.38 to 10.0, 15.0, and 20.0.

Paths for archives of results: ***$HOME /scr488/slt3***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp* and change GroundSurfaceTemperature to 10.0 for run A, 15.0 for run B, and 20.0 for run C.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that modifying the ground surface temperature affects temperature and humidity in a predictable way. (**CAVEAT**: The results from this test have limited implications. For a change in ground surface temperature to be valid, the data files resulting from ITYM should also be regenerated using the current temperature.)

- assumptions: all setup instructions have been carried out.

- constraints: the files *tpa_GST10.out*, *tpa_GST10.out*, and *tpa_GST10.out* do not exist in the run directory.

- output files to compare or examine: *ebsfail.ech*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. use tpa.inp for run A and run *tpa.e* using command "***tpa.e > tpa_GST10.out***"
  4. use tpa.inp for run B and run *tpa.e* using command "***tpa.e > tpa_GST15.out***"
  5. use tpa.inp for run C and run *tpa.e* using command "***tpa.e > tpa_GST20.out***"
  6. compare *ebsfail.ech* from all three runs and TPA5.0y run in slt1 (see spreadsheet *ebsfail_ech.xls*).

- pass/fail criteria: the test passes if:

  1. The modified code runs successfully to completion.

  2. *ebsfail_ech.xls*: There are no differences among the runs for tempwp and temprep and postclosure relhumwp. Preclosure relhumwp is highest when ground surface temperature is 20.0, next highest when ground surface temperature is 17.38 (basecase),

third highest when ground surface temperature is 15.0, and lowest when ground surface temperature is 10.0.

Results of running test:

PASSED.

4. Name: Vary CurrentAnnualPrecipitation[mm/yr] from 162.8 to 100.0 and 200.0.

Paths for archives of results: ***$HOME /scr488/slt4***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp* and change CurrentAnnualPrecipitation[mm/yr] to 100.0 for run A and to 200.0 for run B.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that modifying the current annual precipitation affects temperature and humidity in a predictable way.

- assumptions: all setup instructions have been carried out

- constraints: the files *tpa_CAP100.out* and *tpa_CAP100.out* do not exist in the run directory.

- output files to compare or examine: *ebsfail.ech*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. use *tpa.inp* for run A and run *tpa.e* using command "***tpa.e > tpa_CAP100.out***"
  4. use *tpa.inp* for run B and run *tpa.e* using command "***tpa.e > tpa_CAP200.out***"

5. compare *ebsfail.ech* from both runs and from TPA5.0y in slt1 (see spreadsheet *ebsfail_ech.xls*).

- pass/fail criteria: the test passes if:

1. The modified code runs successfully to completion.

2. *ebsfail.ech*: There are no differences in tempwp, temprep, and relhumwp.

Results of running test:

PASSED.

5. Name: Vary FactorForVentilationHeatlosses[] from 0.7 to 0.86.

Paths for archives of results: ***$HOME /scr488/slt5***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp* and change FactorForVentilationHeatlosses[] to 0.86.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modifying the factor for ventilation heat loss affects temperature and humidity in a predictable way.

- assumptions: all setup instructions have been carried out

- constraints: the files *tpa_Vent-86.out* does not exist in the run directory.

- output files to compare or examine: *ebsfail.ech*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>

2. copy *tpa_y.e* to *tpa.e*
3. run *tpa.e* using command "***tpa.e > tpa_Vent-86.out***"
4. compare files *ebsfail.ech* from this run and from TPA5.0y run in slt1 (see spreadsheet *ebsfail_ech.xls*).

- pass/fail criteria: the test passes if:

1. The modified code runs successfully to completion.

2. *ebsfail.ech*: Tempwp and temprep are lower when ventilation is increased while relhumwp is higher.

Results of running test:

PASSED.

6. Name: Vary CalendarYearOfEmplacement[A.D.] to year 2034 from 2033.

Paths for archives of results: ***$HOME /scr488/slt6***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use *tpa_y.inp* and change CalendarYearOfEmplacement[A.D.] to 2034.

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that modifying year of emplacement affects the results of TPA in a predictable way.

- assumptions: all setup instructions have been carried out

- constraints: the files *tpa_Emplace2034.out* does not exist in the run directory.

- output files to compare or examine: *ebsfail.ech*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_y.e* to *tpa.e*
  3. run *tpa.e* using command "***tpa.e > tpa_Emplace2034.out***"
  4. compare *ebsfail.ech* files from this run and the TPA5.0y run in slt1 (see spreadsheet *ebsfail_ech.xls*).

- pass/fail criteria: the test passes if:

  1. The modified code runs successfully to completion.

  2. *ebsfail.ech*: Tempwp and temprep is slightly lower when year of emplacement increases by one year. Relhumwp is slightly higher at first then becomes slighter lower (after 1250 years for subarea 7).

Results of running test:

PASSED.

NOTES:

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-489	**2. Software Title and Version:** TPA 5.0v	**3. Project No:** 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): uzft.f, szft.f, actinide_kdrd.out
It is desirable to enable the TPA code to produce an intermediate output file (actinide_kdrd.out) that contains the Kd, Rd, surface area, effective porosity, and matrix porosity values used for each radionuclide, layer, zone (unsaturated/saturated), realization combinations for a given run.

5. Change Requested by: P. Bertetti Date: 7-8-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: R. Janetzke

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): Fracture and matrix coefficients Kds and Rds are computed for the elements Am, Np, Pu, Th and U by subroutines uzsf() and szft() by calls to calc_dk() and calc_rd(). Rds only for all nuclides are collected from tpa.inp in szft() by call to prenefmksa(). The collection of these coefficients was done at proper places of the code modeling the flow of the nuclides through the rock layers.
See Attachment A for details.

8. Implemented by: Zbigniew Wojcik	**Date:** July 30, 2004

9. Description of Acceptance Tests:
See Attachment B

10. Tested by:	**Date:** Apr. 13, 2006

CNWRA Form TOP-5 (05/2000)

Attachment A.

The distribution (or partition) coefficient kd is a ratio (fraction) of a contaminant concentration in soil to that in water. The retardation coefficient rd is the ratio of the velocity of water to that of a contaminant. The array kds(i) is computed by subroutine calc_kd() for each rock layer separately, where i is the contaminant Am, Np, Pn, Th, U. Subroutine calc_rd takes kds(i) and computes the array of retardation coefficients rds(i).
Rds are also read from TPA.INP file for the saturated layer and should be the same as Rdd computed by CALC_RD().
The specific surface area ssArea parameter is computed for each rock layer and also needs to be collected with all kds(i) and rds(i).
Run directory: /home/zwojcik/rd/run
Affected modules: uzft.f, szft.f, exec.f, actinide_kdrd.out

1. Made modifications in the uzft.f and in szft.f to save RealizationNumber, Subarea ID and saturated / unsaturated zone, then Layer of Rock and SpecificSurfaceArea, then header listing columns: Nuclide, matrix_KD, matrix_RD, fracture_KD, fracture_RD.
2. Modified uzft() to save the parameters in the new file actinide_kdrd.out: a. Declared the names of the rock layers specific to unsaturated zone; b. Designed with details and implemented the transfer of the new file actinide_kdrd.out for the append operations between calls of subsequent realizations; c) Designed, implemented and tested the mechanism of temporal saving parameters of matrix kds() from the call to calc_kd() (computing the matrix Kd equations) to save them in file actinide_kdrd.out together with the fracture Kd computed later. The loop through rock layers was over the matrix and fracture Kd an Rd computations; d) Done the same for the Rd parameters, however, added new call to calc_rd() in uzft() to get all matrix Rd; e) Followed the required format for the new output file actinide_kdrd.out.
3. Tested the modifications made to uzft(): compared the matrix Rds computed in uzft() as a result of the modification with matrix Rds computed in prenefmksa(). Made the comparison at the corresponding layer rocks and elements. The calc_kd() computes Kds for the nuclides in the sequence: Am, Np, Pu, Th, U. The prenefmksa() extracts these matrix Kds, associates them with the elements Am, Np, Pu, Th, U and then computes matrix Rds.
The Rds computed in prenefmksa() are associated with the right elements Am, Np, Pu, Th, U as in uzft() and are of the same values.
4. Made another, parallel test of correctness of passing matrix Kds from uzft() to prenefmksa() to compute RDs. Took advantage of the call (in uzft.f) to sub setconsmv() saving results of the first call to calc_kd as matrix kd. The values of matrix kd are saved in datc() by layer rock (see common / mvb4 /, include 'mve.i'). The indexes to Kds corresponding to Am, Np, Pu, Th, U extracted by invquery() were the same both in uzft() and in prenefmksa(). So, the indexes to Kds (and Rds) whose values were saved in file actinide_kdrd.out were associated with the right elements Am, Np, Pu, Th, U and with their right values of Kds and Rds existing in prenefmksa().
6. Tested if the values under fields Nuclide, matrixRD, matrixKD, fractureKD, fractureRD computed in uzft.f were written correctly to the file actinide_kdrd.out by comparing the values printed to the screen during execution with the contents of the file actinide_kdrd.out. They were the same.
7. Modified szft.f to save the RD parameters computed by calc_kd() and calc_rd()) into the new file actinide_kdrd.out: a. Declared the names of the rock layers specific to saturated zone; b. Implemented the transfer of the new file actinide_kdrd.out for the append operations between calls of subsequent realizations; c) Designed, implemented and tested the mechanism of transfer of parameters kds() from the call to calc_kd() computing the matrix KD equations to save these matrix parameters in new file actinide_kdrd.out after calling calc_kd() to compute the fracture KD equations. The differences with uzft were: (i) the loop through rock layers was only over the matrix KR an RD computations; (ii) the call to make matrix RDs() parameters were not made from another module; (iii) the fracture parameters were only for the layer 2 of rock, so the matrix parameters had to be transferred to the file actinide_kdrd.out for the layer 2 of rock only.

8. Modified szft.f to save the RD parameters taken from TPA.inp file (not computed by calc_kd() and calc_rd()) into the new file actinide_kdrd.out. Utilized two loop structures over which all the elements and the rock layers are scanned. Identified and saved temporarily the required RDs inside the body of the loop structures. Resolved the differences between the number and names of the nuclides handled when computing Rds by using calc_RD() and when reading RD coefficients from tpa.inp: only 5 nuclides are processed by using calc_kd() and calc_rd(): Am, Np, Pu, Th, U, whereas

all nuclides are processed when reading Rds from tpa.inp.
9. Tested. Compared the matrix Rds for the elements Am, Np, Pu, Th, U computed by calc_rd() in szft() with those collected from tpa.inp for two layers: STFF and SAV. They were the same.
The value of fracture RD computed by calc_rd() was always equal to 1. This is because the value frac_forcefac is always equal to 0, because that frac_forcefac = valuesp(ifforcefac), and that
ifforcefac = ispquery(UZFractureForceFactorForKdToRd).
UZFractureForceFactorForKdToRd = 0 in tpa.inp. So, the values of RDs were as expected.
The outputs of Kds computed by calc_rd() are for only the first area of the first realization, because of the condition in the code:

```
 IF (ir .ne. ir_now) THEN
    Making actinide_kdrd.out
   END IF
```

where ir is the current realization number. This condition is true only for the first area of the first realization, and this explains, why.

Delivarables:
The version of the TPA code providing Kds and Rds for both the unsaturated and saturated zones is in the subdirectory kdrd_all. The new versions of uzft.f, szft.f and exec.f. are necessary can to provide the Kds and Rds for both the unsaturated and saturated zones.

10. To the general requirements to provide the Rds in both unsaturated and saturated zones, Paul requested in addition also the code outputting only the Rds and Kds in the saturated zone. Made updates on the copy of the TPA code described above: commented-out all write statements resulting Kds and Rds from the unsaturated zone, and modified the szft.f to output only the KDs and RDS for the first area only on each realization.

Delivarables:
The version of the TPA code providing Kds and Rds for the saturated zone only is in the subdirectory kdrd.
The initial version of uzft.f can be used to provide the Kds and Rds for the saturated zone only, together with new szft.f and exec.f.

ATTACHMENT B

Test Plan for TPA SCR489

Tested By: Michael Muller Date: Aug 20, 2004
Host Machine: spock Host OS: Solaris
Baseline Version: TPA 5.0v Test Version: TPA 5.0v with SCR mods.

Process Level (PL) Tests

PL-1. Name: scr489_proclevl1
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/scr489_proclelv1
Environment variables: TPA_DATA=. TPA_TEST=.
Special input files or modifications to input files required: none
Special diagnostic code modifications required: none
Program modes to be used (append flags, scenario/model switches,etc.):
NumberOfRealizations: 1
Utility scripts needed to perform the test: none
Utility codes needed in the analysis of the test data: none
Test description:
objective: Compare values in nefiisz.inp to values in file actinide_kdrd.out
assumptions: Numbers will be identical.
constraints: none.
output files to compare/examine: nefii.inp and actinide_kdrd.out
procedure to be used:
Run tpa50v+scr489.
Code for scr489 is in exec.f, uzft.f, and szft.f. Check output from szft.f.
Compare nefiisz.inp and numbers in actinide_kdrd.out
Pass/fail criteria: Success is if numbers in nefiisz.inp and actinide_kdrd.out are the same (for the same nuclides).
Overall test status: FAIL Retested in SCR 523 RJ. 4-13-06

Comments: appears that code saves values for tuff in aluvium variable and vice versa. Also, from output, looks like incorrect index is used to save values for U,Am,Np,Pu, etc.
Suggest av() be changed to alv() for recognition and consistancy.
Also, when looking through code, noted that file actinide_kdrd.out is opened and closed every time it is written to. This is inefficient and it appears that opening/closing it once is possible.
Also noted that tpa version number was hard-coded in write of header of file. This would require editing for each new version.

SL-1. syslevl1
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/scr489_syslevl1

Environment variables: TPA_DATA=. TPA_TEST=.
Program modes to be used (append flags, scenario/model switches,etc.):
NumberOfRealizations: 403
MaximumTime[yr]: 2.5e4
VolcanismDisruptiveScenarioFlag(yes=1,no=0): 1
DirectReleaseOnlyFlag(yes=1,no=0): 1
Test description:
procedure to be used:
Run TPA50v+scr489 for 25Kyears and 403 realizations.
Set: VolcanismDisruptiveScenarioFlag(yes=1,no=0) = 1 and
DirectReleaseOnlyFlag(yes=1,no=0) = 1
objective: To run a long run with many years and realizations and directrelease and volcanism ON.
The values picked are mostly arbitrary (ie. 50yrs and 500 realizations could be used just as well but would take longer to run).
assumptions: 25K years is a sufficiently long time and 403 realizations is sufficiently long.
Pass/fail criteria: Success is when program runs to completion and 'success' line is printed.
Overall test status: PASS

SL-2. syslevl2
Path for run directory: spock:/export/home/muller/tpa/tpa50v/scr484/scr489_syslevl2
Environment variables: TPA_DATA=. TPA_TEST=.
Program modes to be used (append flags, scenario/model switches,etc.):
NumberOfRealizations: 100
MaximumTime[yr]: 5.0e4
Test description:
procedure to be used:
Run TPA50v+scr489 for 50Kyears and 100 realizations.
objective: To run a long run with many years and realizations.
The values picked are mostly arbitrary (ie. 25yrs and 500 realizations could be used just as well but would take longer to run).
assumptions: 50K years is a sufficiently long time and 100 realizations is sufficiently long.
pass/fail criteria: Success is when program runs to completion and 'success' line is printed.
Overall test status: PASS

File actinide_kdrd.out
SpecificSurfaceArea, KD & RD coefficients
TPA 5.0x, Job started: Wed Aug 04 15:32:28 2004

Realization = 1 Subarea = 1 UNSATURATED ZONE

Layer=TSw_ ssAreaMatrix=2.9268E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.6832E+04	4.8405E+08	9.1675E+00	1.0000E+00
Np	4.0790E-03	7.4584E+01	1.3936E-06	1.0000E+00
Pu	1.5389E+00	2.7762E+04	5.2578E-04	1.0000E+00
Th	9.1979E+01	1.6593E+06	3.1426E-02	1.0000E+00
U	8.9352E-02	1.6129E+03	3.0529E-05	1.0000E+00

Layer=CHnv ssAreaMatrix=8.7611E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	8.0317E+04	3.6854E+08	9.1675E+00	1.0000E+00
Np	1.2210E-02	5.7025E+01	1.3936E-06	1.0000E+00
Pu	4.6064E+00	2.1137E+04	5.2578E-04	1.0000E+00
Th	2.7533E+02	1.2633E+06	3.1426E-02	1.0000E+00
U	2.6746E-01	1.2283E+03	3.0529E-05	1.0000E+00

Layer=CHnz ssAreaMatrix=8.0000E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	7.3340E+04	3.7404E+08	9.1675E+00	1.0000E+00
Np	1.1149E-02	5.7861E+01	1.3936E-06	1.0000E+00
Pu	4.2063E+00	2.1453E+04	5.2578E-04	1.0000E+00
Th	2.5141E+02	1.2822E+06	3.1426E-02	1.0000E+00
U	2.4423E-01	1.2466E+03	3.0529E-05	1.0000E+00

Layer=PPw_ ssAreaMatrix=6.6142E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	6.0636E+04	3.9604E+08	9.1675E+00	1.0000E+00
Np	9.2178E-03	6.1205E+01	1.3936E-06	1.0000E+00
Pu	3.4776E+00	2.2715E+04	5.2578E-04	1.0000E+00
Th	2.0786E+02	1.3576E+06	3.1426E-02	1.0000E+00
U	2.0192E-01	1.3198E+03	3.0529E-05	1.0000E+00

Layer=UCF_ ssAreaMatrix=6.9421E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	6.3642E+04	3.9604E+08	9.1675E+00	1.0000E+00
Np	9.6749E-03	6.1205E+01	1.3936E-06	1.0000E+00
Pu	3.6501E+00	2.2715E+04	5.2578E-04	1.0000E+00
Th	2.1816E+02	1.3576E+06	3.1426E-02	1.0000E+00
U	2.1194E-01	1.3198E+03	3.0529E-05	1.0000E+00

Layer=BFw_ ssAreaMatrix=2.8016E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.5683E+04	4.8405E+08	9.1675E+00	1.0000E+00
Np	3.9044E-03	7.4584E+01	1.3936E-06	1.0000E+00
Pu	1.4730E+00	2.7762E+04	5.2578E-04	1.0000E+00
Th	8.8042E+01	1.6593E+06	3.1426E-02	1.0000E+00
U	8.5528E-02	1.6129E+03	3.0529E-05	1.0000E+00

Layer=UFZ_ ssAreaMatrix=2.7376E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.5097E+04	4.8405E+08	9.1675E+00	1.0000E+00
Np	3.8153E-03	7.4584E+01	1.3936E-06	1.0000E+00
Pu	1.4394E+00	2.7762E+04	5.2578E-04	1.0000E+00
Th	8.6033E+01	1.6593E+06	3.1426E-02	1.0000E+00
U	8.3577E-02	1.6129E+03	3.0529E-05	1.0000E+00

Realization = 1 Subarea = 1 SATURATED ZONE

Layer=SAV ssAreaMatrix= 2.6169E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.3990E+04	4.9077E+08	0.0000E+00	0.0000E+00
Np	3.6470E-03	7.5607E+01	0.0000E+00	0.0000E+00
Pu	1.3759E+00	2.8148E+04	0.0000E+00	0.0000E+00
Th	8.2239E+01	1.6824E+06	0.0000E+00	0.0000E+00
U	7.9890E-02	1.6353E+03	0.0000E+00	0.0000E+00

Layer=STFF ssAreaMatrix= 4.8574E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.4530E+04	4.4004E+08	9.1675E+00	1.0000E+00
Np	6.7695E-03	6.7895E+01	1.3936E-06	1.0000E+00
Pu	2.5539E+00	2.5239E+04	5.2578E-04	1.0000E+00
Th	1.5265E+02	1.5085E+06	3.1426E-02	1.0000E+00
U	1.4829E-01	1.4664E+03	3.0529E-05	1.0000E+00

Realization = 1 Subarea = 1 SATURATED ZONE

Layer=SAV.

Nuclide	MobileRd
U	0.1635E+04
Am	0.4908E+09
Np	0.7561E+02
Pu	0.2815E+05
Th	0.1682E+07

Layer=STFF.

Nuclide	ImmobileRd
U	0.1466E+04
Am	0.4400E+09
Np	0.6789E+02
Pu	0.2524E+05
Th	0.1508E+07

Realization = 2 Subarea = 1 UNSATURATED ZONE

Layer=TSw_ ssAreaMatrix=2.9268E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.6358E+04	2.9510E+08	5.5889E+00	1.0000E+00
Np	5.9040E-03	1.0751E+02	2.0172E-06	1.0000E+00
Pu	1.2993E+00	2.3440E+04	4.4392E-04	1.0000E+00
Th	8.1654E+01	1.4730E+06	2.7898E-02	1.0000E+00
U	4.6442E-03	8.4781E+01	1.5868E-06	1.0000E+00

Layer=CHnv ssAreaMatrix=8.7611E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.8965E+04	2.2468E+08	5.5889E+00	1.0000E+00
Np	1.7673E-02	8.2092E+01	2.0172E-06	1.0000E+00
Pu	3.8892E+00	1.7847E+04	4.4392E-04	1.0000E+00
Th	2.4442E+02	1.1215E+06	2.7898E-02	1.0000E+00
U	1.3902E-02	6.4788E+01	1.5868E-06	1.0000E+00

Layer=CHnz ssAreaMatrix=8.0000E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.4712E+04	2.2803E+08	5.5889E+00	1.0000E+00
Np	1.6138E-02	8.3302E+01	2.0172E-06	1.0000E+00
Pu	3.5514E+00	1.8113E+04	4.4392E-04	1.0000E+00
Th	2.2319E+02	1.1383E+06	2.7898E-02	1.0000E+00
U	1.2694E-02	6.5740E+01	1.5868E-06	1.0000E+00

Layer=PPw_ ssAreaMatrix=6.6142E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	3.6966E+04	2.4144E+08	5.5889E+00	1.0000E+00
Np	1.3342E-02	8.8144E+01	2.0172E-06	1.0000E+00
Pu	2.9362E+00	1.9178E+04	4.4392E-04	1.0000E+00
Th	1.8452E+02	1.2052E+06	2.7898E-02	1.0000E+00
U	1.0495E-02	6.9548E+01	1.5868E-06	1.0000E+00

Layer=UCF_ ssAreaMatrix=6.9421E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	3.8799E+04	2.4144E+08	5.5889E+00	1.0000E+00
Np	1.4004E-02	8.8144E+01	2.0172E-06	1.0000E+00
Pu	3.0818E+00	1.9178E+04	4.4392E-04	1.0000E+00
Th	1.9367E+02	1.2052E+06	2.7898E-02	1.0000E+00
U	1.1016E-02	6.9548E+01	1.5868E-06	1.0000E+00

Layer=BFw_ ssAreaMatrix=2.8016E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5658E+04	2.9510E+08	5.5889E+00	1.0000E+00
Np	5.6513E-03	1.0751E+02	2.0172E-06	1.0000E+00
Pu	1.2437E+00	2.3440E+04	4.4392E-04	1.0000E+00
Th	7.8159E+01	1.4730E+06	2.7898E-02	1.0000E+00
U	4.4454E-03	8.4781E+01	1.5868E-06	1.0000E+00

Layer=UFZ_ ssAreaMatrix=2.7376E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5301E+04	2.9510E+08	5.5889E+00	1.0000E+00
Np	5.5224E-03	1.0751E+02	2.0172E-06	1.0000E+00
Pu	1.2153E+00	2.3440E+04	4.4392E-04	1.0000E+00
Th	7.6376E+01	1.4730E+06	2.7898E-02	1.0000E+00
U	4.3440E-03	8.4781E+01	1.5868E-06	1.0000E+00

Realization = 2 Subarea = 1 SATURATED ZONE

Layer=SAV ssAreaMatrix= 3.2900E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.8387E+04	2.8991E+08	0.0000E+00	0.0000E+00
Np	6.6366E-03	1.0564E+02	0.0000E+00	0.0000E+00
Pu	1.4605E+00	2.3028E+04	0.0000E+00	0.0000E+00
Th	9.1785E+01	1.4472E+06	0.0000E+00	0.0000E+00
U	5.2204E-03	8.3309E+01	0.0000E+00	0.0000E+00

Layer=STFF ssAreaMatrix= 4.8586E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.7154E+04	2.6827E+08	5.5889E+00	1.0000E+00
Np	9.8008E-03	9.7826E+01	2.0172E-06	1.0000E+00
Pu	2.1568E+00	2.1309E+04	4.4392E-04	1.0000E+00
Th	1.3555E+02	1.3391E+06	2.7898E-02	1.0000E+00
U	7.7094E-03	7.7164E+01	1.5868E-06	1.0000E+00

Realization = 2 Subarea = 1 SATURATED ZONE

Layer=SAV.

Nuclide	MobileRd
U	0.8331E+02

Am	0.2899E+09
Np	0.1056E+03
Pu	0.2303E+05
Th	0.1447E+07

Layer=STFF.

Nuclide	ImmobileRd
U	0.7716E+02
Am	0.2683E+09
Np	0.9783E+02
Pu	0.2131E+05
Th	0.1339E+07

Realization = 3 Subarea = 1 UNSATURATED ZONE

Layer=TSw_ ssAreaMatrix=2.9268E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.6670E+04	3.0072E+08	5.6955E+00	1.0000E+00
Np	8.6410E-03	1.5688E+02	2.9523E-06	1.0000E+00
Pu	1.5366E+00	2.7721E+04	5.2500E-04	1.0000E+00
Th	5.9877E+01	1.0802E+06	2.0458E-02	1.0000E+00
U	2.0062E-04	4.6192E+00	6.8546E-08	1.0000E+00

Layer=CHnv ssAreaMatrix=8.7611E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.9899E+04	2.2896E+08	5.6955E+00	1.0000E+00
Np	2.5866E-02	1.1968E+02	2.9523E-06	1.0000E+00
Pu	4.5995E+00	2.1106E+04	5.2500E-04	1.0000E+00
Th	1.7923E+02	8.2241E+05	2.0458E-02	1.0000E+00
U	6.0054E-04	3.7556E+00	6.8546E-08	1.0000E+00

Layer=CHnz ssAreaMatrix=8.0000E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	4.5564E+04	2.3238E+08	5.6955E+00	1.0000E+00
Np	2.3619E-02	1.2146E+02	2.9523E-06	1.0000E+00
Pu	4.2000E+00	2.1421E+04	5.2500E-04	1.0000E+00
Th	1.6366E+02	8.3468E+05	2.0458E-02	1.0000E+00
U	5.4837E-04	3.7967E+00	6.8546E-08	1.0000E+00

Layer=PPw_ ssAreaMatrix=6.6142E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	3.7671E+04	2.4605E+08	5.6955E+00	1.0000E+00
Np	1.9527E-02	1.2854E+02	2.9523E-06	1.0000E+00
Pu	3.4724E+00	2.2681E+04	5.2500E-04	1.0000E+00
Th	1.3531E+02	8.8378E+05	2.0458E-02	1.0000E+00
U	4.5338E-04	3.9612E+00	6.8546E-08	1.0000E+00

Layer=UCF_ ssAreaMatrix=6.9421E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	3.9539E+04	2.4605E+08	5.6955E+00	1.0000E+00
Np	2.0496E-02	1.2854E+02	2.9523E-06	1.0000E+00
Pu	3.6446E+00	2.2681E+04	5.2500E-04	1.0000E+00
Th	1.4202E+02	8.8378E+05	2.0458E-02	1.0000E+00
U	4.7586E-04	3.9612E+00	6.8546E-08	1.0000E+00

Layer=BFw_ ssAreaMatrix=2.8016E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5956E+04	3.0072E+08	5.6955E+00	1.0000E+00
Np	8.2711E-03	1.5688E+02	2.9523E-06	1.0000E+00
Pu	1.4708E+00	2.7721E+04	5.2500E-04	1.0000E+00
Th	5.7314E+01	1.0802E+06	2.0458E-02	1.0000E+00
U	1.9204E-04	4.6192E+00	6.8546E-08	1.0000E+00

Layer=UFZ_ ssAreaMatrix=2.7376E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5592E+04	3.0072E+08	5.6955E+00	1.0000E+00
Np	8.0824E-03	1.5688E+02	2.9523E-06	1.0000E+00
Pu	1.4373E+00	2.7721E+04	5.2500E-04	1.0000E+00
Th	5.6006E+01	1.0802E+06	2.0458E-02	1.0000E+00
U	1.8766E-04	4.6192E+00	6.8546E-08	1.0000E+00

Realization = 3 Subarea = 1 SATURATED ZONE

Layer=SAV ssAreaMatrix= 2.7505E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.5665E+04	3.0304E+08	0.0000E+00	0.0000E+00
Np	8.1203E-03	1.5809E+02	0.0000E+00	0.0000E+00
Pu	1.4440E+00	2.7935E+04	0.0000E+00	0.0000E+00
Th	5.6268E+01	1.0885E+06	0.0000E+00	0.0000E+00
U	1.8853E-04	4.6471E+00	0.0000E+00	0.0000E+00

Layer=STFF ssAreaMatrix= 4.8602E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.7681E+04	2.7338E+08	5.6955E+00	1.0000E+00
Np	1.4349E-02	1.4271E+02	2.9523E-06	1.0000E+00
Pu	2.5516E+00	2.5201E+04	5.2500E-04	1.0000E+00
Th	9.9430E+01	9.8198E+05	2.0458E-02	1.0000E+00
U	3.3315E-04	4.2902E+00	6.8546E-08	1.0000E+00

Realization = 3 Subarea = 1 SATURATED ZONE

Layer=SAV.

Nuclide	MobileRd
U	0.4647E+01
Am	0.3030E+09
Np	0.1581E+03
Pu	0.2793E+05
Th	0.1089E+07

Layer=STFF.

Nuclide	ImmobileRd
U	0.4290E+01
Am	0.2734E+09
Np	0.1427E+03
Pu	0.2520E+05
Th	0.9820E+06

Realization = 4 Subarea = 1 UNSATURATED ZONE

Layer=TSw_ ssAreaMatrix=2.9268E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	9.9600E+01	1.7968E+06	3.4030E-02	1.0000E+00
Np	1.9668E-04	4.5481E+00	6.7199E-08	1.0000E+00
Pu	9.3831E-02	1.6937E+03	3.2059E-05	1.0000E+00
Th	2.9939E+01	5.4010E+05	1.0229E-02	1.0000E+00
U	1.3479E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=CHnv ssAreaMatrix=8.7611E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.9814E+02	1.3680E+06	3.4030E-02	1.0000E+00
Np	5.8873E-04	3.7014E+00	6.7199E-08	1.0000E+00
Pu	2.8087E-01	1.2898E+03	3.2059E-05	1.0000E+00
Th	8.9618E+01	4.1121E+05	1.0229E-02	1.0000E+00
U	4.0348E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=CHnz ssAreaMatrix=8.0000E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.7224E+02	1.3884E+06	3.4030E-02	1.0000E+00
Np	5.3759E-04	3.7417E+00	6.7199E-08	1.0000E+00
Pu	2.5647E-01	1.3090E+03	3.2059E-05	1.0000E+00
Th	8.1833E+01	4.1735E+05	1.0229E-02	1.0000E+00
U	3.6843E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=PPw_ ssAreaMatrix=6.6142E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.2508E+02	1.4701E+06	3.4030E-02	1.0000E+00
Np	4.4447E-04	3.9030E+00	6.7199E-08	1.0000E+00
Pu	2.1204E-01	1.3860E+03	3.2059E-05	1.0000E+00
Th	6.7657E+01	4.4190E+05	1.0229E-02	1.0000E+00
U	3.0460E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=UCF_ ssAreaMatrix=6.9421E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	2.3624E+02	1.4701E+06	3.4030E-02	1.0000E+00
Np	4.6650E-04	3.9030E+00	6.7199E-08	1.0000E+00
Pu	2.2256E-01	1.3860E+03	3.2059E-05	1.0000E+00
Th	7.1012E+01	4.4190E+05	1.0229E-02	1.0000E+00
U	3.1971E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=BFw_ ssAreaMatrix=2.8016E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	9.5337E+01	1.7968E+06	3.4030E-02	1.0000E+00
Np	1.8826E-04	4.5481E+00	6.7199E-08	1.0000E+00
Pu	8.9815E-02	1.6937E+03	3.2059E-05	1.0000E+00
Th	2.8657E+01	5.4010E+05	1.0229E-02	1.0000E+00
U	1.2902E-08	1.0002E+00	4.6053E-12	1.0000E+00

Layer=UFZ_ ssAreaMatrix=2.7376E+03 ssAreaFracture=1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	9.3162E+01	1.7968E+06	3.4030E-02	1.0000E+00
Np	1.8397E-04	4.5481E+00	6.7199E-08	1.0000E+00
Pu	8.7766E-02	1.6937E+03	3.2059E-05	1.0000E+00
Th	2.8004E+01	5.4010E+05	1.0229E-02	1.0000E+00
U	1.2608E-08	1.0002E+00	4.6053E-12	1.0000E+00

Realization = 4 Subarea = 1 SATURATED ZONE

Layer=SAV ssAreaMatrix= 3.5900E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.2217E+02	1.7401E+06	0.0000E+00	0.0000E+00
Np	2.4124E-04	4.4362E+00	0.0000E+00	0.0000E+00
Pu	1.1509E-01	1.6403E+03	0.0000E+00	0.0000E+00
Th	3.6722E+01	5.2307E+05	0.0000E+00	0.0000E+00
U	1.6533E-08	1.0002E+00	0.0000E+00	0.0000E+00

Layer=STFF ssAreaMatrix= 4.8572E+03 ssAreaFracture= 1.0000E+00

Nuclide	matrixKD	matrixRD	fractureKD	fractureRD
Am	1.6529E+02	1.6334E+06	3.4030E-02	1.0000E+00

Np	3.2640E-04	4.2255E+00	6.7199E-08	1.0000E+00
Pu	1.5572E-01	1.5398E+03	3.2059E-05	1.0000E+00
Th	4.9685E+01	4.9100E+05	1.0229E-02	1.0000E+00
U	2.2369E-08	1.0002E+00	4.6053E-12	1.0000E+00

Realization = 4 Subarea = 1 SATURATED ZONE

Layer=SAV.

Nuclide	MobileRd
U	0.1000E+01
Am	0.1740E+07
Np	0.4436E+01
Pu	0.1640E+04
Th	0.5231E+06

Layer=STFF.

Nuclide	ImmobileRd
U	0.1000E+01
Am	0.1633E+07
Np	0.4226E+01
Pu	0.1540E+04
Th	0.4910E+06

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-490	**2. Software Title and Version:** TPA 5.0.0b	**3. Project No:** 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): *volcano.f, tpa.inp, tpanames.dbs* and *driftsa.i.*

See Attachment A for selected text from a series of e-mails from B. Hill for the description.

5. Change Requested by: B. Hill Date: 8-20-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 8-20-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

#1 - Parameter name change:
OLD= `'DiameterOfVolcanicCone[m]'`
NEW= `'DiameterOfVolcanicConduit[m]'`
New values used as described in Attachment A.
#2 - In order to keep the intent of the geometric model the suggested change was not made, but rather a fully disrupted drift (similar to dogleg) algorithm was added to the geometric model. This required a new subroutine called *getdrifts*(), located in *volcano.f.*
#3 - Two points were added to the *usersuppliedpwisecdf* distribution in Attachment A to replace the first point:
0.0 0.0
0.1 0.084
#4 - new values used as described in Attachment A.

8. Implemented by: R. Janetzke	**Date:** 9-25-2004

9. Description of Acceptance Tests:

See ATTACHMENTS B & C.

10. Tested by: R. Nes	**Date:** 03-25-2005

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
DELETE	Volcano	DiameterOfVolcanicCone[m]					
ADD	Volcano	DiameterOfVolcanicConduit[m]	Used for calculating the number of packages ejected for an extrusive event in the geometric model. (Applies to ash evolution mode = 0 only)	Uniform	28, 280	Reflect a more accurate designation of the conduit.	

MODIFY TO	Volcano	NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]	Used for calculating the number of packages failed for the intrusive event in the distribution model.	usersuppliedpwisecdf	19 0 0. 0.1 0.084 200 0.094 600 0.117 1000 0.141 1400 0.175 1800 0.213 2110 0.257 2111 0.475 2827 0.562 3147 0.588 3148 0.712 5000 0.781 6300 0.813 7800 0.843 9122 0.881 9123 0.967 9444 0.969 9445 1.000		
MODIFY TO	Ashplumo	VolcanicEventDuration[s]		loguniform	8.64e4 2.59e5		
MODIFY TO	Ashplumo	VolcanicEventPower[W]		loguniform	9.0e9 5.0e11		

ATTACHMENT A

1) Conduit diameters (DiameterOfVolcanicCone) should thus be 28-280 m to represent 1-10 WP ejected with these HLW loadings. Currently, we're using 24.6-77.9 which was based on the SR design.

2) Assuming a rigid dike geometry grossly underestimates the number of failed WP during an intrusive event. Thus, NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[] should always be sampled, regardless of VolcanoModel=1 or 2.

3)
usersuppliedpwisecdf
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]
18
0 0.084
200 0.094
600 0.117
1000 0.141
1400 0.175
1800 0.213
2110 0.257
2111 0.475
2827 0.562
3147 0.588
3148 0.712
5000 0.781
6300 0.813
7800 0.843
9122 0.881
9123 0.967
9444 0.969
9445 1.000

4)
loguniform
VolcanicEventDuration[s]
8.64e4, 2.59e5
**
loguniform
VolcanicEventPower[W]
9.0e9, 5.0e11

ATTACHMENT B

Test Plan for TPA SCR#490

Test Plan Name:

Tested By: Razvan Nes, Albert Lozano Date: 03-25-2005

Host Machine: Frisco, Spock Host OS: Windows 2000 Professional, Unix

Baseline Version: tpa500b Test Version: tpa500c

Process Level (PL) Tests

PL-1. Name: Parameter name change in tpa.inp
Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : N/A
Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:
Test description:
- objective: ensure that old parameter name was replaced with the new one
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: N/A
- step by step test procedure to be used:
  1-visually examine tpa.inp of tpa500b and tpa500c, and identify in each situation where the parameter of interest is located
  2-ensure that old name 'DiameterOf VocanicCone[m]' used in the input file of tpa500b was replaced in tpa500c with 'DiameterOfVolcanicConduit[m], and check also *volcano.f*.
- pass/fail criteria: pass if the replacement was made correctly(i.e. according to PA-SCR-490)

Test Results:
-See ATTACHMENT C;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

PL-2.: Name: Implementation of a fully disrupted drift algorithm, and adding a new subroutine, getdrifts(), in volcano.f
Path for run directory:

Path for archive of results:
Environment variables:
Special input files or modifications to input files required : N/A
Special diagnostic code modifications required : add 'Print ' instructions in volcano.f (see ATTACHMENT C)
Program modes to be used (append flags, scenario/model switches, etc.): set VolcanoModel flag to 1 (Geometric Model)
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:N/A
Test description:
- objective: ensure that old distribution parameters were replaced with the new ones.
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: N/A
- step by step test procedure to be used:
  1-open volcano.f and go where subroutine getdrifts(drxy1out, drxy2out, nWPindrift, maxnumdrifts, ndrifts) is called
  2-put Print statements in volcano.f module of tpa500c, so the code will print drxy1out, x1, y1, drxy2out, x2, y2, nWPindrift
  3-visually compare the data printed in tpa output file tparun.txt as the result of these statements with the ones in *drifts. dat*
- pass/fail criteria: pass, if the two sets of data are identical.

Test Results:
-See ATTACHMENT C;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL): **PASS**

PL-3. Name: New points added in NumberOfMagmaInducedMechanicalFailuresRemainingInDrift distribution of tpa.inp-Volcano

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : N/A
Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:
Test description:
- objective: ensure that old parameter name was replaced with the new one
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: N/A
- step by step test procedure to be used:
  1-visually examine tpa.inp of tpa500b and tpa500c, and identify in each situation where NumberOfMagmaInducedMechanicalFailuresRemainingInDrift

distribution is located
2-visually compare the two distributions and ensure that old distribution used by tpa500b was replaced in tpa500c with the new one, that includes the new points as per PA-SCR-490.
- pass/fail criteria: pass if the replacement was made correctly (i.e. as per PA-SCR-490).

Test Results: -See ATTACHMENT C;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL): **PASS**

PL-4. Name: New values for 'VolcanicEventDuration[s]' and VolcanicEventPower[W]' in tpa.inp-Volcano

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : N/A
Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:

Test description:
- objective: ensure that old distribution parameters were replaced with the new ones.
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: N/A
- step by step test procedure to be used:
  1-visually examine tpa.inp of tpa500b and tpa500c, and identify in each situation where 'VolcanicEventDuration[s]' and VolcanicEventPower[W]' distributions are located
  2-visually compare the two distributions and ensure that old distribution used by tpa500b was replaced in tpa500c with the new ones, that includes the new points as per PA-SCR-490.
- pass/fail criteria: pass if the replacement was made correctly (i.e. as per PA-SCR-490).

Test Results: -See ATTACHMENT C;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL): **PASS**

ATTACHMENT C

PL-1: Input files of tpa 5.0.0b and 5.0.0c, shown below, were visually compared:

-Version 5.0.0b:

```
uniform
DiameterOfVolcanicCone[m]
24.6, 77.9
```

-Version 5.0.0c:

```
uniform
DiameterOfVolcanicConduit[m]
28.0, 280.0
```

Conclusion: Proposed name change was correctly implemented in tpa 5.0.0c, in the input file and tpanames.dbs of the same code version.

Volcano.f file of tpa500c:

```
c rwj 8-22-04; SCR 490;
c       name = 'DiameterOfVolcanicCone[m]'
        name = 'DiameterOfVolcanicConduit[m]'
```

PL-2: Print statements placed in *volcano.f*, and compared tpa output file with *drifts.dat*.

-Print statements in *volcano.f*:

```
                cc rwj 9-25-04; SCR490
                call getdrifts(drxy1out, drxy2out, nWPindrift, maxnumdrifts,
&                       ndrifts)
 print *,"maxnumdrifts = ",maxnumdrifts
 print *,"ndrifts = ",ndrifts
   print *," drxy1out     x1                y1",
&  " drxy2out     x2                y2"," nWPindrift"
   do i=1,ndrifts
     print '(4(1x,1pe15.7),i6)',drxy1out(1,i),drxy1out(2,i),
&    drxy2out(1,i),drxy2out(2,i), nWPindrift(i)
 enddo
 print *," "
   ikey=30231
```

-Printed data in the output file:

drxy1out x1	y1	drxy2out x2	y2	nWPindrift
5.4856719E+05	4.0789380E+06	5.4751062E+05	4.0792695E+06	180
5.4856305E+05	4.0788544E+06	5.4750210E+05	4.0791873E+06	181
5.4855890E+05	4.0787708E+06	5.4749357E+05	4.0791051E+06	181
5.4855476E+05	4.0786872E+06	5.4748505E+05	4.0790228E+06	182

5.4855062E+05	4.0786037E+06	5.4747653E+05	4.0789406E+06	183
5.4854648E+05	4.0785201E+06	5.4746801E+05	4.0788584E+06	184
5.4854233E+05	4.0784365E+06	5.4745948E+05	4.0787762E+06	184
5.4853819E+05	4.0783529E+06	5.4745096E+05	4.0786940E+06	185
5.4853405E+05	4.0782693E+06	5.4744244E+05	4.0786118E+06	186
5.4852990E+05	4.0781857E+06	5.4743392E+05	4.0785295E+06	187
5.4852576E+05	4.0781021E+06	5.4742540E+05	4.0784473E+06	187
5.4852162E+05	4.0780185E+06	5.4741687E+05	4.0783651E+06	188
5.4851747E+05	4.0779349E+06	5.4740835E+05	4.0782829E+06	189
5.4851333E+05	4.0778513E+06	5.4739983E+05	4.0782006E+06	190
5.4850919E+05	4.0777677E+06	5.4739131E+05	4.0781184E+06	190
5.4850505E+05	4.0776841E+06	5.4738279E+05	4.0780362E+06	191
5.4850090E+05	4.0776005E+06	5.4737426E+05	4.0779540E+06	192
5.4849676E+05	4.0775170E+06	5.4737981E+05	4.0778674E+06	190
5.4849261E+05	4.0774334E+06	5.4739430E+05	4.0777779E+06	187
5.4848847E+05	4.0773498E+06	5.4740879E+05	4.0776885E+06	184
5.4848433E+05	4.0772662E+06	5.4742327E+05	4.0775990E+06	181
5.4848018E+05	4.0771826E+06	5.4743776E+05	4.0775096E+06	177
5.4847604E+05	4.0770990E+06	5.4745225E+05	4.0774202E+06	174
5.4847190E+05	4.0770154E+06	5.4746674E+05	4.0773307E+06	171
5.4846775E+05	4.0769318E+06	5.4748099E+05	4.0772414E+06	168
5.4846361E+05	4.0768482E+06	5.4749496E+05	4.0771521E+06	165
5.4845947E+05	4.0767646E+06	5.4750893E+05	4.0770628E+06	162
5.4845532E+05	4.0766810E+06	5.4752290E+05	4.0769735E+06	159
5.4842592E+05	4.0766054E+06	5.4753687E+05	4.0768843E+06	151
5.4839439E+05	4.0765304E+06	5.4755084E+05	4.0767950E+06	144
5.4836286E+05	4.0764554E+06	5.4756481E+05	4.0767057E+06	136
5.4833133E+05	4.0763804E+06	5.4757877E+05	4.0766165E+06	128
5.4829979E+05	4.0763054E+06	5.4759274E+05	4.0765272E+06	120
5.4826826E+05	4.0762304E+06	5.4760671E+05	4.0764379E+06	112
5.4823673E+05	4.0761554E+06	5.4762068E+05	4.0763486E+06	105
5.4820519E+05	4.0760804E+06	5.4763465E+05	4.0762594E+06	97
5.4817366E+05	4.0760054E+06	5.4764861E+05	4.0761701E+06	89
5.4857133E+05	4.0790216E+06	5.4752920E+05	4.0793486E+06	177
5.4857548E+05	4.0791052E+06	5.4755785E+05	4.0794245E+06	173
5.4857962E+05	4.0791888E+06	5.4758651E+05	4.0795004E+06	169
5.4858377E+05	4.0792724E+06	5.4761516E+05	4.0795763E+06	165
5.4858791E+05	4.0793560E+06	5.4764381E+05	4.0796522E+06	161
5.4859258E+05	4.0794394E+06	5.4765057E+05	4.0797350E+06	160
5.4859744E+05	4.0795228E+06	5.4765615E+05	4.0798181E+06	160
5.4860230E+05	4.0796062E+06	5.4766173E+05	4.0799012E+06	160
5.4860715E+05	4.0796895E+06	5.4766731E+05	4.0799844E+06	160
5.4861201E+05	4.0797729E+06	5.4767290E+05	4.0800675E+06	160
5.4861686E+05	4.0798563E+06	5.4767848E+05	4.0801507E+06	160
5.4862172E+05	4.0799396E+06	5.4768406E+05	4.0802338E+06	160
5.4862657E+05	4.0800230E+06	5.4768964E+05	4.0803169E+06	159
5.4863143E+05	4.0801064E+06	5.4769523E+05	4.0804001E+06	159
5.4863629E+05	4.0801897E+06	5.4770081E+05	4.0804832E+06	159
5.4864114E+05	4.0802731E+06	5.4770639E+05	4.0805664E+06	159
5.4864600E+05	4.0803565E+06	5.4771197E+05	4.0806495E+06	116

-Printed data in *drifts. dat* :

```
Emplacement Block
          1
**  Drift Endpoints
**   x1              y1              x2              y2          numWP
 5.48567190E+05 4.07893803E+06 5.47510619E+05 4.07926950E+06   180
```

5.48563047E+05	4.07885444E+06	5.47502097E+05	4.07918728E+06	181
5.48558904E+05	4.07877084E+06	5.47493574E+05	4.07910506E+06	181
5.48554761E+05	4.07868725E+06	5.47485052E+05	4.07902284E+06	182
5.48550618E+05	4.07860366E+06	5.47476530E+05	4.07894062E+06	183
5.48546476E+05	4.07852006E+06	5.47468007E+05	4.07885841E+06	184
5.48542333E+05	4.07843647E+06	5.47459485E+05	4.07877619E+06	184
5.48538190E+05	4.07835288E+06	5.47450963E+05	4.07869397E+06	185
5.48534047E+05	4.07826929E+06	5.47442441E+05	4.07861175E+06	186
5.48529904E+05	4.07818569E+06	5.47433918E+05	4.07852953E+06	187
5.48525761E+05	4.07810210E+06	5.47425396E+05	4.07844731E+06	187
5.48521618E+05	4.07801851E+06	5.47416874E+05	4.07836509E+06	188
5.48517475E+05	4.07793491E+06	5.47408352E+05	4.07828287E+06	189
5.48513332E+05	4.07785132E+06	5.47399829E+05	4.07820065E+06	190
5.48509189E+05	4.07776773E+06	5.47391307E+05	4.07811844E+06	190
5.48505046E+05	4.07768414E+06	5.47382785E+05	4.07803622E+06	191
5.48500902E+05	4.07760054E+06	5.47374262E+05	4.07795400E+06	192
5.48496758E+05	4.07751695E+06	5.47379807E+05	4.07786737E+06	190
5.48492614E+05	4.07743336E+06	5.47394296E+05	4.07777793E+06	187
5.48488470E+05	4.07734977E+06	5.47408785E+05	4.07768849E+06	184
5.48484326E+05	4.07726617E+06	5.47423274E+05	4.07759905E+06	181
5.48480182E+05	4.07718258E+06	5.47437762E+05	4.07750961E+06	177
5.48476039E+05	4.07709899E+06	5.47452251E+05	4.07742017E+06	174
5.48471896E+05	4.07701539E+06	5.47466740E+05	4.07733074E+06	171
5.48467752E+05	4.07693180E+06	5.47480994E+05	4.07724137E+06	168
5.48463609E+05	4.07684821E+06	5.47494963E+05	4.07715210E+06	165
5.48459466E+05	4.07676462E+06	5.47508931E+05	4.07706282E+06	162
5.48455323E+05	4.07668102E+06	5.47522900E+05	4.07697355E+06	159
5.48425924E+05	4.07660535E+06	5.47536868E+05	4.07688427E+06	151
5.48394392E+05	4.07653035E+06	5.47550836E+05	4.07679500E+06	144
5.48362859E+05	4.07645535E+06	5.47564805E+05	4.07670572E+06	136
5.48331326E+05	4.07638035E+06	5.47578773E+05	4.07661645E+06	128
5.48299793E+05	4.07630535E+06	5.47592742E+05	4.07652717E+06	120
5.48268261E+05	4.07623035E+06	5.47606710E+05	4.07643790E+06	112
5.48236728E+05	4.07615535E+06	5.47620679E+05	4.07634862E+06	105
5.48205195E+05	4.07608035E+06	5.47634647E+05	4.07625935E+06	97
5.48173663E+05	4.07600535E+06	5.47648615E+05	4.07617007E+06	89

**
Emplacement Block
2
** Drift Endpoints

** x1	y1	x2	y2	numWP
5.48571334E+05	4.07902162E+06	5.47529205E+05	4.07934856E+06	177
5.48575478E+05	4.07910521E+06	5.47557855E+05	4.07942447E+06	173
5.48579623E+05	4.07918881E+06	5.47586505E+05	4.07950037E+06	169
5.48583767E+05	4.07927240E+06	5.47615155E+05	4.07957628E+06	165
5.48587911E+05	4.07935599E+06	5.47643805E+05	4.07965218E+06	161
5.48592583E+05	4.07943942E+06	5.47650567E+05	4.07973495E+06	160
5.48597439E+05	4.07952279E+06	5.47656149E+05	4.07981809E+06	160
5.48602295E+05	4.07960616E+06	5.47661732E+05	4.07990123E+06	160
5.48607151E+05	4.07968952E+06	5.47667314E+05	4.07998437E+06	160
5.48612007E+05	4.07977289E+06	5.47672896E+05	4.08006752E+06	160
5.48616863E+05	4.07985626E+06	5.47678479E+05	4.08015066E+06	160
5.48621719E+05	4.07993963E+06	5.47684061E+05	4.08023380E+06	160
5.48626574E+05	4.08002300E+06	5.47689643E+05	4.08031694E+06	159
5.48631430E+05	4.08010637E+06	5.47695226E+05	4.08040008E+06	159
5.48636286E+05	4.08018974E+06	5.47700808E+05	4.08048322E+06	159
5.48641142E+05	4.08027311E+06	5.47706390E+05	4.08056636E+06	159
5.48645998E+05	4.08035648E+06	5.47711973E+05	4.08064951E+06	116

Conclusion: Data printed in the tpa output and in *drifts.dat* are identical; subroutine *getdrifts.f* was correctly implemented and works properly.

PL-3: The distribution NumberOfMagmaInducedMechanicalFailuresRemainingInDrift, in the input files of versions 5.0.0b and 5.0.0c, are as follows:

-Version 5.0.0b:

```
loguniform
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]
1.0, 1402.0
```

-Version 5.0.0c:

```
usersuppliedpwisecdf
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]
19
0.      0.000
0.1     0.084
200.    0.094
600.    0.117
1000.   0.141
1400.   0.175
1800.   0.213
2110.   0.257
2111.   0.475
2827.   0.562
3147.   0.588
3148.   0.712
5000.   0.781
6300.   0.813
7800.   0.843
9122.   0.881
9123.   0.967
9444.   0.969
9445.   1.000
```

Conclusion: Visual comparison is confirming (1) old lognormal distribution was replaced with an user-provided one, and (2) two new points (0.0,0.0) were added to the distribution shown in Appendix A.

PL-4: Parameters VolcanicEventDuration and VolcanicEventPower as in the input files of 5.0.0b and 5.0.0c:

-Version 5.0.0b:

```
loguniform
```

```
VolcanicEventDuration[s]
1.8e5, 1.3e6

loguniform
VolcanicEventPower[W]
3.5e9, 5.3e11
```

-Version 5.0.0c:

```
loguniform
VolcanicEventDuration[s]
8.64e4, 2.59e5

loguniform
VolcanicEventPower[W]
9.0e9,  5.0e11
```

Conclusion: New values were correctly implemented in the tpa 5.0.0c input file.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-517	**2. Software Title and Version:** TPA 5.0	**3. Project No:** 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s):

Affected modules: UZFT, SZFT.

Per attached memo (Attachment A) from P. Bertetti. Problems relating to: (I) data file (coefkdeq.dat) used to provide coefficients for calculating sorption coefficients for Am, Np, Pu, Th and U, (ii) specific surface area for tuff and alluvium, and (iii) bulk density and total porosity for calculating radionuclide retardation factors. Also, linear interpolation required between the response function curves for calculating sorption coefficients.

5. Change Requested by: P. Bertetti Date: 8-20-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 8-20-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):
See Attachments B & D.

8. Implemented by: O. Osidele	**Date:** 9-14-2004

9. Description of Acceptance Tests:
The software was tested in accordance with the Test Plan for TPA SCR# 517 (see tp_scr517.wpd). The software, test directories, and test results are contained on a CD labeled "TPA SCR#517 - Test Directories." System Level Test 1 failed, thus generating SCR #523. All other tests passed.

10. Tested by: C. Scherer	**Date:** 11-19-2004

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
ADD	SZFT	AlluviumTotalPorosity_SAV	used for calculating retardation factor for radionuclides in the saturated alluvium layer	uniform	0.15 - 0.3	Range provided by software change requester (P.Bertetti), based on measured values from Fortymile Wash	PB
ADD	SZFT	AlluviumMatrixSpecificSurfaceArea	used for calculating sorption coefficient for radionuclides in the saturated alluvium layer	uniform	1900 - 12100 m^2/Kg	Range provided by software change requester (P.Bertetti), based on sonic core samples from Fortymile Wash	PB

ADD	CORRELATED PARAMETERS	LogCO2PartialPressure_AllUZ_SZLayers[atm], pH_AllUZ_SZLayers[StandardUnits]		correlateinputs	-0.83		PB
MODIFY FROM	UZFT	pH_AllUZ_SZLayers[StandardUnits]		normal	6.3, 9.6		PB
MODIFY TO	UZFT	pH_AllUZ_SZLayers[StandardUnits]		triangular	6.7, 9.2, 7.8		PB
MODIFY FROM	UZFT	LogCO2PartialPressure_AllUZ_SZLayers[atm]		normal	-5.08, -0.77		PB
MODIFY TO	UZFT	LogCO2PartialPressure_AllUZ_SZLayers[atm]		triangular	-4.0, -1.0, -2.5		PB

Attachment A

Description of problem:

Summary of Meeting on Radionuclide Transport Parameters and Coding in TPA

We reviewed a number of topics concerning possible modifications to parameters used in calculating radionuclide Kds and Rds (especially those in which Turner's method is used - Am, Np, Pu, Th and U) and reviewed possible changes to the code to correct deficiencies or weak technical bases. This summary includes what I believe to be the most important points and provides a point of view that reflects the consensus of opinion expressed at the meeting.

1. coefkdeq.dat

The data file (coefkdeq.dat) used to provide coefficients to calculate Ka' values for subsequent use in calculation of Kd and Rd needs to be updated. The original curve fits of surface complexation model results include residual errors that results in a significant mismatch between the SCM curves and TPA-produced versions of the curves. Although this is most evident for Np, the problem affects Pu and U as well. These errors can be reduced significantly by re-fitting the SCM curves and producing and updated coefficient file. Corrections have been made for Np and will be made for U and Pu in the next few weeks (Bertetti). TPA staff will need to incorporate the modified coefkdeq.dat into the final verison of TPA 5.0.

2. Surface area calculations

The effective specific surface areas of the various hydrogeologic layers in the TPA code are used in the calculation and conversion of Ka' to Kd for Am, Np, Pu, Th and U. Specific surface areas are calculated using a relationship found in Arthur (1996), which uses an idealized geometric representation of pore spaces to estimate surface area of whole rock with known porosity and density. The relationship was originally utilized for consolidated crystalline rock.

a. A single constant value is used to represent the pore size distribution of the rock layers within TPA. A more appropriate and defensible method should include a distribution of pore sizes based on measurements. The current value of 0.05×10^{-6} m does produce reasonable surface area values for tuff layers.

b. The pore size value for tuffs is probably not appropriate for the alluvium (SAV layer in TPA) and is not consistent with observations of in Fortymile Wash alluvium, yet the constant value is used for SAV. A recent analysis of surface area for well cuttings and sonic core samples suggest that we can produce a defensible distribution of surface area values for the SAV. Modifications to the TPA code will be required to introduce this new parameter and to modify the surface area calculation for this layer.

c. The values used for porosity and density in the surface area calculation need to be reviewed. The relationship in Arthur appears to call for total porosity and bulk density. Instead, grain density values are used in the code. Also, the code uses effective porosity in the calculation for alluvium. It appears that the tuff values in the code represent total porosity. The code could be modified to include a bulk density calculation (grain density * (1-porosity)) similar to that used in the Kd calculation. This modification should be incorporated into TPA 5.0.

3. Effective porosity for alluvium

The code uses alluvium effective porosity in calculations to determine surface area and Rd. Total porosity should be used. The Rd calculation should be modified accordingly to include a scaling factor or alternate parameter distribution for alluvium porosity. Modifications to the surface area calculation would not be required if alluvium surface area is sampled directly as suggested above.

4. pH and CO_2 distributions

pH and CO_2 distributions produced by the TPA code are slightly different than the distribution produced by the Perfect et al. data set. Because of other issues, it is difficult to analyze the importance of this difference. Recent chemical analyses of Fortymile Wash groundwaters suggest that adding those values might shift the pH and CO_2 range toward the values that TPA currently produces. There are some differences in estimated dose when the new range is implemented, but the differences do not appear to be significant. The parameter range should be updated, but only after other issues are dealt with.

5. Intermediate analysis results

It is difficult to conduct intermediate analyses because the code does not produce a set of stored values for surface area, Kd, and Rd. Recent modifications have been made by Janetzke et al. to provide such output, but it is not available to most versions of TPA 5.0.

Attachment B

The following changes implemented in the TPA 5.0.1 code:

1. Interpolation of response functions for calculating the specific surface area normalized sorption coefficient (Ka').

   Affected source code file: `uzft.f`

   Linear interpolation performed after calculating the bounding Ka' values for the sampled pC02 and pH values. Four new variables introduced:

`dln_kd_aprime1`:	log Ka' (for lower bound pCO2)
`dln_kd_aprime2`:	log Ka' (for upper bound pCO2)
`ipco2idx1`:	index for pCO2 array (lower bound)
`ipco2idx2`:	index for pCO2 array (upper bound)

   Modified section of the code as follows:

```
c   O.Osidele Sep02,2004 SCR517
c
      do i=1,nradioelements  !Am,Np,Pu,Th,U

         j=1
         do while (pco2in.gt.params(1,j,i) .and. j.lt.nrows)
            j=j+1
         end do
         ipco2idx2 = j
         ipco2idx1 = j-1

         if (phin .ge. params(2,ipco2idx2,i) .and.
     &       phin .le. params(3,ipco2idx2,i)) then
            dln_kd_aprime2 = params(4,ipco2idx2,i)          +
     &                       params(5,ipco2idx2,i)*phin     +
     &                       params(6,ipco2idx2,i)*phin**2  +
     &                       params(7,ipco2idx2,i)*phin**3  +
     &                       params(8,ipco2idx2,i)*phin**4  +
     &                       params(9,ipco2idx2,i)*phin**5
            dln_kd_aprime1 = params(4,ipco2idx1,i)          +
     &                       params(5,ipco2idx1,i)*phin     +
     &                       params(6,ipco2idx1,i)*phin**2  +
     &                       params(7,ipco2idx1,i)*phin**3  +
     &                       params(8,ipco2idx1,i)*phin**4  +
     &                       params(9,ipco2idx1,i)*phin**5
            dtemp          = params(1,ipco2idx2,i)-params(1,ipco2idx1,i)
            dtemp          = (pco2in - params(1,ipco2idx1,i))/dtemp
            dtemp          = dtemp*(dln_kd_aprime2 - dln_kd_aprime1)
            dln_kd_aprime  = dln_kd_aprime1 + dtemp
            dkd_aprime     = 10.D0**(dln_kd_aprime)
            kds(i)         = dkd_aprime * ssareain * 1.0D-6   !=m^3/kg
         else
            kds(i) = 0.d0
```

```
          endif
        enddo
c
c   end SCR517
```

2. Installation of data file (`coefkdeq.dat`), provided by P.Bertetti, containing revised coefficients of the polynomial for calculating the Ka' values in 1. above.

   Contents of `coefkdeq.dat` file shown in Attachment C. Modifications made to the Np(V) pH sampling range (pHhigh) and coefficients (a - f) on the first four rows, i.e., for `logPCO2` = {-0.5, -1.0, -1.5, -2.0}.

3. New stochastic parameters for total porosity and specific surface area for the saturated alluvium (SAV) layer.

   Affected source code file: `szft.f`

   `AlluviumTotalPorosity_SAV` and `AlluviumMatrixSpecificSurfaceArea` included in `tpa.inp`, thus:

```
** O.Osidele Sep02,2004 SCR517
uniform
AlluviumTotalPorosity_SAV
1.5e-1, 3.0e-1
**
uniform
AlluviumMatrixSpecificSurfaceArea[m2/kg]
2.0e3, 1.0e4
**
** end SCR517
```

   `szft.f` modified to apply these new parameters only to the saturated alluvium layer:

```
c  O.Osidele Sep02,2004 SCR517
      dimension imtotalporosity(maxlayers)
      dimension imssarea(maxlayers)
c  end  SCR517

c    O.Osidele Sep02,2004 SCR517
        call clearchar( 60, fname )
        fname= 'AlluviumTotalPorosity_'//salayernam(ilayer)(1:3)
        imtotalporosity(ilayer)   =  ispquery( fname )
        call clearchar( 60, fname )
        fname= 'AlluviumMatrixSpecificSurfaceArea[m2/kg]'
        imssarea(ilayer)   =  ispquery( fname )
c    end SCR517

c   O.Osidele Sep02,2004 SCR517
            if (ilayer .eq. 2) then
```

```
            porosity = valuesp(imtotalporosity(ilayer))
            ssarea   = valuesp(imssarea(ilayer))
         else
            porosity = valuesp(imporosity(ilayer))
            ssarea   = 3.0d0*porosity / (density*poreradius)
         end if
c   end SCR517
```

4. Bulk density calculation (grain density * (1 - porosity)) already exists in subroutine `calc_rd` in `uzft.f`. This request (see Attachment A, 2c) was not implemented.

Attachment C

Contents of `coefkdeq.dat` data file:

```
# Coefficients for equations for KD values for five radioelements: Am, Np, Pu, Th, U. Refer
to equations provided by D.Turner. Implementation by S. Mohanty
# Equation parameters and summary of fit results for model curves at discrete PCO2.  Derived
using complete MINTEQA2 generated data set with polynomial fitting by Microsoft Excel 97.
# Expressed in terms of log10 (Ka',in mL/m^2) = a + bx + cx^2 + dx^3 + ex^4 + fx^5 = log10
(Kd/Sa), where x is pH.
#   SCR #427:  correct coefficient values and increase precision (css - 2-14-2003)
#       model requires precision of at least 8 decimal places
# date: 2_13_2003 TPA 5.0betaN    <-- must have word "date" in last header line only.
5     10    !Number of radioelements, Number of data rows for each radioelement
Am(III)
logPCO2(atm) pHLow pHhigh  a              b               c              d              e
  f
  -0.5    6.0    8.50     307.59001700   -200.73337400    48.86857390   -5.34389002   0.24664848
-0.00310416
  -1.0    6.0    9.00  -1270.65128000    961.11970500  -288.77291100   43.05229710  -3.17369574
0.09226157
  -1.5    6.0    9.00  -1045.53642000    775.07897900  -228.07702300   33.27615880  -2.39638932
0.06789750
  -2.0    6.0    9.25   -529.70097000    382.57883000  -109.82740500   15.64244660  -1.09501774
0.02991442
  -2.5    6.0    9.25      9.99115550    -19.12208470     8.43510534   -1.57254303   0.14374613
-0.00530121
  -3.0    6.0    9.50     207.97473500   -163.91087800    50.26749810   -7.53911613   0.56336067
-0.01690361
  -3.5    6.0    9.50     275.22137700   -211.82535300    63.68167270   -9.37809594   0.68606024
-0.02004885
  -4.0    6.0   10.00     277.38065700   -210.45818600    62.29763580   -9.01473543   0.64646365
-0.01846756
  -4.5    6.0   10.25     130.72585800    -98.62225380    28.50975860   -3.95833162   0.27147852
-0.00743480
  -5.0    6.0   10.50      33.74073080    -25.65826470     6.78522964   -0.75797035   0.03813970
-0.00069526
Np(V)
logPCO2(atm) pHLow pHhigh  a              b               c              d              e
  f
  -0.5    6.0    8.00     562.54981909   -500.89579959   176.89291309  -31.07712098   2.71862591
-0.09472022
  -1.0    6.0    8.25    1247.11170086  -1023.28658622   333.71423224  -54.15807008   4.37697101
-0.14095145
  -1.5    6.0    8.50    1167.89757131   -934.90857095   296.99958911  -46.88540807   3.68114075
-0.11502710
  -2.0    6.0    8.75     889.34085898   -699.35389929   217.86487385  -33.68430687   2.58768006
-0.07904888
  -2.5    6.0    9.25     604.15463949   -471.18717183   145.25628277  -22.19529238   1.68365358
-0.05074650
  -3.0    6.0    9.50     764.24156979   -579.32259744   173.40177062  -25.68199425   1.88477442
-0.05486468
  -3.5    6.0    9.50     359.65220164   -271.53092875    80.62144476  -11.82780553   0.85976307
-0.02479575
  -4.0    6.0   10.00     201.90140192   -151.49269268    44.42444548   -6.42016723   0.45942406
-0.01304250
  -4.5    6.0   10.25     144.58349394   -107.42340532    30.99109298   -4.39069911   0.30744094
-0.00852804
  -5.0    6.0   10.50      95.81229583    -70.41985478    19.87058564   -2.73585264   0.18548048
-0.00496593
Pu(V)
```

logPCO2(atm)	pHLow	pHhigh	a	b	c	d	e	f
-0.5	6.0	8.50	1246.30948721	-903.72709304	257.51364332	-36.06686622	2.48869143	-0.06789596
-1.0	6.0	9.00	-587.02195729	460.07381777	-143.09761162	22.00344618	-1.66475939	0.04939950
-1.5	6.0	9.00	-1184.45306764	883.86678055	-261.02854931	38.07646118	-2.73662325	0.07737175
-2.0	6.0	9.25	-50.02594030	30.68415531	-7.14589011	0.71916125	-0.01921190	-0.00076903
-2.5	6.0	9.25	393.21942695	-296.88006200	88.46809928	-13.05328221	0.95901834	-0.02814551
-3.0	6.0	9.50	-95.11976538	67.08508393	-18.86016332	2.60556000	-0.17203212	0.00424400
-3.5	6.0	9.50	-230.00692092	165.06322240	-46.98805430	6.59970619	-0.45311977	0.01211012
-4.0	6.0	10.00	-120.56773140	82.02325299	-22.11369394	2.92664506	-0.18608722	0.00447629
-4.5	6.0	10.25	7.90514519	-13.32252306	5.80401936	-1.10171044	0.10010108	-0.00352281
-5.0	6.0	10.50	74.84983790	-61.92895673	19.68327403	-3.04713289	0.23370762	-0.00711033

Th(IV)

logPCO2(atm)	pHLow	pHhigh	a	b	c	d	e	f
-0.5	6.0	8.50	-312.14711523	243.99009612	-73.03800105	10.68670601	-0.76572596	0.02148313
-1.0	6.0	9.00	-178.60426661	137.73479859	-39.62233542	5.50279873	-0.36964490	0.00956996
-1.5	6.0	9.00	-22.15437259	17.78354930	-3.27591815	0.06714595	0.03117773	-0.00208040
-2.0	6.0	9.25	22.19042131	-14.82976722	6.12630097	-1.25638885	0.12171609	-0.00447272
-2.5	6.0	9.25	0.00987343	3.44007829	0.13956325	-0.28092710	0.04270240	-0.00192857
-3.0	6.0	9.50	-30.36665828	27.32153765	-7.32247331	0.87766304	-0.04670166	0.00081467
-3.5	6.0	9.50	-50.36155981	42.99824237	-12.20001276	1.63047122	-0.10434437	0.00256662
-4.0	6.0	10.00	-59.35569634	49.98525001	-14.35431507	1.96006372	-0.12936953	0.00332113
-4.5	6.0	10.25	-62.85636897	52.70342414	-15.19121240	2.08779456	-0.13903535	0.00361134
-5.0	6.0	10.50	-63.80070118	53.43751658	-15.41765407	2.12244405	-0.14166587	0.00369062

U (VI) <-- "U " 2 character radioelement name needed.

logPCO2(atm)	pHLow	pHhigh	a	b	c	d	e	f
-0.5	6.0	8.50	2003.97493902	-1485.67029530	433.57092214	-62.15156614	4.37263234	-0.12097330
-1.0	6.0	9.00	478.51153159	-327.82314738	86.48866922	-10.82526728	0.63173885	-0.01350561
-1.5	6.0	9.00	-504.79538068	393.52598368	-121.95095503	18.80798789	-1.43871348	0.04335225
-2.0	6.0	9.25	-558.47416786	413.85367777	-121.73861427	17.81411938	-1.29298327	0.03698197
-2.5	6.0	9.25	-445.08506681	316.43450502	-89.18854317	12.50756382	-0.86945763	0.02375106
-3.0	6.0	9.50	-456.35553823	317.97599454	-87.72698192	12.02812351	-0.81637025	0.02175635
-3.5	6.0	9.50	-258.61826289	168.96719847	-43.47518218	5.54955303	-0.34845941	0.00843921
-4.0	6.0	10.00	210.89440197	-174.75673790	55.82991857	-8.60831699	0.64797946	

```
-0.01924467
  -4.5    6.0  10.25     608.99699685   -459.98846072   136.36765428  -19.81478449    1.41668878
-0.04002967
  -5.0    6.0  10.50     475.33711389   -350.55771236   101.20336237  -14.27289372    0.98819149
-0.02700394
```

Attachment D

Test run results:

The changes itemized in Attachment B were implemented in succession. Using the same seed value for parameter sampling, a single realization was run for the original code, and after each successive modification. The peak mean dose and the time of peak obtained are as follows:

Test run#	Changes (Attachment B)	Peak Mean Dose (rem/yr)	Time of peak (yr)
1	(baseline code)	5.36340E-04	8101.3
2	{1}	2.92080E-05	2420.4
3	{1, 2}	2.92080E-05	2420.4
4	{1, 2, 3}	2.89260E-05	2539.8

12/10/4

Test Plan/Report for TPA SCR #517

Test Plan Name: Test Changes to Actinide Kd/Rd Calculations

Tested By: Carol S. Scherer

Date: November 19, 2004

Host Machine: SUN Ultra-4 server: Spock
Net Force x86 AT: Guardian

Host OS: Sun Solaris 5.8
Windows NT 4.0

Baseline Version: TPA 5.0z

Test Version: TPA 5.0.0a

Testing Setup:

Directories/paths used for testing:
$HOME = d:\css\tparun
Path for run directory:***$HOME***

Environment variables:

**TPA_TEST = $HOME **
**TPA_DATA = $HOME **

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 517 - Test Directories*" (attached).

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories under subdirectory ***scr517\modtpavalues***: ***basecase500a, means-AMSSA-10000, means-AMSSA-2000, means-ATP-15, means-ATP-3, meanscase500a, tpa50zruns\basecase50z, and tpa50zruns\meanscase50z***

2. Copy **TPA** version 5.0z to the **$HOME** directory. Run *tpa.exe*. Copy files from the run in **$HOME*scr517\modtpavalues\tpa runs\basecase50z***. Copy *tpameans.out* to *tpa.inp*. Run *tpa.exe*. Copy files from run to **$HOME*scr517\modtpavalues\tpa runs\ meanscase50z***.

3. Copy **TPA** version 5.0.0a to the run directory. Run *tpa.exe*. Copy files from run to **$HOME*scr517\modtpavalues\basescase500a*** Copy *tpameans.out* to *tpa.inp*. Run *tpa.exe*. Copy files from run to **$HOME*scr517\modtpavalues\meanscase500a***

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

1. Name: Compare Modified Code To Previous Version Of The Code.

   Paths for archives of results: ***$HOME \scr517\modtpavalues***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use **$HOME*scr517\modtpavalues\basescase500a*** *tpa_meanscase500a-mod.inp* and **$HOME*scr517\modtpavalues\tpa runs\basecase50z*** *tpa_means50z.inp*.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to show that the modified **TPA** code generates different results and the results differ in the way expected

   - assumptions: all setup instructions have been carried out.

   - constraints: the files *tpa_meanscase500a-maidhood* and *tpa_means50z.inp* do not exist in the run directory.

   - output files to compare or examine: **$HOME*scr517\modtpavalues\basescase500a*** *tpa_base500a-maidhood*, **$HOME*scr517\modtpavalues\basescase500a*** *actinide_kdrd.out*, **$HOME*scr517\modtpavalues\tparuns\basecase50z*** *tpa_basecase50z.out*, and **$HOME*scr517\modtpavalues\tpa runs\basecase50z***

actinide_kdrd_basez.out.

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_orig50z.exe* to *tpa.exe*
  3. run *tpa.e* using command "***tpa.e > tpa_means50z.out***"
  4. copy output files to **$HOME*scr517\tpa50zruns\meanscase50z***
  5. copy *tpa_orig500a.exe* to *tpa.exe*
  6. run *tpa.e* using command "***tpa.e > tpa_meanscase500a-maidhood***"
  7. copy output files to **$HOME*scr517\meanscase500a***
  8. compare the display output files and the actinide output files listed above

- pass/fail criteria: the test passes if:

  1. Both TPA runs complete successfully.

  2. There are differences in the values listed in the display output files.

  3. Values differ for kds and rds in the actinide_kdrd.out files for the actinides in the saturated zone.

  4. The correct values are listed in the actinide_kdrd.out files.

Results of running test:

FAILED. The correct values for szft rds were not listed in the actinide_kdrd.out files. (See NOTES at end of this test report.)

2. Name: Compare Different Values For AlluviumMatrixSpecificSurfaceArea.

Paths for archives of results: ***$HOME \scr517\modtpavalues***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use **$HOME*scr517\modtpavalues\basescase500a*** *tpa_meanscase500a-mod.inp* and make the following modifications:

Test case A: change AlluviuimMatrixSpecificSurfaceArea to 2000; save copy of *tpa.inp* as *tpa_means_AMSSA-2000.inp*

Test case B: change AlluviuimMatrixSpecificSurfaceArea to 10000; save copy of *tpa.inp* as *tpa_means_AMSSA-10000.inp*

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that modifying AlluviumMatrixSpecificSurfaceArea will affect the Rd values for actinides (Am, Np, Pu, Th, and U).

- assumptions: all setup instructions have been carried out.

- constraints: none.

- output files to compare or examine: the *actinide_kdrd.out* file for each testcase

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_orig500a.exe* to *tpa.exe*
  3. copy *tpa_means_AMSSA-2000.inp* to *tpa.inp*
  4. run *tpa.e* using command "***tpa.e > tpa_means_AMSSA-2000.out***"
  5. copy output files to **$HOME*scr517\means-AMSSA-2000***
  6. copy *tpa_means_AMSSA-10000.inp* to *tpa.inp*
  7. run *tpa.e* using command "***tpa.e > tpa_means_AMSSA-10000.out***"
  8. copy output files to **$HOME*scr517\means-AMSSA-10000***
  9. compare the *actinide_kdrd.out* files for each run

- pass/fail criteria: the test passes if:

  1. Each test run completes successfully.

  2. As AlluviumMatrixSpecificSurfaceArea increases, the Rd for the SAV layer decreases. (NOTE: Because of the error reported in System Level Test 1, Alluvium Rds are reported as STFF Rds.)

Results of running test:

PASSED.

3. Name: Compare Different Values For AlluviumTotalPorosity_SAV.

Paths for archives of results: ***$HOME \scr517\modtpavalues***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use **$HOME*scr517\modtpavalues\basescase500a*** *tpa_meanscase500a-mod.inp* and make the following modifications:

Test case A: change AlluviumTotalPorosity_SAV to .15; save copy of *tpa.inp* as *tpa_means_ATP-15.inp*

Test case B: change AlluviumTotalPorosity_SAV to .3; save copy of *tpa.inp* as *tpa_means_ATP-3.inp*

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that modifying AlluviumTotalPorosity_SAV will affect the Rd values for actinides (Am, Np, Pu, Th, and U).

- assumptions: all setup instructions have been carried out.

- constraints: none.

- output files to compare or examine: the *actinide_kdrd.out* file for each testcase

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. copy *tpa_orig500a.exe* to *tpa.exe*
  3. copy *tpa_means_ATP-15.inp* to *tpa.inp*

4. run *tpa.e* using command "***tpa.e > tpa_means_ATP-15.out***"
5. copy output files to **$HOME*scr517\means-ATP-15***
6. copy *tpa_means_ATP-3.inp* to *tpa.inp*
7. run *tpa.e* using command "***tpa.e > tpa_means_ATP-3.out***"
8. copy output files to **$HOME*scr517\means-ATP-3***
9. compare the *actinide_kdrd.out* files for each run

- pass/fail criteria: the test passes if:

1. Each test run completes successfully.

2. As AlluviumTotalPorosity_SAV increases, the Rd for the SAV layer decreases. (NOTE: Because of the error reported in System Level Test 1, Alluvium Rds are reported as STFF Rds.)

Results of running test:

PASSED.

NOTES: System Level Test 1 failed because of error in source code in *szft.f*. The 2nd call to calc_rd in SZFT uses porosity and density values for alluvium, not tuff. The wrong values are printed out *actinide_kdrd.out*; alluvium Rd values are shown as tuff Rd values, and vice versa. It also turns out that the values printed out in actinide_kdrd.out are not the values needed to check the calculated values for kds and rds (actinides) using *coefkdeq.dat*. SCR #523 was generated to correct the code in *szft.f* and to reformat *actinide_kdeq.dat*.

1. SCR No. (*Software Developer Assigns*): PA-SCR-518	2. Software Title and Version: TPA 5.0.0	3. Project No: 20.06002.01.113

4. Affected Software Module(s), Description of Problem(s): dcags.f, ebsfail.f, exec.f, invent.f, tpa.inp, tpanames.dbs, and uzft.f

Correct the following problems:

- Correct spelling of sampled parameters DepthOfResuspendableLayer[] (should be Resuspendible) and ExponetForLocCorrOfOuterOverpack (should be Exponent). Change sampled parameter CalendarYearOfEmplacement[A.D.] to AverageCalendarYearAssumedForEmplacement[A.D.]
- Adding code to account for reversible colloids sometimes produces a nefii.inp file that, while it contains correct values, causes NEFMKS to bomb (tries to process data for too many timesteps and causes an array out of bounds for BF in FACER).
- Exec.f writes repository temperature to nfenv.rlt after dividing the value by 100.0. This is different from the way repository temperature is written to ebsfail.ech. The divide by 100.0 for seepage threshold should also be removed. Also, there are two compile warnings for unused variables when exec is compiled.
- Thermal ouput in burnup.dat was divided by 475 kg. initial U mass (as for PWR assesmbly) but should have been divided by 200 kg. for BWR assembly.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
R. Benke, C. Scherer, J. Menchaca, O. Povetko Date: 9-1-2004	R. Janetzke Date: 9-1-2004 Ron Janetzke

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Parameter names changed in dcags.f, ebsfail.f, invent.f, and tpa.inp. The variable gwttmin (minimum ground water travel time) was changed from 10.0 years to 20.0, thus preventing uzft.f from accepting legs that generate nefii.inp files that overwhelm NEFMKS. At line 3229 in exec.f, the statement "tRep = temprep(i) / 100.0" was changed to "tRep=temprep(i)". At line 3228, the statement "ThrSeep = ThrSeepage / 100.0" was changed to "ThrSeep = ThrSeepage". The declarations for a_line and irhc were removed. Burnup.dat was updated with modified thermal output values.

8. Implemented by:	Date:
C. Scherer Carol S. Scherer	9/8/2004

9. Description of Acceptance Tests:

See Attachment 1

10. Tested by:	Date:
O.Osidele Felix Osidele	2/2/2005

CNWRA Form TOP-5 (05/2000)

Attachment 1

Test Plan for TPA SCR#518

Tested by: Olufemi Osidele | Date: February 1, 2005

Host Machine: SUN Ultra-4 server: Spock | Host OS: Sun Solaris 5.9

Baseline Version: 5.0.0 | Test Version: 5.0.0e

General Remarks

Directory path for codes: base version: ~oosidele/tpa500, ~oosidele/tpa500_mod
test version: ~oosidele/tpa500e

Environment variables: base version: setenv TPA_TEST ~/tpa500
setenv TPA_DATA ~/tpa500
setenv TPA_TEST ~/tpa500_mod
setenv TPA_DATA ~/tpa500_mod

test version: setenv TPA_TEST ~/tpa500e
setenv TPA_DATA ~/tpa500e

Test Description

1. <u>Sampled parameters</u>

Objectives:

(i) Correct spelling of sampled parameters DepthOfResuspendableLayer[] (should be Resuspendible) and ExponetForLocCorrOfOuterOverpack (should be Exponent).

(ii) Change sampled parameter CalendarYearOfEmplacement[A.D.] to AverageCalendarYearAssumedForEmplacement[A.D.].

Affected module(s): DCAGS, EBSFAIL, INVENT

Assumptions: None

Output files to compare or examine: None

Test procedure:

Search for misspelled (or old) and corrected (or new) parameter names in the *~oosidele/tpa500* and *~oosidele/tpa500e* directories using the following command:

```
grep -i <search string> *.f tpa.inp ccdf/*.f codes/*.f
codes/gentpa/*.f codes/itym/src/*.f
```

Pass/Fail criterion(ia):

Misspelled (or old) parameter names should be replaced by the corrected (or new) names in the test version of the code.

Test results:

See file *grepSearch.txt* on attached CD for screen dump of search results. Affected files are: *dcags.f*, *ebsfail.f*, *invent.f*, and *tpa.inp*. Misspelled (or old) parameter names replaced by the corrected (or new) names in *~oosidele/tpa500e*.

Test status: **PASS**

2. Minimum groundwater travel time

Objective: To test the revised assignment of minimum groundwater travel time (`gwttmin`).

Affected module(s): UZFT

Assumptions: None

Output files to compare or examine: *nefii.out*, *nefiiuz.out*.

Test procedure:

(i) Examine code modifications in *~oosidele/tpa500e/uzft.f*;

(ii) Run the base version (*~oosidele/tpa500/tpa.e*) for 200 realizations and dump screen output to file;

(iii) Assign `gwttmin = 20.0` in the base version; re-run base version (*~oosidele/tpa500_mod/tpa.e*) with the same sampling seed as in step (ii); dump screen output to file.

Pass/Fail criterion(ia):

The test version of the code should have the revised assignment statement for `gwttmin`. Re-run of the base version (with modified assignment of `gwttmin`) should not crash.

Test results:

See file */tparun016/tparun016.out* on attached CD for screen dump of test run (step (ii) above). Test run crashed on realization 74 of 200. Last line of file */tparun016/nefii.out* displays the error message:

```
DIMENSIONS EXCEEDED FOR THE TRANSFER FRACTIONS ARRAY, BF
*** PROGRAM STOP FROM FACER
```

See file */tparun017/tparun017.out* on attached CD for screen dump of re-run (step (iii) above). Re-run did not crash.

Test status: **PASS.**

3. <u>Repository temperature output</u>

Objective: To correct the repository temperature (`tRep`) and seepage threshold (`ThrSeep`) calculated prior to output to *nfenv.rlt*. The divide by `100` should be removed.

Affected module(s): EXEC

Assumptions: None

Output files to compare or examine: *nfenv.rlt* and *ebsfail.ech.*

Test procedure:

(i) Examine code modifications in *~oosidele/tpa500e/exec.f*;

(ii) Run the base version (*~oosidele/tpa500/tpa.e*); compare `temprep` columns in *nfenv.rlt* and *ebsfail.ech.*

(iii) Run the test version (*~oosidele/tpa500e/tpa.e*); compare `temprep` columns in *nfenv.rlt* and *ebsfail.ech.*

Pass/Fail criterion(ia):

The divide by `100` should be removed from the statements to calculate `tRep` and `ThrSeep` in the test version. Values written to the `temprep` column in *nfenv.rlt* and *ebsfail.ech* should be the same.

Test results:

See files */tparun016/nfenv.rlt* and */tparun016/ebsfail.ech* on attached CD for outputs of test run (step (ii) above). The `temprep` columns differ by a factor of 100.

See files */tparun018/nfenv.rlt* and */tparun018/ebsfail.ech* on attached CD for outputs of test run (step (iii) above). The `temprep` columns contain the same values.

Test status: **PASS**

4. Thermal output data

Objective: To test the updated thermal output values in burnup.dat.

Affected module(s): INVENT

Assumptions: None

Output files to compare or examine: None

Test procedure:

Compare the `bwr` column of *burnup.dat* in the base and test versions.

Pass/Fail criterion(ia):

Thermal output from BWR assembly (in the `bwr` column) for the test version should be 2.375 times (i.e., 475/200) the values for the base version.

Test results:

The *burnup.dat* file is exactly the same in the base and test versions.

Test status: **FAIL** (SCR# 554 generated to address this).

UPDATE REQUIREMENTS for TPA.INP
SCR518

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for caluating..., used to relate... etc)	Distribution	Range	Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)
Modify From	NFENV	CalendarYearOfEmplacment[A.D.]					
Modify To	NFENV	AverageCalendarYearAssumedForEmplacment[A.D.]					
Modify From	EBSFAIL	ExponetForLocCorrOfOuterOverpack					
Modify To	EBSFAIL	ExponentForLocCorrOfOuterOverpack					
Modify From	DCAGS	DepthOfResuspendableLayer[cm]					
Modify To	DCAGS	DepthOfResuspendibleLayer[cm]					

1. SCR No. (*Software Developer Assigns*): PA-SCR-519	**2. Software Title and Version:** TPA 5.0.0h	**3. Project No:** 20.06002.01.113
4. Affected Software Module(s), Description of Problem(s): *ashremob.f, dcags.f, ebsfail.f, ebsrel.f, exec.f, failt.f, nfenv.f, tpa.inp* See Attachment B.		
5. Change Requested by: R. Benke, C. Scherer, J. Menchaca, O. Povetko Date: 9-1-2004	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 9-1-2004 R. Janetzke	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment C.		
8. Implemented by: C. Scherer Carl S. Scherer	**Date:** 2/24/2005	
9. Description of Acceptance Tests: **retest scr478** See Attachment D.		
10. Tested by: Jose M. Menchaca Jose M. Menchaca	**Date:** 04/22/2005	

CNWRA Form TOP-5 (05/2000)

ATTACHMENT A

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)
Modify From	SZFT	AlluviumMatrix SpecificSurfaceArea[m2/kg]		uniform	2.0e3, 1.0e4	Bechtel SAIC Company, LLC. Geochemical and Isotopic Constraints on Groundwater Flow Directions, Mixing, and Recharge at Yucca Mountain, Nevada. ANL-NBS-HS-000021, Rev. 01. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2004. Bertetti, F.P., J.D. Prikryl and B.A. Werling. Development of Updated Total-system Performance Assessment Parameter Distributions for Radionuclide Transport in the Saturated Zone. CNWRA Report (in review). San Antonio, Texas: CNWRA. 2004.	P. Bertetti
Modify To	SZFT	AlluviumMatrix SpecificSurfaceArea[m2/kg]		uniform	1.9e3, 1.21e4	"	P. Bertetti

Modify From	UZFT	pH_AllUZ_SZLayers[StandardUnits]		normal	6.2, 9.4	"	P. Bertetti
Modify To	UZFT	pH_AllUZ_SZLayers[StandardUnits]		triangular	6.7, 7.8, 9.2	"	P. Bertetti
Modify From	UZFT	LogCO2PartialPressure_AllUZ_SZLayers[atm]		normal	-4.1, -1.9	"	P. Bertetti
Modify To	UZFT	LogCO2PartialPressure_AllUZ_SZLayers[atm]		triangular	-4.0, -2.5, -1.0	"	P. Bertetti
Modify From	CORRELATED PARAMETERS	LogCO2PartialPressure_AllUZ_SZLayers[atm] pH_AllUZ_SZLayers[StandardUnits]		correlateinputs	-0.83	"	P. Bertetti
Modify To	CORRELATED PARAMETERS	LogCO2PartialPressure_AllUZ_SZLayers[atm] pH_AllUZ_SZLayers[StandardUnits]		correlateinputs	-0.95	"	P. Bertetti
Delete	DCAGS	AirborneMassLoadAboveFreshAshBlanket[g/m3]					
Delete	DCAGS	AirborneMassLoadAboveSoil[g/m3]					

Delete	NFENV	EffectiveThermalConductivityOfBasket&SFinWP[W/m-C)]					
Modify From	UZFT	CH_Total_Thickness_9SubArea[m]		constant	128.0		
Modify To	UZFT	CH_Total_Thickness_9SubArea[m]		constant	138.0		
Delete	EBSFAIL	InnerInhibitingCarbonateToCl					O. Pensado
Delete	EBSFAIL	InnerInhibitingSulfateToCl					O. Pensado
Delete	EBSFAIL	OuterWPBetaKineticsParamterforOxygen					SCR #478
Delete	EBSFAIL	InnerWPBetaKineticsParamterforOxygen					SCR #478
Delete	NFENV	Indrift_Cl_PreTemperaturePeak[mol/L]					SCR #478
Delete	NFENV	Indrift_Cl_PostTemperaturePeak[mol/L]					SCR #478

Delete	NFENV	Indrift_Fl_PreTemperaturePeak[mol/L]					SCR #478
Delete	NFENV	Indrift_Fl_PostTemperaturePeak[mol/L]					SCR #478
Delete	NFENV	Indrift_CO3_PreTemperaturePeak[mol/L]					SCR #478
Delete	NFENV	Indrift_CO3_PostTemperaturePeak[mol/L]					SCR #478
Delete	NFENV	Indrift_pH_PreTemperaturePeak[]					SCR #478
Delete	NFENV	Indrift_pH_PostTemperaturePeak[]					SCR #478
Delete	DSFAIL	Wastepackage_DeltaEcrit_PreTemperaturePeak[VSHE]					SCR #478
Delete	DSFAIL	Wastepackage_DeltaEcrit_PostTemperaturePeak[VSHE]					SCR #478

Attachment B

1) Fix findpkmndose() to not print vectors not executed via start/stop realization settings.

2) **Change name of results file from pkmndose.out to pkmndose.res.**

3) New parameter values for *tpa.inp* (Paul Bertetti):
AlluviumMatrixSpecificSurfaceArea[m2/kg]; uniform; 1.9e3, 1.21e4;
pH_AllUZ_SZLayers[StandardUnits]; triangular; 6.7, 7.8, 9.2;
LogCO2PartialPressure_AllUZ_SZLayers[atm]; triangular; -4., -2.5, -1. Correlation for latter two parameters is -0.95.

The alluvium specific surface area distribution should be a uniform distribution from 1.9 to 12.1 m2/g (or 1900 to 12100 m2/kg). These values are based on mineralogical and surface area analyses of well cuttings and sonic core samples from EWDP wells, NC-EWDP-02D, NC-Washburn-1X, and NC-EWDP-19PB.

Out final analysis of recent groundwater chemical data indicate that the range and distribution for pH and CO2 should be modified for TPA. We recommend a TRIANGULAR probability distribution for both pH and CO2.

For pH the values are: minimum = 6.7, maximum = 9.2, and mode = 7.8. For CO2 the values are: minimum = -4.0, maximum = -1.0, and mode = -2.5. pH and CO2 should be correlated at -0.95.

These probability distributions for pH and CO2 are based on analysis of sampled groundwater chemistries from the saturated zone within the DOE site-scale model boundary. The values are listed in BSC, 2004 and Bertetti et al., 2004.

4) Modifications needed for dcags.f:

a) remove dead code from *dcags.f.* related to doss, factor1, factor2
b) change statement "thickness=gramsashpercm2/1.65d0" to "thickness=gramsahspercm2/rhoash" where rhoash is the value from tpa.inp AshBulkDensity[g/m3]
c) delete "*100" in "resuspendiblefraction(it)=thickness*100*dexp(-dlbr*(tim(it)-tim(itoe)))/resuspendibledepth"
d) update header comments

5) Remove unused parameters from *tpa.inp* that were put in for SCR #478: InnerInhibitingCarbonateToCl and InnerInhibitingSulfateToCl. Remove unnecessary code related to parameters in *ebsfail.f.* Code in *ebsfail.f* incorrectly used InnerInhibitingCarbonateToCl and InnerInhibitingSulfateToCl when it should use OuterInhibitingCarbonateToCl and OuterInhibitingSulfateToCl. Add calculations using WeldInhibitingCarbonateToCl and WeldInhibitingSulfateToCl to create a weld inhibiting vector in *ebsfail.f.* Write vector to *ebstrhc.inp*. *Failt.f* should read the weld inhibiting vector and pass it to subroutine

calculateWeldFailure instead of using the effective inhibiting vector which is used to calculate WP failure.

6) Add comments to ebsrel.f re : four parameters (SFC-14InventoryPerKgSF[ci], CladC-14inventoryPerKgSF[ci], ZyrOxideAndCrudC-14InvPerKgSF[ci], and GapAndGrainBoundaryInventoryPerKgSF[ci]) in tpa.inp aren't actually used. They are read in by ebsrel.f and written out to ebsrel.inp, which is read by *releaset*. Releaset reads the values but does nothing with them.

7) remove unused parameters in tpa.inp: AirborneMassLoadAboveFreshAshBlanket[g/m3], AirborneMassLoadAboveSoil[g/m3], and EffectiveThermalConductivityOfBasket&SFinWP[W/(m-C)]. Check for dead or unnecessary code using these parameters.

8) In tpa.inp change CH_Total_Thickness_9Subarea[m] to 138.0. (ChnvThickness_9Subarea[m] is set to 0.0.)

9) Add if (flagvolcano .eq. 1) then - endif around block of code in *exec.f* (lines 4187 - 4206 TPA5.0.0i) where number of WPs ejected is printed out.

10) Modifications to *ashremob.f*: remove AshEvolutionMode declaration and value retrieval; change File Name to ashremob.f.

ATTACHMENT C

Description of Change(s) or Problem Resolution

1)Made the following code changes to *exec.f*:

```
9774c9744
< cc       Find average total dose for this time step.
---
> cc       Find avreage total dose for this time step.
9765,9769c9740
< c
< c css 2-15-2005; SCR519:  only process & print realizations
< c        actually executed
< cc         do iThisVector = 1, iLastVector
<          do iThisVector = iFirstVector, iLastVector
---
>          do iThisVector = 1, iLastVector
9772d9742
< c end change:  SCR519
9798,9802c9768
< c
< c css 2-15-2005; SCR519:  only process & print realizations
< c        actually executed
< cc      do i = 1, iLastVector
<       do i = iFirstVector, iLastVector
---
>       do i = 1, iLastVector
9806d9771
< c end change:  SCR519
```

2)Made the following code changes in *exec.f*:

```
9580d9560
< c css 2-14-2005; SCR519:  change name of pkmndose.out to pkmndose.res
9615d9594
< c css 2-14-2005; SCR519:  change name of pkmndose.out to pkmndose.res
9631d9609
< c css 2-14-2005; SCR519:  change name of pkmndose.out to pkmndose.res
9671,9674c9649
< c css 2-14-2005; SCR519:  change name of pkmndose.out to pkmndose.res
< cc      open (outunit, file = 'pkmndose.out', status = 'UNKNOWN')
<       open (outunit, file = 'pkmndose.res', status = 'UNKNOWN')
< c end change:  scr519
---
>       open (outunit, file = 'pkmndose.out', status = 'UNKNOWN')
```

3) Modified specified parameter values in *tpa.inp*.

4) Commented out specified parameters in *tpa.inp*, and made the following code changes to *dcags.f*:

```
142c142,145
```

```
< c               gramsashpercm2 = mass of ash per unit area [g/cm2]
---
> c               gramsashpercm2 = density of ash [g/cm3]
> c               amassash (mxntime) = double precision, mass of ash per
> c                                    unit area as a function of time after
> c                                    the eruption [g/m2]
173,177c176,178
< c css - SCR519 - delete obsolete variables
< ccc     doss                    =
< ccc     factor1                 =
< ccc     factor2                 =
< c end change:  SCR519
---
> c     doss                    =
> c     factor1                 =
> c     factor2                 =
206d206
< c     irhoash                 = index for rhoash (AshBulkDensity)
284,287d283
< c
< c css 2-18-2005; SCR519:  declare index for AshBulkDensity variable
<       integer irhoash
< c
308,314c304,306
< c
< c css 2-18-2005; SCR519:  remove variables used for obsolete code
< c
< cc      double precision doss
< cc      double precision factor1(maxntime)
< cc      double precision factor2(maxntime)
< c end change:  SCR519
---
>       double precision doss
>       double precision factor1(maxntime)
>       double precision factor2(maxntime)
332,335d323
< c
< c css 2-18-2005; SCR519:  declare variable for AshBulkDensity
<       double precision rhoash
< c end change:  SCR519
452a441
>
464,469c453
< c
< c css 2-18-2005; SCR519:  get index for AshBulkDensity variable
<         call clearchar( 60, name )
<         name = 'AshBulkDensity[g/m3]'
<         irhoash = ispquery( name )
< c end change:  SCR519
---
>
541a526
>       thickness=gramsashpercm2/1.65d0
543,549d527
< c css 2-18-2005; SCR519:  replace 1.65d0 with AshBulkDensity
< cc      thickness=gramsashpercm2/1.65d0
<       rhoash    = ivaluesp(irhoash)
<       thickness = gramsashpercm2 / rhoash
< c end change:  SCR519
<
```

```
< c
559,565c537
< c
< c css 2-18-2005; SCR519:  delete "*100"
< c
< cc        resuspendiblefraction(it)=thickness*100
< cc     &                          *dexp(-dlbr*(tim(it)-tim(itoe)))/
< cc     &                          resuspendibledepth
<         resuspendiblefraction(it)=thickness
---
>         resuspendiblefraction(it)=thickness*100
568d539
< c end change:  SCR519
592,593c563,566
< c css 2-18-2005; SCR519:  remove obsolete code - factor1 and factor2
< c     are not used, saved, or passed on
---
> c   track thickness of ash blanket and scale doses based on availability of
> c   ash to the various pathways.  If ash thickness is less than doss then
> c   only inhalation pathway is reduced.  If ash thickness is greater than
> c   doss then the direct exposure and plant ingestion pathways are reduced.
595,611c568,577
< ccc
< ccc   track thickness of ash blanket and scale doses based on availability of
< ccc   ash to the various pathways.  If ash thickness is less than doss then
< ccc   only inhalation pathway is reduced.  If ash thickness is greater than
< ccc   doss then the direct exposure and plant ingestion pathways are reduced.
< ccc
< cc        if(thickness.lt.doss/100) then
< cc          factor1(it)=thickness/(doss/100)
< cc          factor2(it)=1
< cc        elseif (thickness.gt.doss/100) then
< cc          factor1(it)=1
< cc          factor2(it)=(doss/100)/thickness
< cc        else
< cc          factor1(it)=1
< cc          factor2(it)=1
< cc        endif
< c end change:  SCR519
---
>         if(thickness.lt.doss/100) then
>           factor1(it)=thickness/(doss/100)
>           factor2(it)=1
>         elseif (thickness.gt.doss/100) then
>           factor1(it)=1
>           factor2(it)=(doss/100)/thickness
>         else
>           factor1(it)=1
>           factor2(it)=1
>         endif
```

5)Commented out specified parameters in *tpa.inp*, and made the following code changes.

in *ebsfail.f*:

```
295,296d294
< c     inhWeld          = effective concentration of weld inhibitors (nitrate,
< c                        carbonate, sulfate, etc.)
342,345d339
```

```
< c     outweldc        = outer inhibiting nitrate to Cl divided by
< c                       outer inhibiting weld carbonate to Cl
< c     outwelds        = outer inhibiting nitrate to Cl divided by
< c                       outer inhibiting weld sulfate to Cl
517,524d510
< c css 2-24-2005; SCR519:  remove unused variables
< cc      integer ipHtran, ibeta1hi, ibeta1lo, iire1hi, iire1lo, ig1hi,
< cc     & ig1lo, inpH1hi, inpH1lo, ibeta2hi, ibeta2lo,
< cc     & iire2hi, iire2lo, ig2hi, ig2lo, inpH2hi, inpH2lo,
< cc     & iinhToCl1, iinhcToCl1,
< cc     & iinhsToCl1, ideltaEcInh1, iinhToCl2, iinhcToCl2, iinhsToCl2,
< cc     & ideltaEcInh2, iclcritw, iinhToClw, iinhcToClw, iinhsToClw,
< cc     & ideltaEcInhW
527,531c513,518
<      & ig1lo, inpH1hi, inpH1lo, ibeta2hi, ibeta2lo, iire2hi, iire2lo,
<      & ig2hi, ig2lo, inpH2hi, inpH2lo, iinhToCl1, iinhcToCl1,
<      & iinhsToCl1, ideltaEcInh1, iinhToCl2, ideltaEcInh2, iclcritw,
<      & iinhToClw, iinhcToClw, iinhsToClw, ideltaEcInhW
< c end change:  SCR519
---
>      & ig1lo, inpH1hi, inpH1lo, ibeta2hi, ibeta2lo,
>      & iire2hi, iire2lo, ig2hi, ig2lo, inpH2hi, inpH2lo,
>      & iinhToCl1, iinhcToCl1,
>      & iinhsToCl1, ideltaEcInh1, iinhToCl2, iinhcToCl2, iinhsToCl2,
>      & ideltaEcInh2, iclcritw, iinhToClw, iinhcToClw, iinhsToClw,
>      & ideltaEcInhW
539,552c526,532
< c css 2-24-2005; SCR519:  remove unused variables
< cc      double precision pHtran, beta1hi, beta1lo, ire1hi, ire1lo,
< cc     & g1hi, g1lo, npH1hi, npH1lo, beta2hi, beta2lo,
< cc     & ire2hi, ire2lo, g2hi, g2lo, npH2hi, npH2lo,
< cc     & inhToCl1, inhcToCl1, inhsToCl1,
< cc     & deltaEcInh1, inhToCl2, inhcToCl2, inhsToCl2, deltaEcInh2,
< cc     & clcritw, inhToClw, inhcToClw, inhsToClw, deltaEcInhW,
< cc     & g1anod, g2anod, refTanod
<       double precision pHtran, beta1hi, beta1lo, ire1hi, ire1lo, g1hi,
<      & g1lo, npH1hi, npH1lo, beta2hi, beta2lo, ire2hi, ire2lo, g2hi,
<      & g2lo, npH2hi, npH2lo, inhToCl1, inhcToCl1, inhsToCl1,
<      & deltaEcInh1, inhToCl2, deltaEcInh2, clcritw, inhToClw, inhcToClw,
<      & inhsToClw, deltaEcInhW, g1anod, g2anod, refTanod
< c end change:  SCR519
---
>       double precision pHtran, beta1hi, beta1lo, ire1hi, ire1lo,
>      & g1hi, g1lo, npH1hi, npH1lo, beta2hi, beta2lo,
>      & ire2hi, ire2lo, g2hi, g2lo, npH2hi, npH2lo,
>      & inhToCl1, inhcToCl1, inhsToCl1,
>      & deltaEcInh1, inhToCl2, inhcToCl2, inhsToCl2, deltaEcInh2,
>      & clcritw, inhToClw, inhcToClw, inhsToClw, deltaEcInhW,
>      & g1anod, g2anod, refTanod
557,559d536
< c css 2-24-2005; SCR519:  use weld inhibitors
<       double precision inhWeld, outweldc, outwelds
< c end change:  SCR519
674,682d650
< c css 2-24-2005; SCR519:  remove unused variables
< cc      common / corrpar2 / pHtran, beta1hi, beta1lo, ire1hi, ire1lo,
< cc     & g1hi, g1lo, npH1hi, npH1lo, beta2hi, beta2lo,
< cc     & ire2hi, ire2lo, g2hi, g2lo, npH2hi, npH2lo,
< cc     & inhToCl1, inhcToCl1, inhsToCl1,
< cc     & deltaEcInh1, inhToCl2, inhcToCl2, inhsToCl2, deltaEcInh2,
```

```
< cc      & clcritw, inhToClw, inhcToClw, inhsToClw, deltaEcInhW,
< cc      & g1anod, g2anod, refTanod
< c23456789012345678901234567890123456789012345678901234567890123456789012
684,688c652,657
<       & g1hi, g1lo, npH1hi, npH1lo, beta2hi, beta2lo, ire2hi, ire2lo,
<       & g2hi, g2lo, npH2hi, npH2lo, inhToCl1, inhcToCl1, inhsToCl1,
<       & deltaEcInh1, inhToCl2, deltaEcInh2, clcritw, inhToClw, inhcToClw,
<       & inhsToClw, deltaEcInhW, g1anod, g2anod, refTanod
< c end change:  SCR519
---
>       & g1hi, g1lo, npH1hi, npH1lo, beta2hi, beta2lo,
>       & ire2hi, ire2lo, g2hi, g2lo, npH2hi, npH2lo,
>       & inhToCl1, inhcToCl1, inhsToCl1,
>       & deltaEcInh1, inhToCl2, inhcToCl2, inhsToCl2, deltaEcInh2,
>       & clcritw, inhToClw, inhcToClw, inhsToClw, deltaEcInhW,
>       & g1anod, g2anod, refTanod
1168,1176c1137
< c css 2-24-2005; SCR519:  remove unused parameters
< cc         call clearchar( 60, name )
< cc         name = 'InnerInhibitingCarbonateToCl'
< cc         iinhcToCl2 = ispquery( name )
< cc
< cc         call clearchar( 60, name )
< cc         name = 'InnerInhibitingSulfateToCl'
< cc         iinhsToCl2= ispquery( name )
< c end change:  SCR519
---
>
1177a1139,1146
>          name = 'InnerInhibitingCarbonateToCl'
>          iinhcToCl2 = ispquery( name )
>
>          call clearchar( 60, name )
>          name = 'InnerInhibitingSulfateToCl'
>          iinhsToCl2= ispquery( name )
>
>          call clearchar( 60, name )
1447,1450c1416,1417
< c css 2-24-2005; SCR519:  remove unused parameters/variables
< cc       inhcToCl2= valuesp( iinhcToCl2 )
< cc       inhsToCl2= valuesp( iinhsToCl2 )
< c end change:  SCR519
---
>        inhcToCl2= valuesp( iinhcToCl2 )
>        inhsToCl2= valuesp( iinhsToCl2 )
2063,2071c2030,2031
< c css 2-24-2005; SCR519: use Outer inhibiting values instead of Inner
< cc       wnwc=inhToCl2 / inhcToCl2
< cc       wnws=inhToCl2 / inhsToCl2
<        wnwc=inhToCl1 / inhcToCl1
<        wnws=inhToCl1 / inhsToCl1
<        outweldc = inhToCl1 / inhcToClw
<        outwelds = inhToCl1 / inhsToClw
< c SCR519:  add weld inhibiting concentrations
< c end change:  SCR519
---
>        wnwc=inhToCl2 / inhcToCl2
>        wnws=inhToCl2 / inhsToCl2
2077d2036
< c css 2-24-2005; SCR519:  calculate weld inhibitor vector
```

```
2079,2080d2037
<          inhWeld = no3(it) + outweldc * co3(it) + outwelds * so4(it)
< c end change: SCR519
2085a2043,2044
>         write( iebstrhcinp, fmt='(6f12.4)' ) tim(it), tempwp(it),
>      &  temprep(it), relhumwp(it), phwp(it), inhEff
2088,2093d2046
< c css 2-24-2005; SCR519:  weld inhibitor vector to ebstrhc.inp
< cc        write( iebstrhcinp, fmt='(6f12.4)' ) tim(it), tempwp(it),
< cc     &  temprep(it), relhumwp(it), phwp(it), inhEff
<         write( iebstrhcinp, fmt='(6f12.4)' ) tim(it), tempwp(it),
<      &  temprep(it), relhumwp(it), phwp(it), inhEff, inhWeld
< c end change: SCR519
```

in *failt.f*:

```
147,148c147,148
<      &                  cfactor, inhToCl1, inhToCl2,
<      &                  deltaEcInh1, deltaEcInh2, iflagcl
---
>      &                  cfactor, iflagcl, inhToCl1, inhToCl2,
>      &                  deltaEcInh1, deltaEcInh2
166,171c166,167
< c css 2-24-2005; SCR519:  add weld inhibitor vector
< cc        DOUBLE PRECISION inhvec
< cc        COMMON /inhhist/ inhvec(nintv)
<         DOUBLE PRECISION inhvec, inhvecW
<         COMMON /inhhist/ inhvec(nintv), inhvecW(nintv)
< c end change:  SCR519
---
>         DOUBLE PRECISION inhvec
>         COMMON /inhhist/ inhvec(nintv)
230,234d225
< c css 2-24-2005:  SCR519:  add weld inhibitor vector
< cc        call temphstry (timr, tcan, tavg, humd, pHvec, inhvec, nhist)
<         call temphstry (timr, tcan, tavg, humd, pHvec, inhvec,
<      &                  inhvecW, nhist)
< c end change:  SCR519
235a227,228
>         call temphstry (timr, tcan, tavg, humd, pHvec, inhvec, nhist)
>
251,255d243
< c
< c css 2-24-2005; SCR519:  use weld inhibitor vector for this calculation
< cc        CALL calculateWeldFailure(timr, tcan, humd, pHvec,
< cc     &    deltaEcritOL, clconc, inhvec, nhist, weld_failure_flag,
< cc     &    weld_failure_time)
257c245
<      &    deltaEcritOL, clconc, inhvecW, nhist, weld_failure_flag,
---
>      &    deltaEcritOL, clconc, inhvec, nhist, weld_failure_flag,
259d246
< c end change:  SCR519
598c585
<      &       inhToCl1, inhToCl2, deltaEcInh1, deltaEcInh2, iflagcl
---
>      &       iflagcl,inhToCl1, inhToCl2, deltaEcInh1, deltaEcInh2
769,772d755
< c
```

```
< c css 2-24-2005:  SCR519:  add weld inhibitor vector
< cc        subroutine temphstry(timr, tcan, tavg, humd, pHvec, inhvec,
< cc     &                       nhist)
774,775c757
<      &                       inhvecW, nhist)
< c end change:  SCR519
---
>      &                       nhist)
791,792d772
< c       inhvecW: effective concentration of weld inhibitors (nitrate,
< c                carbonate, etc.)
800,802d779
< c css 2-24-2005; SCR519:  add weld inhibitor vector
< cc        DOUBLE PRECISION humd, tavg, tcan, timr, pHvec, inhvec
<         DOUBLE PRECISION humd, tavg, tcan, timr, pHvec, inhvec, inhvecW
803a781,782
>         DOUBLE PRECISION humd, tavg, tcan, timr, pHvec, inhvec
>
806,807d784
< cc        dimension timr(nintv), tcan(nintv), tavg(nintv), humd(nintv),
< cc     &            pHvec(nintv), inhvec(nintv)
809,810c786
<      &            pHvec(nintv), inhvec(nintv), inhvecW(nintv)
< c end change:  SCR519
---
>      &            pHvec(nintv), inhvec(nintv)
827,831d802
< c css 2-24-2005:  SCR519:  add weld inhibitor vector
< cc         read (2,*) timr(i),tcan(i),tavg(i),humd(i),pHvec(i),inhvec(i)
<          read (2,*) timr(i), tcan(i), tavg(i), humd(i), pHvec(i),
<      &              inhvec(i), inhvecW(i)
< c end change:  SCR519
832a804,805
>          read (2,*) timr(i),tcan(i),tavg(i),humd(i),pHvec(i),inhvec(i)
>
1426,1431c1399,1400
< c css 2-24-2005; SCR519:  add weld inhibitor vector
< cc        DOUBLE PRECISION inhvec
< cc        COMMON /inhhist/ inhvec(nintv)
<         DOUBLE PRECISION inhvec, inhvecW
<         COMMON /inhhist/ inhvec(nintv), inhvecW(nintv)
< c end change:  SCR519
---
>         DOUBLE PRECISION inhvec
>         COMMON /inhhist/ inhvec(nintv)
1435c1404
<      &           inhToCl1, inhToCl2,deltaEcInh1, deltaEcInh2, iflagcl
---
>      &           iflagcl, inhToCl1, inhToCl2,deltaEcInh1, deltaEcInh2
2297,2298c2266,2267
<      &             cfactor, inhToCl1, inhToCl2,
<      &             deltaEcInh1, deltaEcInh2, iflagcl
---
>      &             cfactor, iflagcl, inhToCl1, inhToCl2,
>      &             deltaEcInh1, deltaEcInh2
```

6) Add the following comments to *ebsrel.f*:

```
641,646c641
< c
```

```
< c css 2-14-2005; SCR519:  these 4 parameters are written out
< c     to ebsrel.inp and then read in by releaset; however, releaset
< c     does not actually use them
<c
<c   CFUEL
---
>
650c645
<c   CZMETAL
---
>
654c649
<c   CZOXIDE
---
>
658c653
<c   CGAP
---
>
662,664c657
<c
<c end change:  SCR519
<c
---
>
```

7) Commented out parameters in *tpa.inp*, and made the following code changes.

in exec.f:

```
358,361c358
< c
< c css 2-22-2005; SCR519:  remove unused variable
< cc      dimension tempsf( maxntime )
< c end change: SCR519
---
>       dimension tempsf( maxntime )
3138,3157c3135,3145
< c
< c css 2-22-2005; SCR519: remove unused variable tempsf
< cc          call nfenvFl( isa, ntim, tim(1),
< cc     &     qm3peryrperwpinsa(1),
< cc     &     temprep(1), tempbfoA(1), tempbfoB(1),
< cc     &     tempdsoA(1), tempdsoB(1),
< cc     &     tempdsiA(1), tempdsiB(1), tempwp(1),
< cc     &     tempsf(1), relhumwp(1), flds(1),
< cc     &     qm3peryrperwpinsamisswp(1),
< cc     &     qm3peryrperwpinsahitwp(1),
< cc     &     equivdriftdiaAsubarea(1, isa),
< cc     &     equivdriftdiaBsubarea(1, isa),
< cc     &     equivbfdiaAsubarea(1, isa),
< cc     &     equivbfdiaBsubarea(1, isa))
```

```
<           call nfenvFl( isa, ntim, tim(1), qm3peryrperwpinsa(1),
<      &     temprep(1), tempbfoA(1), tempbfoB(1), tempdsoA(1),
<      &     tempdsoB(1), tempdsiA(1), tempdsiB(1), tempwp(1),
<      &     relhumwp(1), flds(1), qm3peryrperwpinsamisswp(1),
<      &     qm3peryrperwpinsahitwp(1), equivdriftdiaAsubarea(1, isa),
<      &     equivdriftdiaBsubarea(1, isa), equivbfdiaAsubarea(1, isa),
---
>           call nfenvFl( isa, ntim, tim(1),
>      &     qm3peryrperwpinsa(1),
>      &     temprep(1), tempbfoA(1), tempbfoB(1),
>      &     tempdsoA(1), tempdsoB(1),
>      &     tempdsiA(1), tempdsiB(1), tempwp(1),
>      &     tempsf(1), relhumwp(1), flds(1),
>      &     qm3peryrperwpinsamisswp(1),
>      &     qm3peryrperwpinsahitwp(1),
>      &     equivdriftdiaAsubarea(1, isa),
>      &     equivdriftdiaBsubarea(1, isa),
>      &     equivbfdiaAsubarea(1, isa),
3159d3146
< c end change:  SCR519
```

in *nfenv.f*:

```
128,143c128,134
< c
< c css 2-22-2005; SCR519:  remove unused parameter tempsf
< cc      subroutine nfenvFl( isa, ntim, tim, qm3peryrperwpinsa,
< cc     &             temprep, tempbfoA, tempbfoB, tempdsoA, tempdsoB,
< cc     &             tempdsiA, tempdsiB, tempwp,
< cc     &             tempsf, relhumwp,
< cc     &             flds, qm3peryrperwpinsamisswp,
< cc     &             qm3peryrperwpinsahitwp, eqDriftDiaA, eqDriftDiaB,
< cc     &             eqBFDiaA, eqBFDiaB  )
<       subroutine nfenvFl( isa, ntim, tim, qm3peryrperwpinsa, temprep,
<      &                    tempbfoA, tempbfoB, tempdsoA, tempdsoB,
<      &                    tempdsiA, tempdsiB, tempwp, relhumwp, flds,
<      &                    qm3peryrperwpinsamisswp,
<      &                    qm3peryrperwpinsahitwp, eqDriftDiaA,
<      &                    eqDriftDiaB, eqBFDiaA, eqBFDiaB  )
< c end change:  SCR519
---
>       subroutine nfenvFl( isa, ntim, tim, qm3peryrperwpinsa,
>      &             temprep, tempbfoA, tempbfoB, tempdsoA, tempdsoB,
>      &             tempdsiA, tempdsiB, tempwp,
>      &             tempsf, relhumwp,
>      &             flds, qm3peryrperwpinsamisswp,
>      &             qm3peryrperwpinsahitwp, eqDriftDiaA, eqDriftDiaB,
>      &             eqBFDiaA, eqBFDiaB  )
170,173c161,162
< cc css 2-22-2005; SCR519:  remove unused parameter
< ccc              tempsf(ntim)      = double precision, time-dependent maximum
< ccc                                    temperature of spent fuel residing in
WP
< cc  end change:  SCR519
---
> c               tempsf(ntim)      = double precision, time-dependent maximum
> c                                   temperature of spent fuel residing in WP
222,225c211
< c
```

```
< c css 2-22-2005; SCR519:  remove unused parameter and variables
< cc      dimension tempsf(ntim)
< c end change:  SCR519
---
>       dimension tempsf(ntim)
385,388c371
< c
< c css 2-22-2005; SCR519:  remove unused variable
< cc      common / nfenv30 / iaksf
< c end change:  SCR519
---
>       common / nfenv30 / iaksf
783,788d765
< c
< c css 2-22-2005; SCR519: remove unused parameter & related code
< cc        call clearchar( 60, name )
< cc        name = 'EffectiveThermalConductivityOfBasket&SFinWP[W/(m-C)]'
< cc        iaksf  = ispquery( name )
< c end change:  SCR519
790a768,771
>         name = 'EffectiveThermalConductivityOfBasket&SFinWP[W/(m-C)]'
>         iaksf  = ispquery( name )
>
>         call clearchar( 60, name )
1270,1274c1251,1252
< c
< c css 2-22-2005; SCR519:  remove unused parameter and variables
< cc      aksf = valuesp( iaksf )
< cc      gint = aksf * shape
< c end change:  SCR519
---
>       aksf = valuesp( iaksf )
>       gint = aksf * shape
1458,1461c1436
< c
< c css 2-22-2005; SCR519:  remove unused parameter and variables
< cc           tempsf(it) = tempin + qwp / (gint*alengthwp )
< c end change:  SCR519
---
>            tempsf(it) = tempin + qwp / (gint*alengthwp )
```

8) Modified specified parameter in *tpa.inp*.

9) Made the following code changes in *exec.f*:

```
4198,4222c4185,4204
< c
< c css 2-18-2005; SCR519:  code should only be executed if
< c     VolcanismDisruptiveScenario (flagvolcano) is set to 1
< c
<         if (flagvolcano .eq. 1) then
<            if (volmodel .eq. 1) then
<                if ( isa .eq. 2) then
<                   call gsamtu( isa, amtupersa )
<                   releasewpfailedtime(1,3) = DMAX1( 0.0d0,
<      &               releasewpfailedtime(1,3) - dble(nwpexhumed) )
<                   print *,' *** ejected WPs: ', nwpexhumed
<                endif
```

```
<            else if (volmodel .eq. 2) then
<               eventsubarea  = ivaluesp( ieventsubarea )
<               if ( isa .eq. eventsubarea) then
<                  call gsamtu( isa, amtupersa )
<                  releasewpfailedtime(1,3) = DMAX1( 0.0d0,
<      &              releasewpfailedtime(1,3) - dble(nwpexhumed) )
<                  print *,' *** ejected WPs: ', nwpexhumed
<               endif
<            else
<               print *, ' ***>>> Error in exec <<<*** '
<               print *, ' volcano model ID is not 1 or 2.'
<               print *, ' volmodel = ', volmodel
<            endif
---
>
>           if (volmodel .eq. 1) then
>             if ( isa .eq. 2) then
>           call gsamtu( isa, amtupersa )
>           releasewpfailedtime(1,3) = DMAX1( 0.0d0,
>      &          releasewpfailedtime(1,3) - dble(nwpexhumed) )
>           print *,' *** ejected WPs: ', nwpexhumed
>             endif
>           else if (volmodel .eq. 2) then
>             eventsubarea  = ivaluesp( ieventsubarea )
>             if ( isa .eq. eventsubarea) then
>               call gsamtu( isa, amtupersa )
>               releasewpfailedtime(1,3) = DMAX1( 0.0d0,
>      &          releasewpfailedtime(1,3) - dble(nwpexhumed) )
>               print *,' *** ejected WPs: ', nwpexhumed
>             endif
>         else
>           print *, ' ***>>> Error in exec <<<*** '
>           print *, ' volcano model ID is not 1 or 2.'
>           print *, ' volmodel = ', volmodel
4224d4205
< c end change:  SCR519
```

10) Made the following code changes in *ashremob.f*:

```
2c2
< c File Name:           ashremob.f
---
> c File Name:           dcags.f
241,246c241,242
< c
< c css 2-18-2005; SCR519:  remove unused variables
< c
< cc      integer iashevolutionmode
< cc      integer iiashevolutionmode
< c end change:  SCR519
---
>
>       integer iiashevolutionmode
247a244
>       integer iashevolutionmode
374,379c371,372
< c
< c css 2-18-2005; SCR519:  remove unused variables
```

```
< c
< cc      save iashevolutionmode
< cc      save iiashevolutionmode
< c end change:  SCR519
---
>       save iashevolutionmode
>       save iiashevolutionmode
501,508d493
< c
< c css 2-18-2005; SCR519:  remove unused code
< c
< cc        call clearchar(60, name)
< cc        name = 'AshEvolutionMode[0=no_ashremob,1=ashremob]'
< cc        iiashevolutionmode = ispquery( name )
< cc        iashevolutionmode = ivaluesp(iiashevolutionmode)
< c end change:  SCR519
510a496,500
>         name = 'AshEvolutionMode[0=no_ashremob,1=ashremob]'
>         iiashevolutionmode = ispquery( name )
>         iashevolutionmode = ivaluesp(iiashevolutionmode)
>
>         call clearchar(60, name)
```

ATTACHMENT D

Test Plan for TPA SCR#519

Test Plan Name:

Tested By: Jose M. Menchaca

Date: April 22, 2005

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.00k

Test Version: TPA 5.00l

Process Level (PL) Tests

PL-1. Name:
Path for run directory: ~jmench/tpa500l/SCR519/
Path for archive of results: ~jmench/tpa500l/SCR519/
Environment variables: setenv TPA_TEST ~/tpa500l
setenv TPA_DATA ~/tpa500l
Special input files or modifications to input files required :

Item5 - forced Environment III values by forcing Drip Shield failure and reducing Rewetting Humidity.
Pertinent Lines in the tpa.inp file:

```
constant
DripShieldThickness[m]
0.000

constant
RewettingHumidity[]
0.50
```

```
Item5 - Turn Seepage Threshold flag off.
```

Pertinent Lines in the tpa.inp file:

```
FlagSeepageThreshold[]
0
```

.

Special diagnostic code modifications required :modified fortran files as needed for verification purposes.

Item 5 Modified ebsfail.f to printout the following values:

wnwc	Ratio of inhibiting nitrate to Cl to inhibiting carbonate to Cl
inhToCl2	inhibiting nitrate to Cl
inhcToCl2	inhibiting carbonate to Cl
wnws	Ratio of inhibiting nitrate to Cl to inhibiting sulfate to Cl
inhsToCl2	inhibiting sulfate to Cl
it	time
inhEff	Effective inhibitor concentration
no3(it)	time dependent nitrogen concentration of water

co3(it)	time dependent carbonate concentration of water
so4(it)	time dependent sulphur concentration of water

Program modes to be used (append flags, scenario/model switches, etc.): Default values
Utility scripts needed to perform the test:
Utility codes needed in the analysis of the test data: Microsoft Excel®

Test Description:

1) Fix findpkmndose() to not print vectors not executed via start/stop realization settings.

Run a multi-vector test run with a start vector and stop vector different than 0 and 1, then verify that only the executed vectors appear in the pkmndose.res file.

PASS

2) **Change name of results file from pkmndose.out to pkmndose.res.**

Look for output filenames at the end of a tpa500k run and a tpa500l run and compare the name differences.

PASS

3) New parameter values for *tpa.inp* (Paul Bertetti): AlluviumMatrixSpecificSurfaceArea[m2/kg]; uniform; 1.9e3, 1.21e4; pH_AllUZ_SZLayers[StandardUnits]; triangular; 6.7, 7.8, 9.2; LogCO2PartialPressure_AllUZ_SZLayers[atm]; triangular; -4., -2.5, -1. Correlation for latter two parameters is -0.95.

Visual inspection of the values of the three parameters listed above and the correlation is sufficient to verify correct implementation.

PASS

4) Modifications needed for dcags.f:

a) remove dead code from *dcags.f.* related to doss, factor1, factor2

b) change statement "thickness=gramsashpercm2/1.65d0" to "thickness=gramsahspercm2/rhoash" where rhoash is the value from tpa.inp AshBulkDensity[g/m3]

c) delete "*100" in "resuspendiblefraction(it)=thickness*100*dexp(-dlbr*(tim(it)-tim(itoe)))/resuspendibledepth"

d) update header comments

Visual inspection of the items listed above is sufficient to verify correct implementation.

PASS (unclear about what was done for "d)" above)

5) Remove unused parameters from *tpa.inp* that were put in for SCR #478: InnerInhibitingCarbonateToCl and InnerInhibitingSulfateToCl. Remove unnecessary code related to parameters in *ebsfail.f.* Code in *ebsfail.f* incorrectly used InnerInhibitingCarbonateToCl and InnerInhibitingSulfateToCl when it should use OuterInhibitingCarbonateToCl and OuterInhibitingSulfateToCl. Add calculations using WeldInhibitingCarbonateToCl and WeldInhibitingSulfateToCl to create a weld inhibiting vector in *ebsfail.f.* Write vector to *ebstrhc.inp. Failt.f* should read the weld inhibiting vector and pass it to subroutine calculateWeldFailure instead of using the effective inhibiting vector which is used to calculate WP failure.

Execute a run with both Environment I and III conditions inspecting the

output from the modified ebsfail.f code described above. The output should show changes when the Environment III conditions are met.

PASS

6) Add comments to ebsrel.f re : four parameters (SFC-14InventoryPerKgSF[ci], CladC-14inventoryPerKgSF[ci], ZyrOxideAndCrudC-14InvPerKgSF[ci], and GapAndGrainBoundaryInventoryPerKgSF[ci]) in tpa.inp aren't actually used. They are read in by ebsrel.f and written out to ebsrel.inp, which is read by *releaset*. Releaset reads the values but does nothing with them.

Visual inspection of the items listed above is sufficient to verify correct implementation.

PASS

7) remove unused parameters in tpa.inp: AirborneMassLoadAboveFreshAshBlanket[g/m3], AirborneMassLoadAboveSoil[g/m3], and EffectiveThermalConductivityOfBasket&SFinWP[W/(m-C)]. Check for dead or unnecessary code using these parameters.

Visual inspection of the items listed above is sufficient to verify correct implementation.

PASS

8) In tpa.inp change CH_Total_Thickness_9SubArea[m] to 138.0. (CHnvThickness_9SubArea[m] is set to 0.0.)

Visual inspection of the items listed above is sufficient to verify correct

implementation.

Changed from 128.0 in Version 5.0.0k to 138.0 in Version 5.0.0.l

PASS

9) Add if (flagvolcano .eq. 1) then - endif around block of code in *exec.f* (lines 4187 - 4206 TPA5.0.0i) where number of WPs ejected is printed out.

Failed: No ejected data were listed.

This problem is addressed in SCR560

10) Modifications to *ashremob.f*: remove AshEvolutionMode declaration and value retrieval; change File Name to ashremob.f.

Visual inspection of the items listed above is sufficient to verify correct implementation.

PASS

1. SCR No. (*Software Developer Assigns*): PA-SCR-520	2. Software Title and Version: TPA 5.0.0d	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): Exec.f, Nfenv.f, Ebsrel.f

1) The drip shield failure time that is used needs to be consistent. In **nfenv**, the chemical concentrations for the waste package are calculated using the **dsfail** generated drip shield failure time instead of the failure time from mechanical failure.
2) The relative humidity calculation generates a point immediately after closure that is significantly higher than other relative humidity values. This problem is most obvious with natural backfill.
3) The vapor pressure calculation returns an infinite value resulting in errors reading intermediate files. This occurs at temperatures at or above 374.3 C.

5. Change Requested by: R. Janetzke	6. Change Authorized by (*Software Developer*): R. Janetzke Date: 10-22-2004 R. Janetzke

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See attachment 1, "Description of Changes or Problem Resolution."

8. Implemented by: G. Adams	Date: 11–4-2004

9. Description of Acceptance Tests:

See Attachment 2, "Test Plan for TPA SCR#520."

10. Tested by: O. Osidele	Date: 11-15-2004

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Attachment 1

Description of Changes or Problem Resolution

1) **Consistent drip shield failure time**

Modified *exec.f* to move the mechanical failure calculations to before the call to **nfenv**. This change provides a consistent drip shield failure time for the concentration calculations in **nfenv**. Also modified *ebsrel.f* such that if there is no failure during the simulation period, then the time of drip shield failure is set to a time later than the simulation period. Previously, calculations that key on drip shield failure time would be performed at the last time step even though failure of the drip shield did not occur.

2) **Relative humidity calculation**

Modifications made within **nfenv**. Added a smoothing algorithm to the relative humidity calculation such that the relative humidity for the period immediately after closure is weighted to use the preclosure relative humidity.

3) **Vapor pressure calculation**

Modifications made within **nfenv** to limit the temperature range for the vapor pressure calculation. The calculations for the vapor pressure at temperatures above 374.3C are limited to the vapor pressure at 374.3 C.

Attachment 2

Test Plan for TPA SCR#520

Tested by: Olufemi Osidele | Date: November 15, 2004

Host Machine: SUN Ultra-4 server: Spock | Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0.0d | Test Version: TPA 5.0.0e

General Remarks

Directory path for codes: base version: ~oosidele/tpa500d
test version: ~oosidele/tpa500e

Environment variables: base version: setenv TPA_TEST ~/tpa500d
setenv TPA_DATA ~/tpa500d

test version: setenv TPA_TEST ~/tpa500e
setenv TPA_DATA ~/tpa500e

To compare simulation results, the base and test versions were run with the same *tpa.inp* input file. Supporting files are provided in the CD attached to this report.

Test Description

1. Drip shield failure time

Objectives:

(i) To test the program flow revision that executes mechanical failure calculations before calling NFENV.
(ii) To test the code modification that sets drip shield failure to a time after the simulation period if no failure occurs during the simulation period

Affected module(s): EXEC, EBSREL

Assumptions: Before determining the drip shield failure time in EBSREL, the seismic failure array is reset to null to reflect no drip shield failure.

Output files to compare or examine: None

Test procedure:

(i) Examine code modifications in the test version;
(ii) Modify codes for the base and test versions to write to screen: the computed drip shield failure time (`drip shield failure time (yr)`), and the simulation period (`end of simulation (yr)`);
(iii) Compare screen outputs from the base and test versions (see files *screenoutput_v500d.txt*, and *screenoutput_v500e.txt*).

Pass/Fail criterion(ia):

The screen outputs from the test version should indicate that MECHDRIVER is called before NFENV. For the test version, the drip shield failure time should be greater than the simulation period (unlike the base case in which both are the same).

PASS

2. Relative humidity calculation

Objective: To test the revised calculation of relative humidity at the final time step of the simulation.

Affected module(s): NFENV

Assumptions: None

Output files to compare or examine: nearfield.res and nfenv.rlt

Test procedure:

(i) Examine code modifications in the test version;
(ii) Examine the output files for time histories of output variables: `avrh` in *nearfield.res*, and `relhumwp` for each subarea in *nfenv.rlt* (see files *nearfldres_v500d.txt*, *nearfldres_v500e.txt*, *nfenvrlt_v500d.txt*, and *nfenvrlt_v500e.txt*);
(iii) Compare relative humidity values calculated at the end of the simulation period.

Pass/Fail criterion(ia):

The final relative humidity values calculated with the test version should be significantly smaller than the values obtained with the base code. Also, the final relative humidity values calculated with the test version should be about the same as the values calculated for the immediately preceding time steps.

PASS

3. <u>Vapor pressure calculation</u>

Objective: To test the revised logic for calculating vapor pressure for temperatures above 374.3°C.

Affected module(s): NFENV

Assumptions: Temperature set to 374.3°C for simulation times after 2000 yr to 3000 yr, and 380°C for simulations times after 3000 yr to 4000 yr.

Output files to compare or examine: None

Test procedure:

(i) Examine code modifications in the test version;

(ii) Modify codes for the base and test versions to print to screen, the simulation time, temperature and regressor variable (x) from the subroutine `pvap()`;

(iii) Copy screen outputs to spreadsheet (see *scr520_test_pvap.xls*);

(iv) Compare screen outputs from the base and test versions.

Pass/Fail criterion(ia):

For temperatures greater than 374.3°C, the regressor variable (x) calculated with the base version code should be negative, and that calculated with the test version should be zero.

PASS

1. SCR No. (*Software Developer Assigns*): PA-SCR-522	2. Software Title and Version: TPA 5.0.0e	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *exec.f , tpa.inp, volcano.f, ashremob.f*

The number of packages affected by a volcanic event is unclear due to apparently inconsistent displays in the TPA output. Allow *ashremob.f* to accept the amtuejected parameter in order to calculate the dose in rem per year.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
R. Janetzke	R. Janetzke Date: 10-22-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The distribution volcano model was rewritten to handle the number of packages in each category differently. The new model determines the ejected quantity independent from the failed in drift quantity. But, where the failed in drift packages are only considered for ground water transport the ejected cans are considered for both airborne and ground water transport, if there are sufficient number of packages in a subarea to account for both quantities. If there is an insufficient number of packages then the fraction of failed packages in the subarea is automatically set to 1 for the ground water transport and the number of sampled ejected packages is made available to the direct release calculations as before. The number of ejected cans may be double counted (once for ground water and once for direct release), but this is insignificant to total dose according to the model expert.

For the *ashremob.f* module the amtuejected was added to the argument list to be used in the calculation of rem per year.

8. Implemented by:	Date:
R. Janetzke	1-30-05

9. Description of Acceptance Tests:

See ATTACHMENTs A & B.

10. Tested by:	Date:
R. Nes	03-25-2005

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description** **1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justification** **1. site references (journals, sci. notebooks, publishings)** **2. is uncertainty covered by the distribution / range ?** **3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
modify from	volcano	Numberof magmainducedmechanilfailuresremainingindrift[]					
modify to	volcano	Normaizedmagmainducedmechanicalfaiuresremainingindrift[]					

ATTACHMENT A

Test Plan for TPA SCR#522

Test Plan Name:

Tested By: Razvan Nes

Date: 03-25-2005

Host Machine: Frisco

Host OS: Windows 2000 Professional

Baseline Version: tpa500e

Test Version: tpa500f

Process Level (PL) Tests

PL-1. Name: New distribution volcano model in tpa500f, **case 1** (no. of ejected WP's plus no. of WP's failed in drift is less than the total no. of WP's in the subarea, i.e. 1567)

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : the following apply to both tpa500e and tpa500f versions:

- input file was set for single-realization runs
- subarea of interest: 2
- SelectAppendFiles = 6, to append auxilliary output files volcano.ech and volcano.rlt
- set parameters of uniform distribution DefectiveFractionOfWPs/cell to 1.0E-24 and 1.0E-22 (tpa.inp file, EBSREL).
- in tpa.inp VOLCANO, set the parameters of the uniform distribution of the number of ejected WP's NumberOfWPsEntrainedByEjecta[] to (9.999, 10.001), i.e. 10 ejected WP's.
- in tpa.inp VOLCANO, set the distribution of the number of WP's failed in drift NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] to a uniform distribution (0.03190805, 0.03190815), which corresponds to 50 WP's failed in drift.

Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.):

- set VolcanoModel flag to 2 (Distribution Model)
- set all disruptive scenario flags 0, except VolcanismDisruptiveScenarioFlag which was set 1.

Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:N/A
Test description:

- objective: ensure that in tpa500f the WP's failed in drift are treated differently from the ones ejected, unlike in tpa500e (i.e. as per PA-SCR-522)
- assumptions: N/A
- constraints: N/A

- output files to compare or examine: tpa.out, volcano.rlt, wpsfail.res
- step by step test procedure to be used:
  1- exercise tpa500e and tpa500f in single-realization runs
  2 -examine and compare the above-mentioned output files (see ATTACHMENT B).
- pass/fail criteria: pass if the WP's failed in drift are treated as per PA-SCR-522.

Test Results: -See ATTACHMENT B;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

PL-2.: Name: New distribution volcano model in tpa500f, **case 2** (no. of ejected WP's plus no. of WP's failed in drift equals the total no. of WP's in the subarea, i.e. 1567)

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : the following apply to both tpa500e and tpa500f versions:
- input file was set for single-realization runs
- subarea of interest: 2
- SelectAppendFiles = 6, to append auxilliary output files volcano.ech and volcano.rlt
- set parameters of uniform distribution DefectiveFractionOfWPs/cell to 1.0E-24 and 1.0E-22 (tpa.inp file, EBSREL).
- in tpa.inp VOLCANO, set the parameters of the uniform distribution of the number of ejected WP's NumberOfWPsEntrainedByEjecta[] to (999.9, 1000.1), i.e. 1000 ejected WP's.
- in tpa.inp VOLCANO, set the distribution of the number of WP's failed in drift NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] to a uniform distribution (0.3618375, 0.3618385), which corresponds to 567 WP's failed in drift.

Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.):
- set VolcanoModel flag to 2 (Distribution Model)
- set all disruptive scenario flags 0, except VolcanismDisruptiveScenarioFlag which was set 1.

Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:N/A
Test description:
- objective: ensure that in tpa500f the WP's failed in drift are treated differently from the ones ejected, unlike in tpa500e (i.e. as per PA-SCR-522)
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: tpa.out, volcano.rlt, wpsfail.res

- step by step test procedure to be used:
  1- exercise tpa500e and tpa500f in single-realization runs
  2 -examine and compare the above-mentioned output files (see ATTACHMENT B).
- pass/fail criteria: pass if the WP's failed in drift are treated as per PA-SCR-522.

Test Results: -See ATTACHMENT B;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

PL-3: Name: New distribution volcano model in tpa500f, **case 3** (no. of ejected WP's plus no. of WP's failed in drift greater than the total no. of WP's in the subarea, i.e. 1567)

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : the following apply to tpa500e and tpa500f versions:
- input file was set for single-realization runs
- subarea of interest: 2
- SelectAppendFiles = 6, to append auxilliary output files volcano.ech and volcano.rlt
- set parameters of uniform distribution DefectiveFractionOfWPs/cell to 1.0E-24 and 1.0E-22 (tpa.inp file, EBSREL).
- in tpa.inp VOLCANO, set the parameters of the uniform distribution of the number of ejected WP's NumberOfWPsEntrainedByEjecta[] to (799.9, 800.1), i.e. 800 ejected WP's.
- in tpa.inp VOLCANO, set the distribution of the number of WP's failed in drift NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] to a uniform distribution (0.5743455, 0.5743465), which corresponds to 900 WP's failed in drift.

Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.):
- set VolcanoModel flag to 2 (Distribution Model)
- set all disruptive scenario flags 0, except VolcanismDisruptiveScenarioFlag which was set 1.

Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:N/A
Test description:
- objective: ensure that in tpa500f the WP's failed in drift are treated differently from the ones ejected, unlike in tpa500e (i.e. as per PA-SCR-522)
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: tpa.out, volcano.rlt, wpsfail.res
- step by step test procedure to be used:

1- exercise tpa500e and tpa500f in single-realization runs
2 -examine and compare the above-mentioned output files (see ATTACHMENT B).
- pass/fail criteria: pass if the WP's failed in drift are treated as per PA-SCR-522.

Test Results: -When no. of ejected WP's plus no. of WP's failed in drift is equal to or greater than the total no. of WP's in the subarea, the number of WP's failed in drift equals the total no. of WP's in the subarea, regardless the no. of ejected (see ATTACHMENT B).
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

PL-4. Name: New distribution volcano model in tpa500f, **case 4** (no. of ejected WP's plus no. of WP's failed in drift less than the total no. of WP's in the subarea, i.e. 1567), assuming all WP's initially having zero outer wall thickness.

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : the following apply to tpa500f version:
- input file was set for single-realization runs
- subarea of interest: 2
- SelectAppendFiles = 6, to append auxilliary output files volcano.ech and volcano.rlt
-set parameters of uniform distribution DefectiveFractionOfWPs/cell to 1.0E-24 and 1.0E-22 (tpa.inp file, EBSREL).
-set in tpa.inp

```
constant
OuterWPThickness[m]
0.0
```

- in tpa.inp VOLCANO, set the parameters of the uniform distribution of the number of ejected WP's NumberOfWPsEntrainedByEjecta[] to (9.999, 10.001), i.e. 10 ejected WP's.
- in tpa.inp VOLCANO, set the distribution of the number of WP's failed in drift NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] to a uniform distribution (0.03190805, 0.03190815), which corresponds to 50 WP's failed in drift.

Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.):
-set VolcanoModel flag to 2 (Distribution Model)
-set all disruptive scenario flags 0, except VolcanismDisruptiveScenarioFlag which was set 1.
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data:N/A
Test description: - objective: ensure that in tpa500f the WP's affected by igneous activity

(ejected or failed in drift) are subtracted from the total number of WP's failed in the subarea.
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: wpsfail.res
- step by step test procedure to be used:
  1- exercise tpa500f in single-realization runs
  2 -examine and compare the above-mentioned output file (see ATTACHMENT B).
- pass/fail criteria: pass if the subtraction was made correctly.

Test Results: - At the time of the event, wpsfailed.res shows 60 affected WP's. At the end of the compliance period (i.e. 10,000 yr), the rest of 1507 WP's fail in drift due to corrosion (see ATTACHMENT B);
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

PL-5. Name: New distribution volcano model in tpa500f, **case 5** (no. of ejected WP's plus no. of WP's failed in drift less than the total no. of WP's in the subarea, i.e. 1567), assuming 100% defective fraction of WP's.

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : the following apply to tpa500f version:
- input file was set for single-realization runs
- subarea of interest: 2
- SelectAppendFiles = 6, to append auxilliary output files volcano.ech and volcano.rlt
-set in tpa.inp

```
uniform
DefectiveFractionOfWPs/cell
0.99998,  0.99999
```

- in tpa.inp VOLCANO, set the parameters of the uniform distribution of the number of ejected WP's NumberOfWPsEntrainedByEjecta[] to (9.999, 10.001), i.e. 10 ejected WP's.
- in tpa.inp VOLCANO, set the distribution of the number of WP's failed in drift NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] to a uniform distribution (0.03190805, 0.03190815), which corresponds to 50 WP's failed in drift.

Special diagnostic code modifications required : N/A
Program modes to be used (append flags, scenario/model switches, etc.):
-set VolcanoModel flag to 2 (Distribution Model)
-set all disruptive scenario flags 0, except VolcanismDisruptiveScenarioFlag which was set 1.
Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data:N/A

Test description:
- objective: ensure that in tpa500f the WP's affected by igneous activity (ejected or failed in drift) are subtracted from the total number of WP's failed in the subarea.
- assumptions: N/A
- constraints: N/A
- output files to compare or examine: wpsfail.res, tpa.out
- step by step test procedure to be used:
  1- exercise tpa500f in single-realization runs
  2 -examine and compare the above-mentioned output file (see ATTACHMENT B).
- pass/fail criteria: pass if the subtraction was made correctly.

Test Results:
- In this case tpa.out shows 10 ejected WP's and 1567 (all) failed from initial event. Result file wpsfailed.res shows no failed WP's, just recording the time of the igneous event(see ATTACHMENT B);
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

PL-6. Name: New argument added to the argument list for *ashremob.f* module

Path for run directory:

Path for archive of results:

Environment variables:

Special input files or modifications to input files required : N/A

Special diagnostic code modifications required : N/A

Program modes to be used (append flags, scenario/model switches, etc.): N/A

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data:N/A

Test description:
- objective: ensure that new argument *amtuejected* was added to the argument list for *ashremob.f* module
- assumptions: N/A
- constraints: N/A
- files to compare or examine: *ashremob.f*, *exec.f*;
- step by step test procedure to be used:
  1- exercise tpa500f in single-realization runs
  2 -examine and compare the above-mentioned files (see ATTACHMENT B).
- pass/fail criteria: pass if the new argument *amtuejected* was added as per PA-SCR-522.

Test Results:
-See ATTACHMENT B;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

ATTACHMENT B

PL-1: -**tpa.out files:**

-TPA 500e output file

```
-----------------------------------------------------------------------
    subarea   2 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
        Mean Annual Infiltration at Start(AAI0):    9.7117E+00
exec: calling nfenvFl
exec: calling dsfail
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Weld Failure
     *** No Corrosion WP Failure ***
exec: calling volcano
 *** failed WPs:  10   out of  1567  ***
 *** ejected WPs:  10
```

-TPA 500f output file

```
-----------------------------------------------------------------------
    subarea   2 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
        Mean Annual Infiltration at Start(AAI0):    9.7117E+00
exec: calling nfenvFl
exec: calling dsfail
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Weld Failure
     *** No Corrosion WP Failure ***
exec: calling volcano
exec: failed WPs from Volcanic  event =     60 at time =   6715.4 yr
 *** failed WPs:  60   out of  1567  ***
 *** ejected WPs:  10
```

- **volcano.rlt files**:

- TPA 500e volcano.rlt file

```
REALIZATION    1

ALL SUBAREAS

amtuejected =   7.8903E+01

subarea   volcanicamtufailed
     1         0.0000E+00
```

2	2.5176E-01
3	0.0000E+00
4	0.0000E+00
5	0.0000E+00
6	0.0000E+00
7	0.0000E+00
8	0.0000E+00
9	0.0000E+00
10	0.0000E+00

Fraction of Waste Packages Failed by Volcanism

	time	subarea1	subarea2	subarea3	subarea4	subarea5
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
185	6.8750E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
186	7.0382E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
187	7.2053E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
188	7.3763E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
189	7.5513E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
190	7.7304E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
191	7.9137E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
192	8.1013E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
193	8.2933E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
194	8.4897E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
195	8.6908E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
196	8.8966E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
197	9.1072E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
198	9.3227E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
199	9.5433E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
200	9.7690E+03	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00
201	1.0000E+04	0.0000E+00	6.4023E-03	0.0000E+00	0.0000E+00	0.0000E+00

- TPA 500f volcano.rlt file

REALIZATION 1

ALL SUBAREAS

amtuejected = 7.8903E+01

subarea	volcanicamtufailed
1	3.6807E+02
2	4.7340E+02
3	1.9410E+02
4	1.0800E+02
5	1.9083E+02
6	2.1374E+02
7	8.1569E+01
8	2.1273E+02
9	2.4597E+02
10	2.2532E+02

Fraction of Waste Packages Failed by Volcanism

	time	subarea1	subarea2	subarea3	subarea4	subarea5
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
185	6.8750E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
186	7.0382E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
187	7.2053E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
188	7.3763E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
189	7.5513E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
190	7.7304E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
191	7.9137E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
192	8.1013E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
193	8.2933E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
194	8.4897E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
195	8.6908E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
196	8.8966E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
197	9.1072E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
198	9.3227E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
199	9.5433E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
200	9.7690E+03	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02
201	1.0000E+04	3.1908E-02	3.8290E-02	3.1908E-02	3.1908E-02	3.1908E-02

	time	subarea6	subarea7	subarea8	subarea9	subarea10
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
185	6.8750E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
186	7.0382E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
187	7.2053E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
188	7.3763E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
189	7.5513E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
190	7.7304E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
191	7.9137E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
192	8.1013E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
193	8.2933E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
194	8.4897E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
195	8.6908E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
196	8.8966E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
197	9.1072E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
198	9.3227E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
199	9.5433E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
200	9.7690E+03	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02
201	1.0000E+04	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02	3.1908E-02

- **wpsfail.res files:**

-TPA 500e wpsfail.res file:

vector	time	#corrode	#seismic	#fault	#igact
unitless	yr	unitless	unitless	unitless	unitless

```
 1        6.7154E+03    0.0000E+00    0.0000E+00    0.0000E+00    1.0000E+01
```

-TPA 500f wpsfail.res file:

```
 vector      time         #corrode      #seismic      #fault        #igact
 unitless     yr          unitless      unitless      unitless      unitless

 1        6.7154E+03    0.0000E+00    0.0000E+00    0.0000E+00    6.0000E+01
```

PL-2: -<u>tpa.out files:</u>

-TPA 500e output file

```
-----------------------------------------------------------------------
    subarea   2 of  10           realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
        Mean Annual Infiltration at Start(AAI0):    9.7117E+00
exec: calling nfenvFl
exec: calling dsfail
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Weld Failure
     *** No Corrosion WP Failure ***
exec: calling volcano
 *** failed WPs:  1000   out of  1567  ***
 *** ejected WPs:  1000
```

-TPA 500f output file

```
-----------------------------------------------------------------------
    subarea   2 of  10           realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
        Mean Annual Infiltration at Start(AAI0):    9.7117E+00
exec: calling nfenvFl
exec: calling dsfail
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Weld Failure
     *** No Corrosion WP Failure ***
exec: calling volcano
exec: failed WPs from Volcanic  event =   1567 at time =   6715.4 yr
 *** failed WPs: all WPs failed ( 1567 ) ***
 *** ejected WPs:  1000
```

- <u>volcano.rlt files</u>:

- TPA 500e volcano.rlt file

REALIZATION 1

ALL SUBAREAS

amtuejected = 7.8903E+03

subarea	volcanicamtufailed
1	0.0000E+00
2	2.8549E+00
3	0.0000E+00
4	0.0000E+00
5	0.0000E+00
6	0.0000E+00
7	0.0000E+00
8	0.0000E+00
9	0.0000E+00
10	0.0000E+00

Fraction of Waste Packages Failed by Volcanism

	time	subarea1	subarea2	subarea3	subarea4	subarea5
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
185	6.8750E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
186	7.0382E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
187	7.2053E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
188	7.3763E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
189	7.5513E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
190	7.7304E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
191	7.9137E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
192	8.1013E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
193	8.2933E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
194	8.4897E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
195	8.6908E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
196	8.8966E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
197	9.1072E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
198	9.3227E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
199	9.5433E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
200	9.7690E+03	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00
201	1.0000E+04	0.0000E+00	6.3842E-01	0.0000E+00	0.0000E+00	0.0000E+00

	time	subarea6	subarea7	subarea8	subarea9	subarea10
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
185	6.8750E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
186	7.0382E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
187	7.2053E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
188	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
189	7.5513E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
190	7.7304E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
191	7.9137E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
192	8.1013E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

193	8.2933E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
194	8.4897E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
195	8.6908E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
196	8.8966E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
197	9.1072E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
198	9.3227E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
199	9.5433E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
200	9.7690E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
201	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

- TPA 500f volcano.rlt file

REALIZATION 1

ALL SUBAREAS

amtuejected = 7.8903E+03

subarea	volcanicamtufailed
1	4.1739E+03
2	1.2364E+04
3	2.2011E+03
4	1.2248E+03
5	2.1640E+03
6	2.4238E+03
7	9.2499E+02
8	2.4124E+03
9	2.7892E+03
10	2.5551E+03

Fraction of Waste Packages Failed by Volcanism

	time	subarea1	subarea2	subarea3	subarea4	subarea5
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
185	6.8750E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
186	7.0382E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
187	7.2053E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
188	7.3763E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
189	7.5513E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
190	7.7304E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
191	7.9137E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
192	8.1013E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
193	8.2933E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
194	8.4897E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
195	8.6908E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
196	8.8966E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
197	9.1072E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
198	9.3227E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
199	9.5433E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
200	9.7690E+03	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01
201	1.0000E+04	3.6184E-01	1.0000E+00	3.6184E-01	3.6184E-01	3.6184E-01

time	subarea6	subarea7	subarea8	subarea9	subarea10
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
185	6.8750E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
186	7.0382E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
187	7.2053E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
188	7.3763E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
189	7.5513E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
190	7.7304E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
191	7.9137E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
192	8.1013E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
193	8.2933E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
194	8.4897E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
195	8.6908E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
196	8.8966E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
197	9.1072E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
198	9.3227E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
199	9.5433E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
200	9.7690E+03	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01
201	1.0000E+04	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01	3.6184E-01

- **wpsfail.res files:**

-TPA 500e wpsfail.res file

vector	time	#corrode	#seismic	#fault	#igact
unitless	yr	unitless	unitless	unitless	unitless
1	6.7154E+03	0.0000E+00	0.0000E+00	0.0000E+00	1.0000E+03

-TPA 500f wpsfail.res file

vector	time	#corrode	#seismic	#fault	#igact
unitless	yr	unitless	unitless	unitless	unitless
1	6.7154E+03	0.0000E+00	0.0000E+00	0.0000E+00	1.5670E+03

PL-3 : -tpa.out files:

-TPA 500e output file

```
-----------------------------------------------------------------------
    subarea   2 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
        Mean Annual Infiltration at Start(AAI0):    9.7117E+00
```

```
exec: calling nfenvFl
exec: calling dsfail
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Weld Failure
     *** No Corrosion WP Failure ***
exec: calling volcano
 *** failed WPs:  801   out of  1567  ***
 *** ejected WPs:  800
```

-TPA 500f output file

```
-----------------------------------------------------------------------
    subarea   2 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
        Mean Annual Infiltration at Start(AAI0):    9.7117E+00
exec: calling nfenvFl
exec: calling dsfail
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Weld Failure
     *** No Corrosion WP Failure ***
exec: calling volcano
exec: failed WPs from Volcanic  event =   1567 at time =   6715.4 yr
 *** failed WPs: all WPs failed ( 1567 ) ***
 *** ejected WPs:  800
```

- **volcano.rlt files:**

- TPA 500e volcano.rlt file

```
REALIZATION    1


ALL SUBAREAS

amtuejected =   6.3120E+03

subarea   volcanicamtufailed
     1         0.0000E+00
     2         4.5316E+00
     3         0.0000E+00
     4         0.0000E+00
     5         0.0000E+00
     6         0.0000E+00
     7         0.0000E+00
     8         0.0000E+00
     9         0.0000E+00
    10         0.0000E+00

Fraction of Waste Packages Failed by Volcanism

       time         subarea1     subarea2     subarea3     subarea4     subarea5

   1  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
   2  2.3102E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
```

183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
185	6.8750E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
186	7.0382E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
187	7.2053E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
188	7.3763E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
189	7.5513E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
190	7.7304E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
191	7.9137E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
192	8.1013E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
193	8.2933E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
194	8.4897E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
195	8.6908E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
196	8.8966E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
197	9.1072E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
198	9.3227E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
199	9.5433E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
200	9.7690E+03	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00
201	1.0000E+04	0.0000E+00	5.1090E-01	0.0000E+00	0.0000E+00	0.0000E+00

	time	subarea6	subarea7	subarea8	subarea9	subarea10
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
185	6.8750E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
186	7.0382E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
187	7.2053E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
188	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
189	7.5513E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
190	7.7304E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
191	7.9137E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
192	8.1013E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
193	8.2933E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
194	8.4897E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
195	8.6908E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
196	8.8966E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
197	9.1072E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
198	9.3227E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
199	9.5433E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
200	9.7690E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
201	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

- TPA 500f volcano.rlt file

```
REALIZATION     1


ALL SUBAREAS

amtuejected =    6.3123E+03

subarea    volcanicamtufailed
     1          6.6252E+03
     2          1.3413E+04
     3          3.4939E+03
     4          1.9441E+03
```

5	3.4349E+03
6	3.8473E+03
7	1.4682E+03
8	3.8292E+03
9	4.4274E+03
10	4.0558E+03

Fraction of Waste Packages Failed by Volcanism

	time	subarea1	subarea2	subarea3	subarea4	subarea5
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
185	6.8750E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
186	7.0382E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
187	7.2053E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
188	7.3763E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
189	7.5513E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
190	7.7304E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
191	7.9137E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
192	8.1013E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
193	8.2933E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
194	8.4897E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
195	8.6908E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
196	8.8966E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
197	9.1072E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
198	9.3227E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
199	9.5433E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
200	9.7690E+03	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01
201	1.0000E+04	5.7435E-01	1.0000E+00	5.7435E-01	5.7435E-01	5.7435E-01

	time	subarea6	subarea7	subarea8	subarea9	subarea10
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
185	6.8750E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
186	7.0382E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
187	7.2053E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
188	7.3763E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
189	7.5513E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
190	7.7304E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
191	7.9137E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
192	8.1013E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
193	8.2933E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
194	8.4897E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
195	8.6908E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
196	8.8966E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
197	9.1072E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
198	9.3227E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
199	9.5433E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
200	9.7690E+03	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01
201	1.0000E+04	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01	5.7435E-01

- **wpsfail.res files:**

-TPA 500e wpsfail.res file

```
 vector      time          #corrode     #seismic     #fault       #igact
 unitless    yr            unitless     unitless     unitless     unitless

1            6.7154E+03    0.0000E+00   0.0000E+00   0.0000E+00   8.0100E+02
```

-TPA 500f wpsfail.res file

```
vector     time          #corrode      #seismic     #fault       #igact
unitless   yr            unitless      unitless     unitless     unitless

1          6.7154E+03    0.0000E+00    0.0000E+00   0.0000E+00   1.5670E+03
```

PL-4: - <u>wpsfail.res file</u>:

-TPA 500f wpsfail.res file

```
vector     time          #corrode      #seismic      #fault       #igact
unitless   yr            unitless      unitless      unitless     unitless

1          6.7154E+03 0.0000E+00     0.0000E+00       0.0000E+00       6.0000E+01

1          1.0000E+04 1.5070E+03     0.0000E+00       0.0000E+00       0.0000E+00
```

PL-5: - <u>wpsfail.res file</u>:

-TPA 500f wpsfail.res file

```
vector     time          #corrode      #seismic      #fault          #igact
unitless   yr            unitless      unitless      unitless        unitless

1          6.7154E+03    0.0000E+00    0.0000E+00    0.0000E+00      0.0000E+00
```

- <u>tpa.out file</u>:

```
-----------------------------------------------------------------------
    subarea   2 of  10           realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
        Mean Annual Infiltration at Start(AAI0):    9.7117E+00
exec: calling nfenvFl
exec: calling dsfail
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Weld Failure
     *** No Corrosion WP Failure ***
```

```
exec: calling volcano
exec: failed WPs from INITIAL   event =   1567 at time =      0.0 yr
 *** failed WPs: all WPs failed ( 1567 ) ***
 *** ejected WPs:  10
```

PL-6: -ashremob.f file

```
C      ASHREMOB HISTORY:
c                          created by D.J. Sylvester, SwRI
c           1-30-05 rwj    SCR522; Add amtuejected to argument list.
c=====================================================================
cc rwj 1-29-05; SCR 522
c     subroutine ashremob( irl, mxntime, mxnnucldr, ntim, tim, nnucldr,
c    &                     namesdr, dMAT, dMAP, remperyrpernuclgs )
      subroutine ashremob( irl, mxntime, mxnnucldr, ntim, tim, nnucldr,
     &                     namesdr, dMAT, dMAP, amtuejected,
     &                     remperyrpernuclgs )
c=====================================================================
```

-exec.f file:

```
 call ashremob( ir, maxntime, 43, ntim, tim(1), 43,
     &                  namesisotopesave(1),
     &       AAT, AAP, amtuejected, remperyrgsnr)
```

1. SCR No. (*Software Developer Assigns*): PA-SCR-523	2. Software Title and Version: TPA 5.0.0f	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *szft.f, uzft.f, exec.f, tpa.inp, prenefmks.h, ashremob.f, remob_lut.dat.*

1) The **szft** module uses alluvium RD values for tuff RD parameters. This occurs in the interface to the *calc_rd* subroutine.
2) The *actinide_kdrd.out* file needs to be recreated to supply intermediate values for alluvium parameters.
3) The input file *tpa.inp* does not have most recent values for colloid concentrations or colloid retardation factors (from SCR#484).
4) The parameter AlluviumMatrixPoreRadius_SAV[m] is no longer used, but there is code in *szft.f* referencing it and it is still in *tpa.inp*.
5) Calculations of **concentfactoreoli**, **portionflvh**, and **portioneolh** are incorrect in *ashremob.f*
6) Update *remob_lut.dat* file.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
C. Scherer R. Nes	R. Janetzke Date: 11-22-2004

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See Attachment A for items 1-5.
See Attachment B for item 6.

8. Implemented by:	Date:
C. Scherer R. Janetzke	2-9-2005 2-8-2005

9. Description of Acceptance Tests:

10. Tested by:	Date:
J. Menchaca	5-4-05

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)
Delete	SZFT	AlluviumMatrixPoreRadius_SAV[m]					PB

Update Range	UZFT	FractureColloidRetardationFactor_TSw_[]	Retardation factor for colloids.	usersupplie dpwisecdf	15 1.0, 0.0 1.01, 0.01 1.5, 0.04 2.0, 0.06 4.0, 0.12 6.0, 0.15 10.23, 0.25 14.86, 0.35 26.00, 0.5 34.35, 0.60 45.39, 0.70 59.98, 0.80 219.0, 0.90 418.6, 0.95 800.0, 1.00	Modified from DOE distribution (ANL-NBS-HS-000031 Rev 1, Table 7) Linearly interpolated in Log space between tabulated values and with DOE truncation removed. Presumes 1% are unretarded.	DAP, SLP
Update Range	UZFT	FractureColloidRetardationFactor_CHnv[]	"	usersupplie dpwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidRetardationFactor_CHnz[]	"	usersupplie dpwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidRetardationFactor_PPw_[]	"	usersupplie dpwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidRetardationFactor_UCF_[]	"	usersupplie dpwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidRetardationFactor_BFw_[]	"	usersupplie dpwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidRetardationFactor_UFZ_[]	"	usersupplie dpwisecdf	"	"	DAP, SLP
Update Range	UZFT	MatrixColloidRetardationFactor_TSw_[]	"	usersupplie dpwisecdf	20 1.0, 0.0 1.01, 0.01 1.50, 0.07 2.0, 0.12 4.0, 0.22	Modified from DOE distribution ANL-NBS-HS-000031 Rev 1, Table 8. Linearly interpolated in	DAP, SLP

					6.0, 0.29 8.0, 0.33 14.4, 0.4 22.14, 0.45 34.0, 0.5 56.15, 0.55 92.85, 0.6 153.5, 0.65 253.9, 0.7 419.7, 0.75 694.0, 0.8 1148, 0.85 1897, 0.9 3138, 0.95 5188.0, 1.0	Log space between tabulated values and with DOE truncation removed. Presumes 1% are unretarded.	
Update Range	UZFT	MatrixColloidRetardationFactor_CHnv[]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	MatrixColloidRetardationFactor_CHnz[]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	MatrixColloidRetardationFactor_PPw_[]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	MatrixColloidRetardationFactor_UCF_[]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	MatrixColloidRetardationFactor_BFw_[]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	MatrixColloidRetardationFactor_UFZ_[]	"	usersupplied pwisecdf	"	"	DAP, SLP

Update Range	UZFT	FractureColloidConcentration_TSw_[kg/m3]	Colloid Concentration	usersupplied pwisecdf	16 1.0e-6, 0.0 2.51e-6, 0.1 6.31e-6, 0.2 1.58e-5, 0.3 3.98e-5, 0.4 1.0e-4, 0.5 2.51e-4, 0.6 6.31e-4, 0.7 1.0e-3, 0.75 2.15e-3, 0.8 4.64e-3, 0.85 1.0e-2, 0.9 2.24e-2, 0.94 5.0e-2., 0.98 0.1, 0.99 0.2, 1.0	MDL-EBS-PA-000004 Rev 0, Table 5, linearly interpolated in log space. Best available information.	DAP, SLP
Update Range	UZFT	FractureColloidConcentration_CHnv[kg/m3]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidConcentration_Chnz[kg/m3]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidConcentration_PPw_[kg/m3]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidConcentration_UCF_[kg/m3]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidConcentration_BFw_[kg/m3]	"	usersupplied pwisecdf	"	"	DAP, SLP
Update Range	UZFT	FractureColloidConcentration_UFZ_[kg/m3]	"	usersupplied pwisecdf	"	"	DAP, SLP

Update Range	UZFT	MatrixColloidConcentration_TSw_[kg/m3]	"	usersupplied pwisecdf	16 1.6e-7, 0.0 3.02e-7, 0.1 1.01e-6, 0.2 2.53e-6, 0.3 6.37e-6, 0.4 1.60e-5, 0.5 4.02e-5, 0.6 1.01e-4, 0.7 1.6e-4, 0.75 3.44e-4, 0.8 7.42e-4, 0.85 1.6e-3, 0.9 3.58e-3, 0.94 8.0e-3, 0.98 0.016, 0.99 0.032, 1.0	MDL-EBS-PA-000004 Rev 0, Table 5 after scaling by a filtration factor. See scientific notebook 133, pages 85 to 90	DAP, SLP
Update Range	UZFT	MatrixColloidConcentration_CHnv[kg/m3]	"	usersupplied pwisecdf	16 3.1e-7, 0.0 7.78e-7, 0.1 1.96e-6, 0.2 4.99e-6, 0.3 1.23e-5, 0.4 3.1e-5, 0.5 7.78e-5, 0.6 1.96e-4, 0.7 3.1e-4, 0.75 6.66e-4, 0.8 1.44e-4, 0.85 3.1e-3, 0.9 6.94e-3, 0.94 1.55e-2., 0.98 0.031, 0.99 0.062, 1.0	"	DAP, SLP

Update Range	UZFT	MatrixColloidConcentration_Chnz[kg/m3]	"	usersupplied pwisecdf	16 1.1e-7, 0.0 2.768e-7, 0.1 6.94e-7, 0.2 1.74e-6, 0.3 4.38e-6, 0.4 1.1e-5, 0.5 2.76e-5, 0.6 6.94e-5, 0.7 1.1e-4, 0.75 2.37e-4, 0.8 5.10e-4, 0.85 1.1e-3, 0.9 2.46e-3, 0.94 5.5e-3, 0.98 0.011, 0.99 0.022, 1.0	"	DAP, SLP

Update Range	UZFT	MatrixColloidConcentration_PPw_[kg/m3]	"	usersupplied pwisecdf	16 4.1e-7, 0.0 1.03e-6, 0.1 2.59e-6, 0.2 6.48e-6, 0.3 1.63e-5, 0.4 4.1e-5, 0.5 1.03e-4, 0.6 2.59e-4, 0.7 4.1e-4, 0.75 8.81e-4, 0.8 1.90e-3, 0.85 4.1e-3, 0.9 9.18e-3, 0.94 2.05e-2, 0.98 0.041, 0.99 0.082, 1.0	"	DAP, SLP

Update Range	UZFT	MatrixColloidConcentration_UCF_[kg/m3]	"	usersupplie dpwisecdf	16 3.3e-7, 0.0 8.28e-7, 0.1 2.08e-6, 0.2 5.21e-6, 0.3 1.31e-5, 0.4 3.3e-5, 0.5 8.28e-5, 0.6 2.08e-4, 0.7 3.3e-4, 0.75 7.09e-4, 0.8 1.53e-3, 0.85 3.3e-3, 0.9 7.39e-3, 0.94 0.0165, 0.98 0.033, 0.99 0.066, 1.0	"	DAP, SLP

Update Range	UZFT	MatrixColloidConcentration_BFw_[kg/m3]	"	usersupplied pwisecdf	16 7.1e-8, 0.0 1.78e-7, 0.1 4.48e-7, 0.2 1.122e-6, 0.3 2.82e-6, 0.4 7.1e-6, 0.5 1.78e-5, 0.6 4.48e-5, 0.7 7.1e-5, 0.75 1.53e-4, 0.8 3.29e-4, 0.85 7.1e-4, 0.9 1.59e-3, 0.94 3.55e-3, 0.98 7.1e-3, 0.99 0.0142, 1.0	"	DAP, SLP
Update Range	UZFT	MatrixColloidConcentration_UFZ_[kg/m3]"constant	0			not used in basecase	DAP, SLP

Update Range	SZFT	ColloidRetardationFactor_SAV_[]	Colloid Retardation factor in Alluvium.	usersupplied pwisecdf	20 1.0, 0.0 1.01, 0.01 1.50, 0.07 2.0, 0.12 4.0, 0.22 6.0, 0.29 8.0, 0.33 14.4, 0.4 22.14, 0.45 34.0, 0.5 56.15, 0.55 92.85, 0.6 153.5, 0.65 253.9, 0.7 419.7, 0.75 694.0, 0.8 1148, 0.85 1897, 0.9 3138, 0.95	Modified from DOE distribution (ANL-NBS-HS-000031 Rev 1, Table 7) Linearly interpolated in Log space between tabulated values and with DOE truncation removed. Presumes 1% are unretarded.	DAP, SLP
Update Range	SZFT	ColloidRetardationFactor_STFF[]	Colloid Retardation factor in fractures in the fractured volcanic leg of saturated zone.	usersupplied pwisecdf	15 1.0, 0.0 1.01, 0.01 1.5, 0.04 2.0, 0.06 4.0, 0.12 6.0, 0.15 10.23, 0.25 14.86, 0.35 26.00, 0.5 34.35, 0.60 45.39, 0.70 59.98, 0.80 219.0, 0.90 418.6, 0.95 800.0, 1.00	Modified from DOE distribution ANL-NBS-HS-000031 Rev 1, Table 8. Linearly interpolated in Log space between tabulated values and with DOE truncation removed. Presumes 1% are unretarded. DAP, SLP	

Update Range	SZFT	ColloidConcentration_SAV_[kg/m3]	Colloid concentration in alluvium.	usersupplie dpwisecdf	16 1.0e-6, 0.0 2.51e-6, 0.1 6.31e-6, 0.2 1.58e-5, 0.3 3.98e-5, 0.4 1.0e-4, 0.5 2.51e-4, 0.6 6.31e-4, 0.7 1.0e-3, 0.75 2.15e-3, 0.8 4.64e-3, 0.85 1.0e-2, 0.9 2.24e-2, 0.94 5.e-2., 0.98 0.1, 0.99	MDL-EBS-PA-000004 Rev 0, Table 5, linearly interpolated in log space. Best available information.	DAP,
Update Range	SZFT	ColloidConcentration_STFF[kg/m3]	Colloid concentration in fractures the factured volcanic leg	"	"	DAP, SLP	

ATTACHMENT A

1) The following block of comments and code was inserted before the 2nd call to calc_kd:

```
c
c css - 1-31-2005; SCR523:  use TUFF values, not ALLUVIUM values
c     leftover from previous loop
         density    = valuesp(imdensity(ilayer))
         porosity   = valuesp(imporosity(ilayer))
         poreradius = valuesp(imporeradius(ilayer))
         ssarea     = 3.0d0*porosity / (density*poreradius)
c end change: SCR523
```

2) Code that created and wrote to the file *actinide_kdrd.out* was commented out. Code that creates and writes to four new files was added to *exec.f*, *uzft.f*, and *szft.f*. *Prenefmks.h* was modified to allow ir to be passed as an input parameter. A new routine setup_kdrd_files was added to *exec.f*. In *szft.f*, the following code was added:

after 1st calls to calc_kd and calc_rd:

```
c
c css - 2-1-2005; SCR523:  modify contents of actinide_kdrd.out
      open(unit=iszkdrd, file='sz_kdrd.out',
     &     STATUS='OLD',ACCESS='APPEND')
      if (firstheader1) then
         firstheader1 = .false.
         write(labels, '(a12)') '(12(a13,2x)'
         strptr1 = 1
         strptr2 = 76
         do i=1,5
            labels(strptr1:strptr1+14) = radelems(i)
            labels(strptr2:strptr2+14) = radelems(i)
            strptr1 = strptr1 + 15
            strptr2 = strptr2 + 15
         end do
         write(iszkdrd, '(12(a13,2x),a150)')
     &         'realization  ', 'layer        ', 'media        ',
     &         'logCO2       ', 'CO2          ', 'ph           ',
     &         'porosity     ', 'ssarea       ', 'density      ',
     &         'aperture     ', 'frac_forcefac', 'pore_radius  ',
     &         labels
         write(iszkdrd, *) ' '
      end if
      write(iszkdrd, '(i3,12x,i1,14x,a2,13x,19(e12.4,3x))')
     &      ir, ilayer, '1', dlogco2pp_uzsz,
     &      co2pp_uzsz, ph_uzsz, porosity, ssarea, density,
     &      aperture, frac_forcefac, poreradius,
     &      (kds(i),i=1,5), (rds(i),i=1,5)
      close(iszkdrd)
c end change:  SCR523
```

after 2nd calls to calc_kd and calc_rd:

```
c
c css - 2-1-2005; SCR523:  modify contents of actinide_kdrd.out
c
      open(unit=iszkdrd, file='sz_kdrd.out',
     &     STATUS='OLD',ACCESS='APPEND')
      write(iszkdrd, '(i3,12x,i1,14x,a2,13x,19(e12.4,3x))')
     &      ir, ilayer, '2', dlogco2pp_uzsz,
     &      co2pp_uzsz, ph_uzsz, porosity, ssarea, density,
     &      aperture, frac_forcefac, poreradius,
     &      (kds(i),i=1,5), (rds(i),i=1,5)
      close(iszkdrd)
c end change:  SCR523
```

after call to mod_rdrdi:

```
c
c css - 2-1-2005; SCR523:  modify contents of actinide_kdrd.out
c
      open(unit=iszrevers, file='sz_revers.out',
     &     STATUS='OLD',ACCESS='APPEND')
      if (firstheader1) then
         firstheader1 = .false.
         write(fmtstr, '(a, i2, a)')
     &         '(3(a13,2x),', numelm*2, '(a2,13x))'
         write(iszrevers, fmtstr)
     &         'realization  ', 'subarea      ',  'layer        ',
     &         (elementlist(ii),ii=1,numelm),
     &         (elementlist(ii),ii=1,numelm)
      end if
      write(fmtstr, '(a,i2,a)')
     &      '(i3,12x,i2,13x,i2,13x,',  numelm*2, '(e12.4,3x))'
      do kk=1,nefleg
         write(iszrevers, fmtstr) ir, isa, kk,
     &         (rd(ii,kk),ii=1,numelm), (rdi(ii,kk),ii=1,numelm)
      end do
      close(iszrevers)
c end change:  SCR523
```

The following code was added to uzft.f:

after 1st calls to calc_kd and calc_rd:

```
c
c css - 2-3-2005; SCR523:  modify contents of actinide_kdrd.out
      open(unit=iuzkdrd, file='uz_kdrd.out',
     &     STATUS='OLD',ACCESS='APPEND')
      if (firstheader1) then
         firstheader1 = .false.
         write(labels, '(a12)') '(12(a13,2x)'
         strptr1 = 1
         strptr2 = 76
         do i=1,5
            labels(strptr1:strptr1+14) = radelems(i)
            labels(strptr2:strptr2+14) = radelems(i)
            strptr1 = strptr1 + 15
            strptr2 = strptr2 + 15
```

```
         end do
         write(iuzkdrd, '(12(a13,2x),a150)')
     &         'realization  ', 'layer        ', 'media        ',
     &         'logCO2       ', 'CO2          ', 'ph           ',
     &         'porosity     ', 'ssarea       ', 'density      ',
     &         'aperture     ', 'frac_forcefac', 'pore_radius  ',
     &         labels
         write(iuzkdrd, *) ' '
      end if
      write(iuzkdrd, '(i3,12x,i1,14x,a2,13x,19(e12.4,3x))')
     &      ir, ilayer, '1', dlogco2pp_uzsz,
     &      co2pp_uzsz, ph_uzsz, porosity, ssarea, density,
     &      aperture, frac_forcefac, poreradius,
     &      (kds(i),i=1,5), (rds(i),i=1,5)

      close(iuzkdrd)
c end change:  SCR523
```

after 2nd calls to calc_kd and cald_rd:

```
c
c css - 2-3-2005; SCR523:  modify contents of actinide_kdrd.out
      open(unit=iuzkdrd, file='uz_kdrd.out',
     &     STATUS='OLD',ACCESS='APPEND')
      write(iuzkdrd, '(i3,12x,i1,14x,a2,13x,19(e12.4,3x))')
     &      ir, ilayer, '2', dlogco2pp_uzsz,
     &      co2pp_uzsz, ph_uzsz, porosity, ssarea, density,
     &      aperture, frac_forcefac, poreradius,
     &      (kds(i),i=1,5), (rds(i),i=1,5)
      close(iuzkdrd)
c end change:  SCR523
```

after line containing "903 CONTINUE":

```
c
c css - 4-3-2005; SCR523:  modify contents of actinide_kdrd.out
c
      open(unit=iuzrevers, file='uz_revers.out',
     &     STATUS='OLD',ACCESS='APPEND')
      if (firstheader1) then
         firstheader1 = .false.
         write(fmtstr, '(a, i2, a)') '(4(a13,2x),', numelm, '(a2,13x))'
         write(iuzrevers, fmtstr) 'realization ', 'subarea      ',
     &                            'leg         ', 'media        ',
     &         (elementlist(ii),ii=1,numelm)
      end if
      write(fmtstr, '(a,i2,a)')
     &      '(i2,13x,i2,13x,i2,13x,i2,13x',  numelm, '(e12.4,3x))'
      do kk=1,nefleg
         write(iuzrevers, fmtstr) ir, isa, kk,
     &         media, (nefrd(ii,kk), ii=1,numelm)
      end do
      close(iuzrevers)
c end change:  SCR523
```

The following code was added to exec.f:

after line 1146:

```
c css - 1-31-2005; SCR523:  modify contents of actinide_kdrd.out file
c    make multiple files and rename
     call setup_kdrd_files()
c end change: SCR523
```

at the end of the file:

```
c==+=================================================================
      subroutine setup_kdrd_files()
c=====================================================================
c     NAME:      setup_kdrd_files
c
c     PURPOSE:   initialize files that contain calculated values for
c                kds, rds, and reversible kds and rds for saturated
c                and unsaturated zones
c
c     METHOD:
c        Subroutine added 2-1-2005 for SCR523
c
c     INPUT:
c           none
c
c     OUTPUT:
c            none
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c     --- TEST DRIVER ---
c      include 'setup_kdrd_files.t'

c     --- HEADER ---
c      include 'setup_kdrd_files.h'

       implicit none

cccccc
c     GLOSSARY:
c
cccccc
      character*330 header1
      character*645 header2

      integer i
      integer iszkdrd
      integer iszrevers
      integer iuzkdrd
      integer iuzrevers

      common / szkdrd / iszkdrd, iszrevers
      common / uzkdrd / iuzkdrd, iuzrevers

      integer igetunitnumber
      external igetunitnumber
c
c     Start here.
c
```

```
 iszkdrd = igetunitnumber('exec     ')
 open(unit=iszkdrd,file='sz_kdrd.out',status='unknown')
 write(iszkdrd, '(a)') 'File: sz_kdrd.out'
 write(iszkdrd, '(a)')
&      'Input and calculated values used to ' //
&      'calculate KDs & RDs for saturated zone'
 write(iszkdrd,*) ' '
 write(iszkdrd, '(a)')
&      'SZFT:  kds/rds (Am, Np, Pu, Th, and ' //
&      'U are calculated)'
 write(iszkdrd, '(a)') '     Layer:  1=tuff, 2=alluvium'
 write(iszkdrd, '(a)') '     Media:  1=matrix, 2=fracture'
 write(iszkdrd, '(a)') '     for tuff layer, porosity is ' //
&      'ImmobilePorosity_STFF and surface area is ' //
&      'surface area = 3*porosity/(density*poreradius)'
 write(iszkdrd, '(a)') '     for alluvium layer, porosity ' //
&      'is AlluviumTotalPorosity_SAV and surface area is ' //
&      'AlluviumMatrixSpecificSurfaceArea_SAV'
 do i=1,330
    header1(i:i) = ' '
 end do
 header1(181:184) = 'kds:'
 header1(256:259) = 'rds:'
 write(iszkdrd, '(a330)') header1
 write(iszkdrd, *) ' '
 close(iszkdrd)

 iuzkdrd = igetunitnumber('exec     ')
 open(unit=iuzkdrd,file='uz_kdrd.out',status='unknown')
 write(iuzkdrd, '(a)') 'File: uz_kdrd.out'
 write(iuzkdrd, '(a)')
&      'Input and calculated values used to ' //
&      'calculate KDs & RDs for unsaturated zone'
 write(iuzkdrd,*) ' '
 write(iuzkdrd, '(a)')
&      'UZFT:  kds/rds (Am, Np, Pu, Th, and ' //
&      'U are calculated)'
 write(iuzkdrd, '(a)') '     Layer:  1=TSw, 2=CHnv ' //
&      '3=CHnz, 4=PPw, 5=UCF, 6=BFw, 7=UFZ'
 write(iuzkdrd, '(a,50x,a)') '     Media:  1=matrix, 2=fracture'
 do i=1,330
    header1(i:i) = ' '
 end do
 header1(181:184) = 'kds:'
 header1(256:259) = 'rds:'
 write(iuzkdrd, '(a330)') header1
 write(iuzkdrd, *) ' '
 close(iuzkdrd)

 iszrevers = igetunitnumber('exec     ')
 open(unit=iszrevers,file='sz_revers.out',status='unknown')
 write(iszrevers, '(a)') 'File: sz_revers.out'
 write(iszrevers, '(a)')
&      'Input and calculated values used to ' //
&      'calculate KDs & RDs accounting for ' //
&      'reversibles for saturated zone'
 do i=1,645
    header2 = ' '
 end do
 header2(1:16)     = 'SZFT Reversibles'
```

```
      header2(46:48)    = 'rd:'
      header2(346:349) = 'rdi:'
      write(iszrevers,*) ' '
      write(iszrevers, '(a645)') header2
      write(iszrevers,*) ' '
      close(iszrevers)

      iuzrevers = igetunitnumber('exec     ')
      open(unit=iuzrevers,file='uz_revers.out',status='unknown')
      write(iuzrevers, '(a)') 'File: uz_revers.out'
      write(iuzrevers, '(a)')
     &      'Input and calculated values used to ' //
     &      'calculate KDs & RDs accounting for ' //
     &      'reversibles for unsaturated zone'
      write(iuzrevers,*) ' '
      write(iuzrevers, '(a)') 'UZFT Reversibles' //
     &      ' (from nefrd(elem,leg) - only legs selected for NEFTRAN)'
      write(iuzrevers,*) ' '
      close(iuzrevers)

      return
      end
```

3) *Tpa.inp* was updated with the most recent values for colloid concentrations and colloid retardation factors.

4) The parameter AlluviumMatrixPoreRadius_SAV[m] was commented out in *tpa.inp* and the code referencing it was commented out in *szft.f*.

5) The following changes were made in *ashremob.f*:

```
concentfactoeoli = iashplumerealindex /
```
was changed to
```
  concentfactoeoli = masshlweol(iashplumerealindex) /
```

```
portionflvh = partmassloadfluv(it) / hlwgmp3toth(it)
portioneolh = partmassloadeoli(it) / hlwgmp3toth(it)
```
was changed to
```
portionflvh = partmassloadfluv(it) / hlwgmp3toth(it) * wgtfactorfluvial
portioneolh = partmassloadeoli(it) / hlwgmp3toth(it) * wgtfactoreolian
```

ATTACHMENT B

remob_lut.dat

```
c_HLW_I,C_ash_I,m_HLW_f,m_ash_f,area_f,m_HLW_e,m_ash_e,area_e
g/m2,g/m2,g,g,m2,g,g,m2
1.87E-04,7.06E+00,3.19E+07,3.19E+16,5.80E+07,9.89E+05,3.73E+10,4.60E+07
1.66E-32,6.54E-26,1.32E+07,1.32E+16,1.56E+08,0.00E+00,0.00E+00,0.00E+00
2.17E-11,1.29E-04,1.56E+07,1.56E+16,1.95E+08,5.95E+04,3.51E+11,7.00E+07
8.08E-16,8.03E-10,2.81E+07,2.81E+16,2.34E+08,1.19E+05,1.18E+11,6.60E+07
6.93E-05,3.73E+02,7.61E+06,7.61E+15,9.10E+07,2.09E+06,1.13E+13,8.38E+08
4.43E-09,7.59E-03,2.24E+07,2.24E+16,1.09E+08,4.14E+04,7.05E+10,3.90E+07
4.20E-37,2.60E-31,4.59E+07,4.59E+16,1.57E+08,0.00E+00,0.00E+00,0.00E+00
5.07E-06,1.23E+01,1.41E+07,1.41E+16,2.01E+08,1.88E+06,4.56E+12,3.44E+08
6.46E-07,1.99E-02,5.56E+07,5.56E+16,7.50E+07,0.00E+00,0.00E+00,0.00E+00
4.54E-12,1.30E-05,6.44E+06,6.44E+15,2.43E+08,9.87E+05,2.81E+12,9.00E+07
4.12E-18,3.45E-12,3.31E+07,3.31E+16,2.03E+08,2.33E+05,1.94E+11,7.10E+07
2.27E-05,1.57E+00,4.14E+07,4.14E+16,5.90E+07,4.09E+06,2.83E+11,5.00E+07
9.34E-08,6.07E-02,1.39E+07,1.39E+16,6.30E+07,1.93E+06,1.25E+12,1.35E+08
1.84E-06,8.22E-01,5.16E+07,5.16E+16,3.08E+08,4.64E+05,2.07E+11,1.80E+08
8.29E-07,9.51E-01,5.74E+07,5.74E+16,2.15E+08,1.66E+07,1.90E+13,4.29E+08
1.49E-09,4.75E-04,4.66E+07,4.66E+16,2.04E+08,9.97E+05,3.16E+11,1.39E+08
5.08E-10,3.61E-04,1.19E+07,1.19E+16,2.59E+08,1.57E+06,1.11E+12,1.01E+08
5.20E-06,2.69E+01,9.02E+06,9.02E+15,3.08E+08,4.55E+05,2.36E+12,3.29E+08
1.10E-24,4.18E-19,8.52E+06,8.52E+15,7.80E+07,0.00E+00,0.00E+00,0.00E+00
3.03E-07,3.44E-01,2.53E+06,2.52E+15,1.40E+07,1.83E+07,2.08E+13,2.80E+08
2.89E-06,3.70E+00,7.54E+06,7.54E+15,7.10E+07,5.26E+06,6.72E+12,3.15E+08
8.51E-06,2.34E+00,2.23E+07,2.23E+16,2.50E+07,3.94E+07,1.08E+13,2.76E+08
2.04E-11,3.01E-05,6.24E+07,6.24E+16,2.49E+08,2.98E+04,4.37E+10,3.60E+07
1.18E-24,2.09E-18,9.27E+06,9.27E+15,1.66E+08,2.69E+02,4.73E+08,2.00E+06
1.05E-11,8.58E-06,1.65E+07,1.65E+16,1.51E+08,8.28E+03,6.74E+09,2.20E+07
5.36E-11,7.60E-06,4.78E+07,4.78E+16,1.47E+08,2.06E+07,2.92E+12,1.99E+08
3.42E-06,2.77E-01,1.69E+07,1.69E+16,1.11E+08,2.72E+06,2.19E+11,6.40E+07
1.23E-10,5.45E-04,1.50E+07,1.50E+16,1.28E+08,1.55E+06,6.81E+12,1.86E+08
2.55E-02,3.32E+04,5.44E+07,5.44E+16,8.10E+07,2.32E+07,3.01E+13,1.13E+09
3.74E-08,1.51E-02,3.03E+07,3.03E+16,7.40E+07,9.02E+05,3.63E+11,1.41E+08
5.83E-20,2.33E-14,2.98E+06,2.98E+15,3.00E+07,2.83E+06,1.13E+12,8.90E+07
4.76E-12,2.16E-05,8.44E+06,8.44E+15,5.60E+07,7.93E+05,3.60E+12,2.69E+08
4.07E-08,4.57E-03,2.29E+07,2.29E+16,9.30E+07,1.57E+06,1.76E+11,1.77E+08
7.20E-09,9.55E-03,1.06E+07,1.06E+16,2.41E+08,2.41E+04,3.19E+10,5.20E+07
1.40E-10,3.10E-05,3.55E+07,3.55E+16,2.03E+08,5.39E+05,1.19E+11,1.28E+08
1.83E-14,1.17E-07,2.10E+06,2.10E+15,1.10E+07,1.00E+07,6.39E+13,2.29E+08
9.48E-04,5.03E+01,6.43E+07,6.43E+16,1.25E+08,8.51E+06,4.52E+11,1.64E+08
1.52E-09,1.46E-04,1.75E+07,1.75E+16,7.90E+07,7.48E+06,7.13E+11,1.23E+08
1.04E-05,2.37E+00,1.76E+07,1.76E+16,8.20E+07,3.77E+06,8.64E+11,1.56E+08
5.43E-07,9.18E-02,1.81E+07,1.81E+16,5.90E+07,4.60E+06,7.76E+11,1.44E+08
1.92E-08,3.73E-03,3.04E+07,3.04E+16,1.64E+08,8.65E+04,1.68E+10,9.00E+06
1.10E-15,1.26E-09,1.85E+07,1.85E+16,2.20E+08,3.25E+06,3.71E+12,2.16E+08
1.73E-16,2.09E-10,1.34E+07,1.34E+16,2.36E+08,4.01E+05,4.82E+11,1.11E+08
8.38E-05,2.36E+01,7.41E+06,7.41E+15,5.40E+07,4.70E+06,1.32E+12,2.57E+08
2.30E-03,1.20E+03,6.43E+06,6.43E+15,1.36E+08,1.56E+06,8.11E+11,2.26E+08
1.42E-05,7.51E+00,8.19E+06,8.19E+15,9.40E+07,4.31E+06,2.28E+12,1.98E+08
2.50E-03,7.30E+03,2.34E+07,2.34E+16,2.40E+08,1.45E+06,4.23E+12,4.27E+08
8.23E-10,2.09E-05,6.09E+07,6.09E+16,1.42E+08,1.23E+06,3.11E+10,6.70E+07
6.52E-09,4.01E-03,1.65E+07,1.65E+16,3.06E+08,1.02E+06,6.26E+11,2.48E+08
1.44E-07,1.36E-02,1.70E+07,1.70E+16,8.70E+07,1.47E+05,1.39E+10,3.90E+07
3.05E-19,1.18E-13,3.03E+07,3.03E+16,2.17E+08,1.28E+06,4.90E+11,4.10E+07
3.76E-06,1.82E+00,1.46E+07,1.46E+16,9.70E+07,7.34E+06,3.56E+12,2.40E+08
3.78E-19,6.95E-13,1.09E+07,1.09E+16,8.00E+06,1.29E+07,2.35E+13,1.20E+08
6.81E-23,4.58E-17,6.50E+07,6.50E+16,1.46E+08,0.00E+00,0.00E+00,0.00E+00
2.43E-08,6.83E-02,1.56E+07,1.56E+16,3.09E+08,1.48E+06,4.16E+12,2.69E+08
3.72E-09,4.51E-03,1.20E+07,1.20E+16,2.32E+08,9.31E+05,1.13E+12,2.29E+08
1.28E-20,2.91E-16,5.87E+07,5.87E+16,6.20E+07,0.00E+00,0.00E+00,0.00E+00
7.82E-07,7.10E-01,5.92E+07,5.92E+16,9.40E+07,1.07E+07,9.69E+12,3.89E+08
1.11E-19,1.35E-14,3.92E+07,3.92E+16,1.66E+08,6.29E+06,7.63E+11,1.01E+08
1.13E-03,2.40E+03,2.66E+07,2.66E+16,8.40E+07,5.14E+06,1.09E+13,5.46E+08
6.70E-11,1.78E-05,5.20E+07,5.20E+16,5.40E+07,2.48E+06,6.53E+11,8.70E+07
7.09E-63,2.85E-58,6.60E+07,6.60E+16,1.19E+08,5.00E+03,2.00E+08,1.00E+06
2.32E-27,1.69E-22,1.81E+07,1.81E+16,1.86E+08,6.13E+05,4.45E+10,1.80E+07
3.99E-06,5.27E+00,5.99E+07,5.99E+16,2.44E+08,2.57E+05,3.39E+11,1.27E+08
```

4.58E-05,3.89E+02,7.22E+06,7.22E+15,1.03E+08,3.87E+06,3.28E+13,6.26E+08
4.26E-54,2.05E-48,4.10E+07,4.10E+16,1.70E+08,7.43E+02,3.56E+08,1.00E+06
2.36E-05,2.79E+01,2.10E+07,2.10E+16,2.39E+08,1.60E+07,1.90E+13,5.15E+08
6.18E-07,1.52E+00,7.75E+06,7.75E+15,7.80E+07,3.22E+06,7.91E+12,4.45E+08
1.95E-26,8.66E-21,9.16E+06,9.16E+15,8.20E+07,0.00E+00,0.00E+00,0.00E+00
4.37E-10,6.93E-05,9.24E+06,9.24E+15,1.02E+08,4.56E+04,7.22E+09,2.50E+07
9.14E-09,5.34E-03,6.07E+07,6.07E+16,2.17E+08,4.40E+05,2.57E+11,1.32E+08
1.43E-05,9.38E+00,2.87E+07,2.87E+16,1.51E+08,2.58E+06,1.69E+12,2.32E+08
6.08E-35,7.65E-30,2.99E+07,2.99E+16,1.79E+08,0.00E+00,0.00E+00,0.00E+00
2.69E-06,2.08E+01,6.79E+06,6.79E+15,2.50E+08,5.85E+06,4.51E+13,5.48E+08
1.22E-03,7.88E+02,4.52E+07,4.52E+16,6.90E+07,6.18E+06,4.01E+12,3.21E+08
3.84E-06,1.50E+01,6.43E+06,6.43E+15,2.26E+08,3.11E+06,1.22E+13,4.85E+08
1.11E-09,2.10E-03,3.14E+07,3.14E+16,2.75E+08,6.81E+06,1.29E+13,1.46E+08
1.56E-05,1.92E+00,1.26E+07,1.26E+16,8.80E+07,2.51E+06,3.08E+11,1.31E+08
2.82E-10,4.94E-05,1.19E+07,1.19E+16,5.20E+07,3.11E+06,5.45E+11,1.93E+08
1.51E-04,4.09E+00,3.83E+07,3.83E+16,1.10E+08,9.82E+06,2.67E+11,2.71E+08
9.22E-09,3.56E-03,2.14E+07,2.14E+16,1.61E+08,9.27E+05,3.56E+11,1.44E+08
2.34E-05,1.87E+01,5.24E+07,5.24E+16,3.08E+08,3.87E+06,3.09E+12,4.50E+08
5.79E-10,3.91E-04,4.18E+07,4.18E+16,1.21E+08,7.78E+03,5.23E+09,2.10E+07
1.32E-03,9.48E+01,1.25E+07,1.25E+16,7.10E+07,5.22E+06,3.76E+11,2.18E+08
1.28E-21,1.43E-16,2.03E+07,2.03E+16,2.17E+08,3.43E+05,3.83E+10,5.80E+07
8.06E-04,3.02E+03,6.09E+06,6.09E+15,8.20E+07,3.73E+06,1.40E+13,1.01E+09
3.06E-27,2.40E-21,3.14E+07,3.14E+16,1.82E+08,0.00E+00,0.00E+00,0.00E+00
4.28E-22,2.08E-15,6.65E+06,6.65E+15,1.10E+08,2.27E+06,1.09E+13,1.03E+08
9.62E-39,5.53E-32,1.60E+07,1.60E+16,1.26E+08,0.00E+00,0.00E+00,0.00E+00
9.84E-08,1.34E-02,1.24E+07,1.24E+16,5.50E+07,3.14E+05,4.24E+10,1.50E+07
7.04E-06,1.81E+00,1.96E+07,1.96E+16,2.64E+08,4.37E+05,1.12E+11,1.53E+08
9.82E-07,6.37E-02,1.75E+07,1.75E+16,8.90E+07,9.91E+05,6.40E+10,4.20E+07
4.21E-08,1.62E-01,2.36E+07,2.36E+16,1.57E+08,1.67E+06,6.38E+12,3.86E+08
9.81E-11,1.89E-04,2.65E+06,2.65E+15,1.60E+07,6.71E+06,1.28E+13,1.66E+08
1.74E-04,3.65E+02,3.42E+07,3.42E+16,7.70E+07,1.06E+06,2.22E+12,2.53E+08
2.06E-03,3.47E+02,2.59E+07,2.59E+16,7.70E+07,1.43E+07,2.42E+12,5.39E+08
5.15E-09,6.81E-02,5.90E+06,5.90E+15,1.90E+07,1.83E+06,2.41E+13,1.85E+08
1.62E-14,5.80E-09,9.81E+06,9.81E+15,1.02E+08,8.78E+03,3.13E+09,1.60E+07
1.02E-04,1.33E+02,6.47E+07,6.47E+16,1.12E+08,9.90E+06,1.30E+13,6.25E+08
5.42E-19,1.04E-13,2.20E+07,2.20E+16,7.60E+07,7.79E+02,1.49E+08,1.00E+06
3.24E-08,1.23E-03,2.90E+07,2.90E+16,5.30E+07,3.15E+06,1.19E+11,5.30E+07
1.30E-35,5.10E-29,1.10E+07,1.10E+16,1.13E+08,2.58E+06,1.01E+13,7.80E+07
6.05E-09,3.59E-02,1.51E+07,1.51E+16,2.12E+08,6.72E+03,3.96E+10,3.60E+07
2.22E-05,2.20E+01,2.78E+07,2.78E+16,1.08E+08,1.92E+05,1.90E+11,1.35E+08
1.04E-05,5.59E+01,7.36E+06,7.36E+15,1.07E+08,2.29E+06,1.23E+13,5.66E+08
8.69E-42,1.49E-35,2.20E+07,2.20E+16,1.64E+08,1.61E+05,2.75E+11,8.50E+07
1.27E-12,7.86E-07,4.83E+07,4.83E+16,3.10E+07,7.90E+05,4.85E+11,5.80E+07
2.07E-07,5.03E-01,1.51E+07,1.51E+16,1.20E+08,1.03E+06,2.50E+12,4.07E+08
7.47E-30,2.30E-25,5.78E+07,5.78E+16,8.20E+07,0.00E+00,0.00E+00,0.00E+00
1.39E-19,3.97E-13,7.25E+06,7.25E+15,1.83E+08,2.43E+04,6.89E+10,1.20E+07
6.43E-11,5.39E-05,1.41E+07,1.41E+16,1.10E+07,1.94E+07,1.61E+13,1.61E+08
1.23E-07,8.50E-03,3.90E+07,3.90E+16,2.30E+07,6.11E+06,4.22E+11,6.80E+07
5.75E-07,3.74E-01,1.36E+07,1.36E+16,1.69E+08,2.16E+06,1.40E+12,1.41E+08
1.54E-05,6.90E+00,4.90E+07,4.90E+16,1.96E+08,3.77E+06,1.68E+12,5.06E+08
1.48E-07,1.70E-01,6.55E+07,6.55E+16,2.95E+08,9.06E+06,1.04E+13,3.21E+08
7.84E-08,2.49E-02,2.52E+07,2.52E+16,1.83E+08,1.97E+07,6.23E+12,1.07E+08
2.02E-10,1.43E-04,1.09E+07,1.09E+16,2.60E+08,2.54E+06,1.80E+12,1.53E+08
3.25E-07,1.69E+00,7.80E+06,7.80E+15,2.77E+08,1.71E+06,8.85E+12,3.32E+08
1.95E-19,7.41E-14,8.01E+06,8.01E+15,1.14E+08,1.10E+04,4.14E+09,1.20E+07
5.83E-25,6.66E-19,1.87E+07,1.87E+16,2.13E+08,2.35E+04,2.67E+10,2.40E+07
5.97E-06,7.65E+00,6.57E+06,6.57E+15,9.40E+07,6.20E+06,7.93E+12,2.91E+08
1.22E-07,3.37E-02,5.94E+07,5.94E+16,2.96E+08,2.04E+06,5.61E+11,1.76E+08
1.38E-05,2.03E+01,6.25E+07,6.24E+16,1.84E+08,5.01E+05,7.36E+11,3.03E+08
2.05E-09,3.62E-03,9.33E+06,9.33E+15,2.70E+08,1.20E+06,2.11E+12,2.69E+08
8.85E-08,7.24E-02,1.60E+07,1.60E+16,7.20E+07,2.78E+05,2.27E+11,1.18E+08
3.51E-14,5.00E-09,7.38E+07,7.37E+16,2.32E+08,8.45E+04,1.20E+10,2.70E+07
1.10E-04,8.87E+00,1.85E+07,1.85E+16,1.23E+08,1.11E+06,8.93E+10,1.61E+08
6.73E-10,2.96E-03,1.58E+07,1.58E+16,9.30E+07,7.73E+05,3.39E+12,3.39E+08
2.44E-11,3.20E-05,7.42E+07,7.42E+16,2.61E+08,1.13E+06,1.47E+12,1.08E+08
1.48E-07,5.99E-02,3.08E+07,3.08E+16,1.42E+08,9.20E+05,3.70E+11,6.00E+07
3.19E-09,1.28E-03,9.61E+06,9.61E+15,1.96E+08,2.04E+05,8.13E+10,1.20E+08
3.85E-17,1.76E-10,9.21E+06,9.21E+15,2.27E+08,2.46E+02,1.12E+09,6.00E+06
2.21E-05,2.47E+00,1.77E+07,1.77E+16,7.80E+07,6.63E+06,7.43E+11,3.27E+08
7.53E-10,1.00E-03,1.06E+07,1.06E+16,1.11E+08,1.67E+05,2.20E+11,1.65E+08
8.10E-06,1.78E+00,1.34E+07,1.34E+16,2.20E+07,2.27E+07,5.00E+12,3.49E+08
5.72E-19,3.67E-12,1.18E+07,1.18E+16,1.93E+08,1.55E+03,9.91E+09,3.10E+07
5.92E-07,3.16E-02,7.22E+07,7.22E+16,1.26E+08,8.98E+05,4.77E+10,8.70E+07
1.23E-06,1.18E-01,2.48E+07,2.48E+16,1.58E+08,6.72E+04,6.40E+09,2.50E+07
1.76E-15,4.06E-10,1.82E+07,1.82E+16,2.19E+08,2.07E+05,4.73E+10,1.20E+07

5.40E-08,9.14E-03,1.55E+07,1.54E+16,1.59E+08,7.23E+06,1.22E+12,1.76E+08
3.88E-50,7.57E-45,2.94E+07,2.94E+16,1.78E+08,3.20E+03,6.20E+08,1.00E+06
1.03E-03,1.18E+03,1.82E+07,1.82E+16,2.65E+08,4.13E+06,4.72E+12,5.17E+08
4.06E-04,4.89E+02,1.30E+07,1.30E+16,1.36E+08,1.23E+06,1.47E+12,3.10E+08
2.08E-11,5.89E-06,1.16E+07,1.16E+16,2.21E+08,6.65E+04,1.87E+10,3.50E+07
2.39E-04,1.25E+02,8.56E+06,8.56E+15,1.62E+08,1.19E+06,6.19E+11,3.48E+08
5.89E-46,3.13E-40,1.24E+07,1.24E+16,1.71E+08,1.53E+04,8.08E+09,6.00E+06
1.12E-14,3.28E-08,2.45E+07,2.45E+16,2.51E+08,1.28E+06,3.72E+12,2.03E+08
5.87E-06,1.49E-01,5.55E+07,5.55E+16,7.00E+07,8.87E+06,2.24E+11,9.80E+07
8.94E-25,5.52E-19,7.74E+06,7.74E+15,1.86E+08,5.56E+06,3.41E+12,8.50E+07
1.47E-05,1.38E+00,4.39E+06,4.39E+15,2.40E+07,1.26E+07,1.19E+12,1.96E+08
1.59E-06,6.11E-01,2.89E+07,2.89E+16,1.49E+08,5.04E+06,1.93E+12,2.87E+08
3.88E-48,1.89E-42,1.35E+07,1.35E+16,1.27E+08,0.00E+00,0.00E+00,0.00E+00
5.69E-34,1.05E-27,2.38E+07,2.38E+16,6.50E+07,3.95E+05,7.22E+11,1.80E+07
1.20E-13,8.04E-08,5.64E+07,5.64E+16,5.10E+07,9.78E+06,6.54E+12,2.84E+08
1.01E-07,2.85E-01,1.35E+07,1.35E+16,2.67E+08,2.43E+06,6.82E+12,2.38E+08
4.93E-10,5.99E-04,1.16E+07,1.16E+16,2.69E+08,1.12E+05,1.36E+11,9.10E+07
1.17E-29,2.66E-25,5.79E+07,5.79E+16,1.07E+08,0.00E+00,0.00E+00,0.00E+00
1.41E-08,1.29E-02,6.97E+07,6.97E+16,2.28E+08,5.62E+05,5.10E+11,1.90E+08
3.74E-16,4.56E-11,4.34E+07,4.34E+16,1.75E+08,2.43E+06,2.95E+11,8.60E+07
4.91E-23,1.05E-16,2.67E+07,2.67E+16,1.29E+08,3.70E+06,7.87E+12,4.50E+07
3.25E-12,8.61E-07,5.43E+07,5.42E+16,1.18E+08,1.16E+06,3.05E+11,1.87E+08
9.20E-17,3.70E-12,6.19E+07,6.19E+16,6.60E+07,0.00E+00,0.00E+00,0.00E+00
1.36E-20,9.88E-16,2.03E+07,2.03E+16,1.89E+08,1.52E+04,1.10E+09,4.00E+06
8.86E-05,1.17E+02,5.82E+07,5.82E+16,2.19E+08,1.50E+06,1.98E+12,1.75E+08
7.81E-04,6.63E+03,9.89E+06,9.89E+15,3.48E+08,1.34E+06,1.14E+13,8.00E+08
2.74E-04,1.32E+02,4.77E+07,4.77E+16,1.06E+08,1.82E+06,8.73E+11,2.71E+08
3.80E-21,4.52E-15,3.47E+07,3.47E+16,2.06E+08,2.99E+04,3.54E+10,2.20E+07
8.83E-18,2.18E-11,9.46E+06,9.46E+15,2.38E+08,1.30E+06,3.20E+12,1.62E+08
5.29E-11,2.35E-05,9.66E+06,9.66E+15,1.04E+08,0.00E+00,0.00E+00,0.00E+00
4.44E-07,7.02E-02,7.12E+06,7.12E+15,6.10E+07,2.05E+06,3.24E+11,1.14E+08
2.46E-14,1.44E-08,6.18E+07,6.18E+16,2.24E+08,3.59E+04,2.09E+10,3.80E+07
1.32E-05,8.65E+00,2.58E+07,2.58E+16,1.31E+08,6.08E+06,3.99E+12,2.77E+08
2.50E-41,3.15E-36,2.63E+07,2.63E+16,1.34E+08,0.00E+00,0.00E+00,0.00E+00
8.39E-05,6.47E+02,1.18E+07,1.18E+16,2.86E+08,9.90E+05,7.63E+12,8.41E+08
3.54E-12,2.31E-06,5.00E+07,5.00E+16,2.01E+08,1.22E+04,7.90E+09,1.90E+07
1.72E-19,6.75E-13,7.51E+06,7.51E+15,2.23E+08,1.34E+06,5.23E+12,1.11E+08
2.50E-05,4.73E+01,3.66E+07,3.66E+16,3.26E+08,6.07E+06,1.15E+13,5.65E+08
3.04E-05,3.73E+00,1.47E+07,1.47E+16,2.02E+08,4.33E+05,5.32E+10,8.30E+07
6.14E-09,1.08E-03,1.47E+07,1.47E+16,2.51E+08,2.74E+05,4.81E+10,9.20E+07
2.45E-05,6.66E-01,3.37E+07,3.37E+16,1.32E+08,1.15E+07,3.13E+11,1.69E+08
1.26E-06,4.85E-01,1.51E+07,1.51E+16,2.04E+08,5.98E+06,2.30E+12,2.59E+08
1.16E-05,9.31E+00,4.91E+07,4.91E+16,2.86E+08,2.29E+05,1.83E+11,1.94E+08
1.26E-07,8.53E-02,3.83E+07,3.83E+16,1.15E+08,4.80E+05,3.22E+11,7.20E+07
4.17E-05,3.00E+00,1.67E+07,1.67E+16,1.39E+08,8.19E+05,5.90E+10,7.50E+07
5.01E-08,5.60E-03,1.63E+07,1.63E+16,1.59E+08,4.46E+06,4.98E+11,1.58E+08
4.37E-03,1.64E+04,4.56E+06,4.56E+15,6.30E+07,5.18E+06,1.94E+13,8.51E+08
4.75E-15,3.73E-09,2.70E+07,2.70E+16,2.01E+08,4.07E+06,3.18E+12,1.05E+08
3.54E-22,1.72E-15,8.85E+06,8.85E+15,1.65E+08,0.00E+00,0.00E+00,0.00E+00
1.75E-04,1.00E+03,1.91E+07,1.91E+16,1.74E+08,1.21E+06,6.91E+12,6.32E+08
5.31E-04,7.17E+01,1.22E+07,1.22E+16,3.10E+07,1.50E+06,2.03E+11,7.40E+07
9.12E-09,2.35E-03,2.00E+07,2.00E+16,1.99E+08,6.47E+05,1.66E+11,1.55E+08
3.16E-12,2.06E-07,1.52E+07,1.52E+16,8.70E+07,2.97E+06,1.92E+11,5.60E+07
2.20E-05,8.43E+01,1.76E+07,1.76E+16,1.35E+08,6.56E+06,2.51E+13,3.78E+08
5.80E-06,1.11E+01,8.92E+06,8.92E+15,2.57E+08,5.72E+05,1.10E+12,3.12E+08
1.03E-13,2.17E-07,3.34E+07,3.34E+16,4.40E+07,1.51E+06,3.18E+12,9.50E+07
1.79E-26,3.04E-21,2.38E+07,2.38E+16,1.17E+08,1.26E+07,2.14E+12,1.22E+08
5.03E-08,6.63E-01,9.40E+06,9.40E+15,1.27E+08,1.83E+04,2.40E+11,1.41E+08
3.80E-05,1.35E+01,7.15E+06,7.15E+15,3.50E+07,3.11E+06,1.11E+12,1.38E+08
2.13E-13,2.81E-07,6.99E+07,6.99E+16,2.67E+08,3.70E+06,4.86E+12,1.70E+08
2.94E-10,5.63E-05,2.55E+07,2.55E+16,5.80E+07,9.84E+02,1.88E+08,1.00E+06
1.58E-30,5.99E-26,3.19E+07,3.19E+16,1.35E+08,0.00E+00,0.00E+00,0.00E+00
4.92E-08,1.93E-01,1.61E+07,1.61E+16,2.94E+08,1.04E+06,4.07E+12,3.39E+08
1.66E-09,9.77E-03,7.10E+06,7.10E+15,1.20E+07,8.41E+06,4.96E+13,3.61E+08
1.17E-04,1.16E+02,2.75E+07,2.75E+16,1.00E+08,8.00E+05,7.90E+11,2.30E+08
2.43E-25,1.32E-18,8.42E+06,8.42E+15,2.21E+08,3.34E+04,1.80E+11,3.40E+07
2.47E-104,4.24E-98,2.13E+07,2.13E+16,1.26E+08,0.00E+00,0.00E+00,0.00E+00
1.43E-09,8.85E-04,3.94E+07,3.94E+16,9.70E+07,7.36E+04,4.52E+10,3.60E+07
1.05E-05,2.54E+01,1.26E+07,1.26E+16,8.30E+07,3.58E+06,8.67E+12,2.85E+08
2.85E-15,8.72E-11,1.67E+07,1.67E+16,8.00E+06,4.33E+07,1.32E+12,1.32E+08
6.75E-27,1.93E-20,6.41E+06,6.41E+15,1.94E+08,6.81E+04,1.94E+11,9.00E+06
5.99E-07,5.01E-01,3.36E+07,3.36E+16,7.90E+07,4.50E+05,3.75E+11,1.69E+08
3.21E-07,2.23E-02,4.54E+07,4.54E+16,1.00E+08,5.19E+04,3.59E+09,9.00E+06
2.68E-09,1.74E-03,1.17E+07,1.17E+16,1.84E+08,3.86E+06,2.50E+12,1.44E+08
4.19E-04,1.87E+02,4.96E+07,4.96E+16,2.83E+08,2.62E+06,1.17E+12,3.96E+08

1.42E-08,1.63E-02,6.95E+07,6.95E+16,2.86E+08,4.61E+06,5.28E+12,2.16E+08
3.55E-06,1.13E+00,4.69E+07,4.69E+16,2.82E+08,7.57E+05,2.40E+11,1.69E+08
8.40E-24,5.98E-18,7.19E+06,7.19E+15,2.01E+08,3.96E+06,2.80E+12,8.20E+07
1.52E-03,7.85E+03,7.02E+06,7.02E+15,8.10E+07,2.49E+06,1.29E+13,8.06E+08
1.42E-19,5.42E-14,5.93E+06,5.93E+15,4.80E+07,2.53E+06,9.56E+11,7.40E+07
5.44E-04,6.18E+02,1.89E+07,1.89E+16,3.02E+08,2.02E+06,2.30E+12,2.94E+08
2.13E-06,2.72E+00,1.04E+07,1.04E+16,2.30E+08,2.34E+06,2.99E+12,2.81E+08
6.48E-06,1.79E+00,4.29E+07,4.29E+16,1.09E+08,1.86E+07,5.12E+12,2.60E+08
2.80E-04,4.11E+02,4.20E+07,4.20E+16,9.10E+07,2.10E+07,3.08E+13,7.72E+08
4.26E-06,7.51E+00,1.02E+07,1.02E+16,3.17E+08,3.63E+05,6.39E+11,3.44E+08
4.99E-12,4.09E-06,1.59E+07,1.58E+16,8.20E+07,8.37E+05,6.81E+11,6.30E+07
4.11E-07,5.84E-02,5.57E+07,5.57E+16,1.55E+08,2.05E+07,2.90E+12,2.14E+08
1.12E-12,9.10E-08,1.84E+07,1.84E+16,1.57E+08,3.00E+05,2.43E+10,1.90E+07
4.87E-06,2.14E+01,1.44E+07,1.44E+16,1.23E+08,1.86E+06,8.17E+12,2.73E+08
1.93E-07,2.52E-01,6.85E+07,6.85E+16,1.84E+08,7.77E+06,1.01E+13,3.04E+08
1.68E-50,6.81E-45,3.12E+07,3.12E+16,1.48E+08,0.00E+00,0.00E+00,0.00E+00
1.25E-06,4.97E-01,9.39E+06,9.39E+15,1.43E+08,4.37E+05,1.74E+11,1.34E+08
1.15E-07,5.23E-01,8.93E+06,8.93E+15,2.15E+08,2.82E+05,1.28E+12,1.42E+08
2.26E-07,2.54E-02,1.58E+07,1.58E+16,1.07E+08,6.29E+06,7.05E+11,1.90E+08
1.18E-06,1.56E+00,1.04E+07,1.04E+16,1.06E+08,3.63E+05,4.80E+11,1.15E+08
6.61E-03,1.46E+03,2.70E+07,2.70E+16,6.90E+07,9.20E+06,2.02E+12,3.61E+08
2.60E-08,1.67E-01,1.18E+07,1.18E+16,1.82E+08,4.57E+03,2.92E+10,3.00E+07
1.57E-09,8.33E-05,2.77E+06,2.77E+15,9.00E+06,6.93E+07,3.68E+12,2.67E+08
1.00E-04,9.55E+00,2.43E+07,2.43E+16,1.62E+08,7.53E+05,7.17E+10,8.90E+07
1.65E-06,3.79E-01,1.45E+07,1.45E+16,1.76E+08,6.70E+06,1.53E+12,1.83E+08
2.38E-18,4.04E-13,2.23E+07,2.23E+16,2.08E+08,1.15E+05,1.93E+10,2.90E+07
1.01E-07,1.96E-02,3.09E+07,3.09E+16,1.73E+08,4.69E+05,9.09E+10,1.36E+08
3.95E-06,4.52E+00,2.03E+07,2.03E+16,2.23E+08,1.84E+06,2.10E+12,3.76E+08
4.08E-28,4.94E-22,1.14E+07,1.14E+16,1.49E+08,8.97E+05,1.08E+12,5.10E+07
6.02E-05,1.70E+01,7.59E+06,7.59E+15,7.70E+07,4.05E+06,1.14E+12,4.15E+08
2.50E-08,1.31E-02,8.96E+06,8.95E+15,1.77E+08,7.85E+05,4.10E+11,2.27E+08
6.65E-07,3.53E-01,1.25E+07,1.25E+16,1.17E+08,1.64E+05,8.67E+10,1.07E+08
1.63E-04,4.76E+02,2.66E+07,2.66E+16,1.53E+08,1.35E+06,3.92E+12,4.70E+08
2.79E-14,7.09E-10,3.74E+07,3.74E+16,8.70E+07,1.98E+07,5.00E+11,1.59E+08
1.89E-03,1.16E+03,9.78E+06,9.78E+15,7.80E+07,8.23E+06,5.05E+12,6.07E+08
5.75E-04,5.40E+01,1.53E+07,1.53E+16,7.90E+07,1.73E+06,1.63E+11,1.39E+08
1.25E-12,4.82E-07,3.38E+07,3.38E+16,2.26E+08,4.07E+04,1.56E+10,3.10E+07
2.22E-13,1.08E-07,2.22E+07,2.22E+16,2.52E+08,6.92E+04,3.36E+10,6.20E+07
7.64E-07,1.41E+00,1.99E+07,1.99E+16,6.80E+07,1.53E+06,2.81E+12,1.31E+08
9.89E-15,6.65E-09,6.63E+07,6.63E+16,1.26E+08,1.05E+05,6.99E+10,2.60E+07
8.85E-11,2.49E-04,5.65E+06,5.65E+15,4.40E+07,3.70E+06,1.04E+13,1.62E+08
5.51E-04,6.66E+02,1.70E+06,1.70E+15,2.00E+07,1.13E+07,1.37E+13,7.21E+08
8.89E-06,2.01E-01,2.75E+07,2.75E+16,1.30E+07,3.29E+07,7.42E+11,1.12E+08
9.35E-05,8.49E+01,6.19E+07,6.19E+16,1.01E+08,8.09E+06,7.34E+12,4.60E+08
4.18E-05,5.07E+00,4.05E+07,4.05E+16,1.20E+08,7.09E+06,8.59E+11,4.54E+08
5.63E-11,1.20E-04,3.10E+07,3.10E+16,2.01E+08,5.67E+05,1.20E+12,3.28E+08
3.02E-38,8.02E-33,5.23E+07,5.23E+16,1.93E+08,8.67E+04,2.28E+10,6.00E+06
3.88E-24,1.56E-19,6.65E+07,6.65E+16,4.20E+07,1.19E+06,4.77E+10,1.20E+07
6.56E-11,4.78E-06,2.27E+07,2.27E+16,1.79E+08,1.41E+05,1.02E+10,1.90E+07
1.57E-07,2.07E-01,5.45E+07,5.45E+16,8.30E+07,6.59E+06,8.67E+12,2.08E+08
4.49E-16,3.83E-09,1.05E+07,1.05E+16,2.50E+08,4.83E+05,4.10E+12,1.32E+08
3.22E-07,1.55E-01,3.93E+07,3.93E+16,2.82E+08,9.72E+06,4.66E+12,2.37E+08
6.55E-07,7.74E-01,2.85E+07,2.85E+16,9.70E+07,8.23E+06,9.73E+12,4.14E+08
1.49E-08,3.67E-02,1.02E+07,1.02E+16,1.43E+08,8.10E+05,1.99E+12,2.39E+08
5.05E-10,2.24E-04,9.72E+06,9.72E+15,1.36E+08,1.72E+04,7.59E+09,1.30E+07
1.67E-05,2.64E+00,9.01E+06,9.01E+15,6.50E+07,1.41E+05,2.23E+10,5.50E+07
1.25E-11,7.33E-06,6.14E+07,6.14E+16,2.15E+08,1.51E+05,8.79E+10,7.30E+07
8.39E-08,5.52E-02,3.18E+07,3.17E+16,2.96E+08,3.14E+04,2.06E+10,6.50E+07
2.14E-09,2.70E-04,3.07E+07,3.07E+16,9.70E+07,4.82E+03,6.03E+08,4.00E+06
1.94E-06,1.50E+01,5.94E+06,5.94E+15,2.26E+08,6.82E+06,5.26E+13,4.85E+08
1.69E-06,1.10E+00,5.04E+07,5.04E+16,8.70E+07,6.65E+05,4.32E+11,1.78E+08
2.08E-08,8.15E-02,9.17E+06,9.17E+15,2.46E+08,3.69E+05,1.44E+12,2.58E+08
2.68E-04,5.05E+02,2.98E+07,2.98E+16,1.03E+08,1.25E+07,2.36E+13,8.12E+08
9.09E-09,1.12E-03,1.52E+07,1.52E+16,2.02E+08,3.62E+03,4.44E+08,3.00E+06
1.54E-06,2.70E-01,8.90E+06,8.90E+15,7.70E+07,6.10E+06,1.07E+12,1.64E+08
1.84E-13,5.03E-09,3.63E+07,3.63E+16,2.16E+08,8.15E+06,2.22E+11,1.14E+08
7.09E-07,2.74E-01,2.08E+07,2.08E+16,1.89E+08,8.89E+05,3.42E+11,7.60E+07
1.36E-06,1.09E+00,4.53E+07,4.53E+16,1.87E+08,1.05E+07,8.37E+12,3.68E+08
1.78E-09,1.21E-03,3.81E+07,3.81E+16,9.70E+07,5.73E+06,3.85E+12,1.02E+08
8.36E-05,6.02E+00,1.44E+07,1.44E+16,6.20E+07,3.38E+06,2.43E+11,2.08E+08
9.51E-13,1.07E-07,2.13E+07,2.13E+16,2.11E+08,2.63E+04,2.94E+09,1.40E+07
3.81E-10,1.44E-03,9.35E+06,9.35E+15,2.38E+08,7.93E+03,2.97E+10,3.00E+07
1.06E-11,8.32E-06,3.21E+07,3.21E+16,2.17E+08,1.05E+05,8.15E+10,1.09E+08
5.91E-08,2.85E-01,8.92E+06,8.92E+15,1.08E+08,9.36E+04,4.51E+11,2.20E+08
1.61E-07,9.22E-01,1.91E+07,1.91E+16,3.10E+08,1.96E+05,1.12E+12,3.11E+08

2.63E-07,3.58E-02,1.27E+07,1.27E+16,3.70E+07,1.10E+05,1.49E+10,2.10E+07
5.00E-43,1.29E-37,1.37E+07,1.37E+16,1.86E+08,1.36E+06,3.50E+11,4.10E+07
3.93E-22,2.55E-17,1.59E+07,1.59E+16,1.20E+08,0.00E+00,0.00E+00,0.00E+00
8.20E-09,3.15E-02,2.36E+07,2.36E+16,2.85E+08,1.61E+06,6.18E+12,3.51E+08
1.01E-05,1.93E+01,8.46E+06,8.46E+15,1.95E+08,8.77E+05,1.68E+12,2.82E+08
4.39E-10,9.26E-04,3.64E+07,3.64E+16,6.20E+07,3.21E+05,6.73E+11,6.10E+07
3.02E-09,5.12E-04,1.96E+07,1.96E+16,4.80E+07,1.78E+07,3.01E+12,1.60E+08
1.50E-08,1.99E-01,9.05E+06,9.05E+15,1.19E+08,4.48E+04,5.89E+11,1.21E+08
3.82E-11,1.37E-05,1.01E+07,1.01E+16,5.40E+07,1.94E+05,6.92E+10,3.60E+07
8.20E-17,1.08E-10,6.34E+07,6.34E+16,2.32E+08,8.02E+06,1.05E+13,1.09E+08
1.01E-32,1.94E-27,2.29E+07,2.29E+16,8.50E+07,0.00E+00,0.00E+00,0.00E+00
3.26E-17,1.24E-12,3.26E+07,3.26E+16,1.00E+08,0.00E+00,0.00E+00,0.00E+00
1.21E-03,4.74E+03,1.43E+07,1.43E+16,2.52E+08,2.89E+06,1.13E+13,7.58E+08
4.32E-36,2.56E-29,1.49E+07,1.49E+16,2.20E+08,3.32E+05,1.96E+12,1.43E+08
1.30E-06,1.29E+00,2.82E+07,2.82E+16,1.78E+08,1.50E+05,1.48E+11,1.11E+08
1.79E-11,9.71E-05,9.27E+06,9.27E+15,2.23E+08,1.40E+04,7.53E+10,8.00E+07
2.65E-06,4.54E+00,1.73E+07,1.73E+16,2.70E+07,2.78E+06,4.74E+12,1.30E+08
1.23E-13,7.59E-08,4.62E+07,4.62E+16,6.50E+07,3.00E+05,1.85E+11,3.60E+07
9.11E-15,2.22E-08,1.48E+07,1.48E+16,2.43E+08,1.18E+06,2.86E+12,1.84E+08
5.19E-46,1.60E-41,5.90E+07,5.90E+16,1.16E+08,0.00E+00,0.00E+00,0.00E+00
7.00E-25,2.00E-18,6.40E+06,6.40E+15,1.32E+08,0.00E+00,0.00E+00,0.00E+00
2.73E-53,2.29E-47,3.22E+07,3.22E+16,1.30E+08,1.08E+04,9.00E+09,4.00E+06
2.64E-49,1.83E-44,3.36E+07,3.36E+16,2.60E+07,2.99E+06,2.06E+11,1.10E+07
3.97E-07,2.58E-01,1.03E+07,1.03E+16,5.90E+07,5.19E+06,3.36E+12,1.68E+08
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1.64E-03,5.21E+02,3.64E+07,3.64E+16,1.05E+08,1.14E+07,3.61E+12,6.78E+08
3.58E-23,2.55E-17,1.02E+07,1.02E+16,1.66E+08,0.00E+00,0.00E+00,0.00E+00
2.24E-06,1.16E+01,4.51E+06,4.51E+15,1.23E+08,4.96E+06,2.57E+13,3.46E+08
1.37E-15,5.19E-10,7.88E+06,7.88E+15,3.80E+07,2.52E+05,9.51E+10,4.60E+07
5.38E-38,6.14E-32,1.62E+07,1.62E+16,1.18E+08,0.00E+00,0.00E+00,0.00E+00
4.43E-08,5.67E-02,9.76E+06,9.76E+15,1.47E+08,2.93E+06,3.74E+12,1.94E+08
5.94E-06,1.64E+00,6.11E+07,6.11E+16,1.62E+08,6.37E+05,1.75E+11,1.58E+08
2.95E-07,4.34E-01,4.76E+07,4.76E+16,2.32E+08,1.50E+07,2.21E+13,4.55E+08
7.42E-06,1.31E+01,9.93E+06,9.93E+15,2.13E+08,9.41E+05,1.66E+12,2.43E+08
9.43E-11,7.71E-05,1.65E+07,1.65E+16,5.10E+07,3.84E+05,3.13E+11,1.22E+08
1.66E-03,2.35E+02,4.50E+07,4.50E+16,9.00E+07,3.49E+07,4.95E+12,7.12E+08
3.31E-06,2.68E-01,8.92E+06,8.92E+15,6.90E+07,1.06E+07,8.54E+11,1.20E+08
4.69E-23,2.07E-16,1.58E+07,1.58E+16,1.68E+08,7.78E+05,3.42E+12,1.17E+08
2.74E-03,3.57E+03,4.70E+07,4.70E+16,9.70E+07,3.05E+07,3.97E+13,7.59E+08
2.04E-10,8.24E-05,2.47E+07,2.47E+16,4.30E+07,6.10E+06,2.46E+12,1.27E+08
3.11E-07,1.24E-01,9.25E+06,9.24E+15,1.76E+08,5.83E+05,2.32E+11,9.80E+07
5.10E-13,2.33E-06,8.67E+06,8.67E+15,1.70E+08,3.46E+05,1.57E+12,1.58E+08
1.02E-20,1.15E-15,6.98E+06,6.98E+15,2.10E+07,9.26E+06,1.04E+12,3.30E+07
8.82E-08,1.17E-01,6.06E+06,6.06E+15,1.90E+07,4.63E+06,6.12E+12,1.70E+08
1.46E-07,3.23E-02,3.62E+07,3.62E+16,1.56E+08,1.11E+05,2.45E+10,5.60E+07
3.66E-10,2.35E-03,1.25E+07,1.25E+16,1.48E+08,1.58E+03,1.01E+10,3.50E+07
2.04E-06,1.08E-01,7.16E+07,7.16E+16,1.91E+08,7.68E+05,4.08E+10,5.30E+07
4.97E-07,4.75E-02,2.37E+07,2.37E+16,1.41E+08,1.51E+04,1.44E+09,7.00E+06
1.02E-02,2.33E+03,1.37E+07,1.37E+16,7.30E+07,7.65E+06,1.75E+12,3.65E+08
1.41E-26,2.39E-21,2.04E+07,2.04E+16,1.34E+08,0.00E+00,0.00E+00,0.00E+00
3.10E-58,6.05E-53,2.92E+07,2.92E+16,9.90E+07,0.00E+00,0.00E+00,0.00E+00
2.49E-06,2.85E+00,1.89E+07,1.89E+16,2.52E+08,3.63E+06,4.15E+12,4.27E+08
2.38E-02,2.86E+04,2.80E+06,2.80E+15,4.20E+07,1.12E+07,1.35E+13,6.17E+08
7.52E-04,2.12E+02,5.98E+05,5.98E+14,1.30E+07,1.14E+07,3.20E+12,5.68E+08
1.42E-09,7.42E-04,8.76E+06,8.76E+15,2.09E+08,9.66E+05,5.04E+11,2.16E+08
4.71E-10,2.50E-04,1.28E+07,1.28E+16,1.23E+08,5.09E+03,2.69E+09,1.30E+07
4.44E-02,1.29E+05,1.20E+07,1.20E+16,5.70E+07,1.59E+07,4.62E+13,8.51E+08
3.83E-05,9.69E-01,6.36E+07,6.36E+16,2.02E+08,2.39E+05,6.04E+09,2.90E+07
5.99E-05,3.67E+01,1.54E+07,1.54E+16,2.95E+08,2.50E+06,1.53E+12,2.43E+08
4.51E-06,4.25E-01,1.66E+07,1.66E+16,1.67E+08,3.38E+05,3.18E+10,3.50E+07
2.75E-05,1.06E+01,3.29E+07,3.28E+16,1.85E+08,1.51E+06,5.80E+11,3.21E+08
1.88E-04,9.10E+01,1.78E+07,1.78E+16,8.10E+07,5.26E+06,2.55E+12,6.26E+08
1.83E-18,3.35E-12,2.30E+07,2.30E+16,4.50E+07,1.24E+06,2.26E+12,1.70E+08
7.49E-04,5.01E+02,5.90E+07,5.90E+16,1.65E+08,7.04E+06,4.70E+12,2.59E+08
9.67E-11,2.73E-04,1.63E+07,1.63E+16,2.66E+08,4.17E+05,1.17E+12,1.64E+08
5.93E-04,7.17E+02,9.98E+06,9.98E+15,2.86E+08,2.06E+06,2.50E+12,5.49E+08
1.63E-09,3.69E-05,5.97E+07,5.97E+16,1.29E+08,1.63E+05,3.68E+09,1.10E+07
1.63E-09,1.49E-03,6.06E+07,6.06E+16,1.03E+08,8.10E+06,7.35E+12,1.49E+08
9.60E-06,1.17E+00,3.93E+07,3.93E+16,2.01E+08,7.26E+06,8.80E+11,2.27E+08
1.84E-23,3.94E-17,3.13E+07,3.13E+16,2.06E+08,7.16E+02,1.52E+09,4.00E+06
2.30E-07,6.06E-02,5.52E+07,5.52E+16,2.18E+08,2.50E+05,6.59E+10,9.20E+07
9.67E-07,3.89E-02,6.55E+07,6.55E+16,5.60E+07,5.98E+05,2.39E+10,2.50E+07
3.70E-23,2.70E-18,1.95E+07,1.95E+16,1.77E+08,0.00E+00,0.00E+00,0.00E+00
2.36E-07,3.11E-01,4.97E+07,4.97E+16,7.40E+07,1.01E+07,1.33E+13,3.14E+08

1.62E-13,1.38E-06,1.05E+07,1.05E+16,2.48E+08,1.56E+05,1.33E+12,1.22E+08
6.74E-18,3.25E-12,4.82E+07,4.82E+16,1.95E+08,0.00E+00,0.00E+00,0.00E+00
7.07E-03,8.36E+03,1.38E+07,1.38E+16,7.70E+07,2.17E+07,2.56E+13,1.22E+09
1.10E-07,2.70E-01,9.35E+06,9.35E+15,1.62E+08,1.66E+06,4.06E+12,3.16E+08
4.52E-20,2.01E-14,9.47E+06,9.47E+15,1.54E+08,1.66E+05,7.33E+10,6.80E+07
1.23E-03,1.95E+02,7.23E+06,7.23E+15,4.10E+07,1.97E+06,3.12E+11,1.20E+08
1.80E-08,1.06E-02,5.16E+07,5.16E+16,1.93E+08,9.93E+06,5.79E+12,1.98E+08
1.46E-22,9.64E-17,3.00E+07,2.99E+16,1.77E+08,0.00E+00,0.00E+00,0.00E+00
1.72E-08,2.15E-03,6.20E+06,6.20E+15,9.00E+06,2.46E+07,3.07E+12,2.29E+08
6.51E-16,5.05E-09,6.99E+06,6.99E+15,1.67E+08,1.41E+06,1.09E+13,1.50E+08
2.97E-05,1.94E+01,4.95E+07,4.95E+16,1.44E+08,1.85E+06,1.20E+12,2.14E+08
8.07E-06,3.16E+01,8.25E+06,8.25E+15,1.80E+08,1.29E+06,5.03E+12,6.10E+08
1.79E-13,3.40E-07,3.96E+07,3.95E+16,2.50E+08,3.54E+05,6.67E+11,1.28E+08
2.93E-28,3.62E-23,8.01E+06,8.01E+15,8.80E+07,4.29E+06,5.27E+11,9.20E+07
2.23E-08,3.93E-03,1.17E+07,1.17E+16,1.41E+08,2.90E+06,5.08E+11,6.30E+07
3.46E-06,9.42E-02,4.39E+07,4.39E+16,1.76E+08,4.33E+06,1.18E+11,1.79E+08
4.11E-06,1.58E+00,1.88E+07,1.88E+16,1.07E+08,2.61E+06,1.01E+12,1.17E+08
2.81E-04,2.25E+02,5.40E+07,5.40E+16,3.38E+08,2.15E+06,1.72E+12,5.00E+08
1.35E-16,9.15E-11,3.88E+07,3.88E+16,1.45E+08,0.00E+00,0.00E+00,0.00E+00
1.97E-05,1.42E+00,1.75E+07,1.75E+16,1.03E+08,3.81E+05,2.74E+10,8.30E+07
1.28E-14,1.44E-09,2.00E+07,2.00E+16,1.62E+08,1.37E+06,1.53E+11,1.41E+08
6.03E-19,2.27E-12,8.55E+06,8.55E+15,2.16E+08,1.42E+04,5.32E+10,2.00E+07
2.00E-06,1.56E+00,3.11E+07,3.11E+16,1.95E+08,3.22E+05,2.51E+11,5.70E+07
1.10E-04,5.28E+02,8.45E+06,8.45E+15,7.80E+07,6.98E+05,3.37E+12,2.35E+08
6.31E-12,3.63E-05,1.82E+07,1.82E+16,2.51E+08,4.69E+05,2.68E+12,2.01E+08
2.03E-09,2.76E-04,1.06E+07,1.06E+16,4.70E+07,1.53E+06,2.06E+11,3.50E+07
6.70E-03,1.72E+03,8.35E+06,8.35E+15,7.00E+07,1.23E+07,3.17E+12,6.37E+08
9.34E-08,6.06E-03,1.35E+07,1.35E+16,8.10E+07,4.92E+06,3.18E+11,7.40E+07
9.51E-09,3.65E-02,2.38E+07,2.37E+16,2.60E+08,1.44E+06,5.50E+12,2.88E+08
4.01E-06,7.67E+00,5.82E+06,5.82E+15,2.15E+08,3.66E+06,7.01E+12,3.16E+08
2.44E-11,5.16E-05,3.55E+07,3.55E+16,1.01E+08,5.15E+04,1.08E+11,3.60E+07
5.95E-06,1.01E+00,3.23E+07,3.23E+16,1.07E+08,7.87E+06,1.33E+12,2.34E+08
5.52E-12,7.30E-05,7.85E+06,7.85E+15,1.66E+08,2.13E+05,2.79E+12,9.20E+07
2.38E-08,8.49E-03,8.56E+06,8.56E+15,6.10E+07,1.73E+06,6.15E+11,6.80E+07
7.56E-06,9.94E+00,7.30E+07,7.30E+16,2.61E+08,1.86E+06,2.43E+12,4.01E+08
8.24E-16,1.58E-10,2.37E+07,2.37E+16,5.80E+07,3.33E+04,6.35E+09,1.10E+07
3.93E-05,1.49E+00,3.07E+07,3.07E+16,5.90E+07,2.09E+06,7.87E+10,9.60E+07
1.24E-06,4.85E+00,9.81E+06,9.81E+15,1.19E+08,6.04E+06,2.36E+13,3.44E+08
3.58E-08,2.12E-01,1.59E+07,1.59E+16,1.54E+08,3.94E+03,2.32E+10,5.10E+07
8.37E-15,8.32E-09,2.66E+07,2.66E+16,1.19E+08,6.90E+03,6.82E+09,4.00E+06
7.90E-07,4.26E+00,7.56E+06,7.55E+15,2.60E+08,2.12E+06,1.14E+13,3.97E+08
1.50E-09,2.57E-03,2.15E+07,2.15E+16,5.10E+07,4.92E+05,8.38E+11,8.40E+07
1.43E-09,8.81E-04,4.97E+07,4.97E+16,5.10E+07,1.62E+05,9.98E+10,3.10E+07
2.13E-07,5.17E-01,3.19E+06,3.19E+15,1.00E+07,1.29E+07,3.13E+13,3.88E+08
7.72E-34,2.38E-29,5.81E+07,5.81E+16,7.90E+07,2.14E+05,6.54E+09,1.80E+07
8.43E-14,2.41E-07,8.29E+06,8.29E+15,2.20E+08,1.72E+06,4.90E+12,1.10E+08
6.72E-06,5.62E+00,3.08E+07,3.08E+16,1.01E+08,2.29E+06,1.91E+12,2.24E+08
4.28E-12,2.97E-07,4.20E+07,4.20E+16,6.60E+07,2.20E+06,1.52E+11,4.60E+07
2.41E-25,1.57E-19,1.43E+07,1.43E+16,1.71E+08,0.00E+00,0.00E+00,0.00E+00
9.99E-21,4.48E-15,4.74E+07,4.74E+16,1.91E+08,1.24E+04,5.54E+09,9.00E+06
1.08E-04,1.24E+02,6.97E+07,6.97E+16,2.95E+08,4.05E+06,4.64E+12,3.62E+08
2.33E-02,7.40E+03,2.46E+07,2.46E+16,8.00E+07,2.32E+07,7.35E+12,6.96E+08
1.45E-04,1.02E+02,1.37E+07,1.37E+16,1.88E+08,8.38E+05,5.93E+11,3.34E+08
5.36E-07,2.78E+00,8.78E+06,8.78E+15,2.08E+08,7.35E+05,3.81E+12,2.70E+08
2.57E-08,9.76E-03,5.62E+06,5.62E+15,1.70E+07,2.41E+06,9.12E+11,7.20E+07
2.93E-07,3.33E-01,1.78E+07,1.78E+16,2.83E+08,3.09E+06,3.50E+12,3.10E+08
2.55E-05,3.26E+01,1.18E+07,1.18E+16,1.23E+08,9.66E+05,1.23E+12,4.22E+08
5.59E-17,1.54E-11,6.01E+07,6.01E+16,2.09E+08,6.54E+03,1.80E+09,5.00E+06
4.28E-04,6.28E+02,5.93E+07,5.93E+16,1.04E+08,3.68E+06,5.41E+12,6.41E+08
9.78E-05,1.72E+02,1.03E+07,1.03E+16,2.32E+08,5.21E+05,9.16E+11,4.12E+08
3.12E-05,2.54E+01,1.32E+07,1.32E+16,2.50E+07,2.80E+06,2.28E+12,1.84E+08
5.27E-06,7.48E-01,7.49E+07,7.49E+16,2.73E+08,6.02E+06,8.53E+11,1.75E+08
2.00E-11,1.62E-06,1.44E+07,1.44E+16,4.50E+07,4.62E+06,3.73E+11,5.40E+07
2.98E-34,1.32E-27,1.51E+07,1.51E+16,1.42E+08,0.00E+00,0.00E+00,0.00E+00
7.50E-07,9.79E-01,5.50E+07,5.50E+16,1.78E+08,2.10E+07,2.73E+13,2.75E+08
7.33E-07,2.97E-01,3.16E+07,3.16E+16,1.06E+08,1.79E+05,7.20E+10,8.10E+07
3.50E-08,1.39E-02,9.65E+06,9.65E+15,2.59E+08,6.13E+04,2.44E+10,5.50E+07
3.83E-21,1.75E-14,8.96E+06,8.96E+15,1.89E+08,7.23E+04,3.28E+11,1.80E+07
2.13E-12,2.39E-07,1.59E+07,1.59E+16,6.50E+07,7.07E+06,7.91E+11,1.50E+08
5.83E-08,7.73E-02,6.84E+06,6.84E+15,2.00E+07,3.92E+06,5.18E+12,2.15E+08
1.31E-06,2.89E-01,3.60E+07,3.60E+16,2.45E+08,6.25E+04,1.38E+10,4.50E+07
1.14E-04,7.29E+02,1.09E+07,1.09E+16,6.60E+07,8.48E+05,5.41E+12,3.27E+08
6.71E-08,3.57E-03,7.06E+07,7.06E+16,1.76E+08,2.13E+06,1.13E+11,1.53E+08
4.70E-03,4.48E+02,1.55E+07,1.55E+16,6.00E+07,9.31E+06,8.88E+11,3.04E+08
9.78E-10,2.25E-04,1.56E+07,1.56E+16,2.36E+08,4.98E+06,1.14E+12,1.55E+08

2.21E-05,3.73E+00,1.85E+07,1.85E+16,9.70E+07,4.16E+06,7.01E+11,3.35E+08
6.26E-35,1.22E-29,2.94E+07,2.94E+16,1.83E+08,0.00E+00,0.00E+00,0.00E+00
2.12E-36,2.43E-30,1.75E+07,1.75E+16,1.84E+08,8.56E+04,9.78E+10,2.70E+07
7.08E-08,8.53E-02,1.33E+07,1.33E+16,1.41E+08,8.84E+05,1.06E+12,3.26E+08
8.42E-09,2.38E-03,1.21E+07,1.21E+16,1.70E+08,4.64E+04,1.31E+10,4.40E+07
9.51E-07,4.97E-01,6.01E+06,6.01E+15,2.65E+08,3.63E+06,1.89E+12,2.19E+08
1.54E-16,8.21E-11,1.27E+07,1.27E+16,1.79E+08,5.77E+02,3.05E+08,2.00E+06
1.58E-24,4.64E-18,2.36E+07,2.36E+16,2.40E+08,3.49E+05,1.02E+12,6.30E+07
7.96E-04,2.01E+01,5.93E+07,5.93E+16,1.52E+08,4.54E+06,1.15E+11,1.88E+08
7.43E-04,4.56E+02,1.60E+07,1.60E+16,1.46E+08,2.02E+06,1.24E+12,4.48E+08
1.81E-10,1.71E-05,1.57E+07,1.57E+16,1.30E+08,1.05E+06,9.88E+10,4.00E+07
1.34E-05,5.16E+00,3.10E+07,3.10E+16,1.99E+08,3.34E+06,1.28E+12,2.28E+08
6.77E-05,3.29E+01,2.18E+07,2.18E+16,1.24E+08,1.30E+06,6.29E+11,3.51E+08
1.66E-08,3.05E-02,2.40E+07,2.40E+16,4.50E+07,3.53E+05,6.46E+11,6.50E+07
5.10E-08,3.42E-02,6.56E+07,6.56E+16,1.52E+08,2.01E+05,1.35E+11,1.27E+08
1.73E-14,4.88E-08,1.60E+07,1.60E+16,2.41E+08,1.02E+05,2.88E+11,5.40E+07
6.11E-07,7.40E-01,1.01E+07,1.01E+16,3.04E+08,2.84E+06,3.43E+12,2.65E+08
1.36E-06,3.09E-02,5.56E+07,5.55E+16,2.80E+07,3.98E+06,8.98E+10,3.80E+07
1.44E-05,1.31E+01,6.45E+07,6.45E+16,1.28E+08,5.62E+06,5.10E+12,4.90E+08
6.02E-07,7.30E-02,3.75E+07,3.75E+16,9.60E+07,9.74E+06,1.18E+12,2.97E+08
2.84E-11,6.06E-05,3.03E+07,3.03E+16,1.58E+08,9.49E+05,2.02E+12,7.80E+07
1.12E-09,2.97E-04,5.57E+07,5.57E+16,2.09E+08,2.61E+05,6.88E+10,8.70E+07
1.14E-10,4.57E-06,6.78E+07,6.78E+16,3.40E+07,3.52E+06,1.41E+11,2.90E+07
1.56E-07,1.13E-02,2.10E+07,2.10E+16,2.33E+08,1.07E+06,7.78E+10,1.08E+08
5.99E-10,7.93E-04,4.96E+07,4.96E+16,1.51E+08,1.13E+07,1.49E+13,2.07E+08
1.18E-06,1.00E+01,1.09E+07,1.09E+16,2.56E+08,5.10E+05,4.32E+12,4.02E+08
9.43E-05,4.52E+01,4.19E+07,4.19E+16,1.83E+08,7.40E+06,3.54E+12,2.88E+08
1.13E-09,1.34E-03,3.32E+07,3.31E+16,2.75E+08,3.62E+06,4.28E+12,2.99E+08
1.17E-10,2.89E-04,9.06E+06,9.06E+15,1.63E+08,9.73E+05,2.39E+12,1.67E+08
1.01E-05,4.46E+00,6.13E+06,6.12E+15,1.70E+07,3.57E+06,1.58E+12,1.66E+08
7.31E-12,1.16E-06,8.99E+06,8.99E+15,4.90E+07,1.64E+05,2.60E+10,2.90E+07
4.16E-06,2.43E+00,5.87E+07,5.87E+16,1.35E+08,3.61E+06,2.10E+12,1.38E+08
4.39E-06,2.88E+00,3.14E+07,3.14E+16,2.57E+08,3.99E+05,2.62E+11,2.84E+08
4.26E-06,5.35E-01,2.64E+07,2.64E+16,3.20E+07,3.86E+06,4.83E+11,7.70E+07
7.39E-12,5.72E-05,1.14E+07,1.14E+16,2.73E+08,9.18E+05,7.08E+12,1.96E+08
2.04E-05,1.32E+01,4.22E+07,4.22E+16,5.20E+07,8.64E+06,5.60E+12,2.32E+08
2.91E-20,1.14E-13,8.69E+06,8.69E+15,2.31E+08,2.52E+04,9.85E+10,5.60E+07
7.88E-10,1.49E-03,3.44E+07,3.44E+16,2.77E+08,7.14E+06,1.35E+13,3.92E+08
7.31E-04,8.97E+01,1.29E+07,1.29E+16,8.70E+07,2.23E+06,2.74E+11,2.37E+08
6.20E-06,1.09E+00,1.26E+07,1.26E+16,1.06E+08,2.28E+06,3.99E+11,2.17E+08
6.01E-04,1.63E+01,4.07E+07,4.07E+16,1.58E+08,7.62E+06,2.07E+11,1.62E+08
6.56E-05,2.52E+01,1.86E+07,1.86E+16,9.30E+07,3.39E+06,1.30E+12,2.52E+08
1.88E-06,1.51E+00,5.29E+07,5.29E+16,2.66E+08,3.33E+06,2.67E+12,4.11E+08
9.45E-47,6.38E-41,4.07E+07,4.07E+16,1.61E+08,4.81E+04,3.23E+10,1.70E+07
3.54E-13,2.56E-08,1.77E+07,1.77E+16,1.63E+08,0.00E+00,0.00E+00,0.00E+00
1.65E-15,1.84E-10,1.75E+07,1.75E+16,1.81E+08,2.48E+06,2.77E+11,1.66E+08
4.07E-12,1.53E-05,8.06E+06,8.06E+15,2.51E+08,1.40E+06,5.22E+12,1.87E+08
1.40E-12,1.10E-06,3.19E+07,3.19E+16,2.44E+08,1.53E+05,1.19E+11,4.50E+07
2.09E-15,1.01E-08,8.88E+06,8.88E+15,2.32E+08,9.50E+04,4.58E+11,1.40E+08
3.07E-10,1.76E-03,1.29E+07,1.29E+16,1.65E+08,6.15E+06,3.52E+13,2.41E+08
1.33E-08,1.81E-03,8.51E+06,8.51E+15,1.20E+07,3.67E+06,4.96E+11,4.90E+07
3.46E-08,8.94E-03,2.05E+07,2.05E+16,2.70E+08,1.24E+04,3.19E+09,1.30E+07
2.26E-04,1.46E+01,1.77E+07,1.77E+16,5.80E+07,8.21E+05,5.30E+10,6.40E+07
3.39E-07,1.30E+00,2.31E+07,2.31E+16,2.61E+08,1.96E+06,7.51E+12,3.38E+08
7.44E-09,1.43E-02,6.24E+06,6.24E+15,1.70E+08,2.94E+06,5.63E+12,2.41E+08
7.33E-16,1.55E-09,3.08E+07,3.08E+16,1.19E+08,0.00E+00,0.00E+00,0.00E+00
8.16E-12,1.38E-06,3.87E+07,3.87E+16,2.46E+08,3.74E+05,6.31E+10,1.06E+08
1.22E-21,1.62E-14,7.93E+06,7.93E+15,2.09E+08,7.14E+01,9.41E+08,5.00E+06
9.17E-08,3.28E-02,1.04E+07,1.04E+16,8.70E+07,1.30E+04,4.61E+09,1.20E+07
6.30E-13,8.26E-07,2.55E+07,2.55E+16,8.20E+07,2.23E+07,2.93E+13,3.44E+08
5.13E-36,9.84E-31,2.31E+07,2.31E+16,1.17E+08,0.00E+00,0.00E+00,0.00E+00
1.19E-14,4.50E-10,3.27E+07,3.27E+16,7.60E+07,0.00E+00,0.00E+00,0.00E+00
5.18E-08,2.03E-01,1.46E+07,1.46E+16,2.33E+08,2.35E+06,9.18E+12,1.70E+08
1.54E-06,9.08E+00,1.34E+07,1.34E+16,4.40E+07,1.51E+06,8.89E+12,1.97E+08
5.42E-07,5.38E-01,2.75E+07,2.75E+16,2.15E+08,6.24E+05,6.17E+11,1.08E+08
7.53E-05,4.06E+02,7.18E+06,7.18E+15,8.90E+07,2.53E+06,1.36E+13,8.41E+08
2.86E-21,4.90E-15,2.10E+07,2.10E+16,1.34E+08,0.00E+00,0.00E+00,0.00E+00
2.35E-31,1.45E-25,4.07E+07,4.07E+16,1.15E+08,7.90E+04,4.85E+10,2.20E+07
2.90E-06,7.05E+00,1.60E+07,1.60E+16,1.67E+08,2.11E+05,5.12E+11,1.59E+08
4.54E-12,1.40E-07,4.98E+07,4.98E+16,5.40E+07,6.00E+06,1.84E+11,2.80E+07
1.96E-14,5.60E-08,9.43E+06,9.43E+15,2.33E+08,2.00E+05,5.67E+11,8.50E+07
4.14E-08,3.47E-02,3.36E+07,3.36E+16,2.18E+08,3.07E+05,2.56E+11,1.29E+08
1.71E-05,1.18E+00,4.45E+07,4.45E+16,8.50E+07,1.62E+06,1.12E+11,1.31E+08
1.35E-07,8.81E-02,1.57E+07,1.57E+16,1.75E+08,9.87E+04,6.40E+10,1.04E+08
3.00E-08,1.34E-02,5.17E+07,5.17E+16,2.73E+08,7.05E+05,3.15E+11,1.41E+08

3.69E-02,4.22E+04,2.59E+07,2.59E+16,7.80E+07,4.92E+07,5.63E+13,1.35E+09
2.42E-45,7.70E-40,2.32E+07,2.32E+16,9.60E+07,5.29E+06,1.68E+12,5.40E+07
4.08E-09,2.90E-03,1.19E+07,1.19E+16,1.97E+08,1.54E+06,1.09E+12,9.30E+07
2.08E-06,1.08E+01,9.69E+05,9.69E+14,3.30E+07,8.37E+06,4.33E+13,3.43E+08
9.94E-06,3.77E+00,8.72E+06,8.72E+15,6.30E+07,1.12E+05,4.22E+10,6.50E+07
3.91E-27,4.47E-21,1.96E+07,1.96E+16,1.80E+08,0.00E+00,0.00E+00,0.00E+00
5.75E-06,7.36E+00,1.25E+07,1.25E+16,2.29E+08,2.50E+05,3.20E+11,2.05E+08
2.26E-18,6.25E-13,5.92E+07,5.92E+16,1.96E+08,2.62E+03,7.21E+08,2.00E+06
1.18E-08,1.75E-02,5.38E+07,5.38E+16,1.81E+08,8.11E+06,1.19E+13,2.30E+08
3.78E-07,6.66E-01,6.78E+06,6.78E+15,9.60E+07,4.07E+06,7.16E+12,3.08E+08
9.05E-14,7.41E-08,1.62E+07,1.62E+16,1.59E+08,6.48E+03,5.28E+09,1.90E+07
1.06E-06,1.50E-01,4.27E+06,4.27E+15,1.40E+07,7.50E+07,1.06E+13,4.12E+08
3.21E-23,2.61E-18,1.87E+07,1.87E+16,1.63E+08,0.00E+00,0.00E+00,0.00E+00
1.08E-04,4.75E+02,1.49E+07,1.49E+16,8.50E+07,1.62E+06,7.12E+12,3.59E+08
2.65E-12,3.47E-06,5.96E+07,5.96E+16,2.49E+08,9.62E+06,1.25E+13,7.90E+07
2.13E-07,8.60E-02,2.89E+07,2.89E+16,7.80E+07,2.71E+06,1.09E+12,7.60E+07
2.51E-05,1.00E+01,8.92E+06,8.92E+15,9.10E+07,9.15E+05,3.64E+11,1.52E+08
8.99E-14,4.10E-07,9.17E+06,9.17E+15,1.11E+08,1.00E+05,4.54E+11,1.28E+08
2.93E-06,3.29E-01,2.44E+07,2.44E+16,2.08E+08,9.51E+04,1.07E+10,2.40E+07
7.38E-07,9.79E-01,9.61E+06,9.61E+15,8.00E+07,1.04E+06,1.38E+12,2.49E+08
5.82E-08,1.29E-02,3.59E+07,3.59E+16,2.25E+08,1.98E+05,4.36E+10,1.00E+08
1.31E-22,8.41E-16,1.16E+07,1.16E+16,1.60E+08,0.00E+00,0.00E+00,0.00E+00
7.54E-37,4.03E-32,6.31E+07,6.31E+16,1.62E+08,0.00E+00,0.00E+00,0.00E+00
8.86E-06,8.46E-01,2.30E+07,2.30E+16,8.30E+07,2.02E+06,1.93E+11,1.71E+08
1.66E-06,3.79E-01,9.19E+05,9.18E+14,9.00E+06,1.94E+07,4.43E+12,3.56E+08
2.24E-07,3.79E-02,1.81E+07,1.81E+16,2.06E+08,4.58E+06,7.72E+11,1.20E+08
2.11E-03,4.09E+02,2.57E+07,2.57E+16,7.60E+07,5.61E+06,1.09E+12,2.40E+08
2.74E-26,3.14E-20,1.62E+07,1.62E+16,1.72E+08,0.00E+00,0.00E+00,0.00E+00
1.04E-05,1.26E+01,1.22E+07,1.22E+16,1.07E+08,1.87E+06,2.25E+12,3.51E+08
3.38E-11,9.57E-06,1.16E+07,1.16E+16,2.13E+08,3.45E+05,9.70E+10,8.20E+07
3.02E-28,1.59E-22,8.33E+06,8.32E+15,1.77E+08,0.00E+00,0.00E+00,0.00E+00
2.09E-15,1.11E-09,1.26E+07,1.26E+16,1.80E+08,1.29E+05,6.82E+10,3.00E+07
1.28E-03,3.74E+03,2.52E+07,2.52E+16,1.11E+08,2.74E+06,8.00E+12,7.50E+08
1.22E-20,3.11E-16,5.16E+07,5.16E+16,1.04E+08,2.69E+06,6.80E+10,4.80E+07
8.10E-38,5.00E-32,1.41E+07,1.41E+16,1.57E+08,0.00E+00,0.00E+00,0.00E+00
3.85E-19,3.64E-14,1.57E+07,1.57E+16,1.13E+08,0.00E+00,0.00E+00,0.00E+00
4.89E-36,1.89E-30,2.87E+07,2.87E+16,1.81E+08,3.40E+03,1.30E+09,2.00E+06
2.53E-06,1.23E+00,1.90E+07,1.90E+16,1.24E+08,3.90E+06,1.89E+12,3.56E+08
1.73E-07,3.18E-01,2.17E+07,2.17E+16,9.70E+07,6.40E+04,1.17E+11,1.13E+08
2.55E-14,1.71E-08,6.54E+07,6.54E+16,1.10E+08,4.24E+05,2.84E+11,4.30E+07
2.80E-05,7.87E+01,1.30E+07,1.30E+16,1.98E+08,4.37E+06,1.23E+13,5.13E+08
5.78E-03,6.99E+03,7.26E+06,7.26E+15,6.80E+07,5.82E+06,7.04E+12,6.99E+08
1.82E-08,4.12E-04,4.06E+07,4.06E+16,1.70E+07,1.97E+07,4.43E+11,7.80E+07
4.90E-08,4.45E-02,6.65E+07,6.65E+16,2.80E+08,3.64E+06,3.30E+12,3.74E+08
5.47E-10,6.65E-05,4.52E+07,4.52E+16,2.09E+08,0.00E+00,0.00E+00,0.00E+00
4.67E-19,9.98E-13,3.15E+07,3.15E+16,2.02E+08,1.00E+02,2.13E+08,1.00E+06
1.62E-30,4.31E-25,5.40E+07,5.40E+16,1.72E+08,0.00E+00,0.00E+00,0.00E+00
1.30E-02,5.20E+02,5.27E+07,5.27E+16,3.50E+07,1.74E+07,6.96E+11,1.11E+08
1.25E-02,9.04E+02,1.40E+07,1.40E+16,6.50E+07,9.45E+06,6.85E+11,3.15E+08
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8.90E-04,7.55E+03,8.70E+06,8.70E+15,2.34E+08,1.61E+06,1.37E+13,5.91E+08
7.58E-06,3.64E+00,4.67E+07,4.67E+16,1.33E+08,2.46E+06,1.18E+12,2.64E+08
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6.91E-05,1.70E+02,7.26E+06,7.26E+15,2.80E+08,3.77E+06,9.26E+12,3.87E+08
5.86E-09,2.60E-03,9.68E+06,9.68E+15,1.46E+08,1.56E+03,6.89E+08,4.00E+06
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7.03E-23,4.64E-17,2.91E+07,2.91E+16,2.25E+08,6.66E+05,4.37E+11,5.10E+07
9.16E-06,1.15E+00,3.05E+07,3.05E+16,1.56E+08,3.16E+05,3.95E+10,3.80E+07
3.54E-04,2.73E+03,8.67E+06,8.67E+15,2.18E+08,4.13E+06,3.19E+13,1.04E+09
6.24E-05,4.06E+01,4.66E+07,4.66E+16,8.50E+07,4.43E+06,2.87E+12,2.30E+08
2.31E-12,9.05E-06,5.62E+06,5.62E+15,1.65E+08,2.52E+06,9.86E+12,1.69E+08
1.89E-32,3.58E-26,3.01E+07,3.01E+16,1.72E+08,0.00E+00,0.00E+00,0.00E+00
1.22E-04,1.49E+01,1.46E+07,1.46E+16,2.14E+08,5.49E+05,6.74E+10,1.25E+08
1.05E-07,1.84E-02,1.07E+07,1.07E+16,1.56E+08,3.84E+06,6.73E+11,2.04E+08
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3.41E-05,1.31E+01,1.64E+07,1.64E+16,4.30E+07,5.85E+06,2.25E+12,1.91E+08
2.00E-17,1.61E-11,4.66E+07,4.66E+16,2.13E+08,2.10E+06,1.68E+12,8.30E+07
2.07E-28,1.40E-22,3.92E+07,3.92E+16,1.32E+08,0.00E+00,0.00E+00,0.00E+00
1.88E-07,1.36E-02,1.79E+07,1.79E+16,1.41E+08,1.27E+04,9.13E+08,6.00E+06
5.95E-20,6.64E-15,8.03E+06,8.02E+15,3.90E+07,1.25E+07,1.39E+12,2.53E+08
6.48E-19,2.44E-12,9.25E+06,9.25E+15,2.41E+08,2.80E+05,1.05E+12,1.03E+08
5.51E-07,4.31E-01,2.87E+07,2.87E+16,1.15E+08,3.24E+06,2.53E+12,2.25E+08
6.07E-12,2.95E-05,8.93E+06,8.93E+15,1.71E+08,3.03E+02,1.46E+09,8.00E+06
1.11E-08,6.37E-02,1.84E+07,1.84E+16,3.10E+08,1.51E+06,8.61E+12,2.38E+08

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3.88E-26,1.00E-20,1.59E+07,1.59E+16,2.05E+08,2.03E+06,5.23E+11,8.70E+07
1.84E-11,1.19E-06,1.80E+07,1.80E+16,1.31E+08,3.39E+05,2.19E+10,5.30E+07
7.06E-07,2.70E+00,1.86E+07,1.86E+16,2.49E+08,6.17E+06,2.36E+13,3.95E+08
4.13E-07,7.92E-01,8.99E+06,8.99E+15,1.81E+08,5.29E+05,1.01E+12,3.03E+08
2.72E-05,5.71E+01,2.38E+07,2.38E+16,2.40E+07,6.49E+06,1.36E+13,2.66E+08
3.54E-11,6.01E-06,3.72E+07,3.72E+16,2.43E+08,2.42E+06,4.09E+11,7.90E+07
3.27E-20,4.33E-13,8.91E+06,8.91E+15,2.12E+08,1.84E+04,2.42E+11,1.13E+08
1.88E-08,6.74E-03,1.08E+07,1.08E+16,6.50E+07,1.05E+04,3.75E+09,8.00E+06
1.12E-06,1.47E+00,6.41E+07,6.41E+16,9.50E+07,1.05E+07,1.38E+13,4.14E+08
1.91E-11,3.66E-06,2.30E+07,2.30E+16,6.40E+07,0.00E+00,0.00E+00,0.00E+00
1.84E-05,6.94E-01,2.63E+07,2.63E+16,6.00E+07,6.22E+06,2.35E+11,9.40E+07
5.46E-09,2.14E-02,1.47E+07,1.47E+16,3.05E+08,2.44E+06,9.55E+12,3.86E+08
1.58E-04,9.33E+02,1.50E+07,1.50E+16,1.80E+08,8.30E+05,4.90E+12,1.91E+08
5.38E-03,5.32E+03,8.17E+06,8.17E+15,5.80E+07,2.02E+07,1.99E+13,7.89E+08
2.29E-05,1.24E+02,7.10E+06,7.10E+15,9.30E+07,2.59E+06,1.40E+13,4.42E+08
8.71E-12,1.49E-05,2.52E+07,2.52E+16,4.20E+07,1.51E+05,2.57E+11,5.10E+07
1.27E-12,7.86E-07,4.45E+07,4.45E+16,8.40E+07,4.24E+02,2.61E+08,1.00E+06
1.59E-43,3.87E-37,1.49E+07,1.49E+16,1.93E+08,2.47E+02,5.98E+08,1.00E+06
1.30E-11,4.01E-07,5.63E+07,5.63E+16,7.70E+07,9.05E+04,2.77E+09,9.00E+06
1.11E-04,3.14E+02,7.78E+06,7.78E+15,3.39E+08,2.33E+06,6.62E+12,4.91E+08
5.69E-06,4.75E+00,3.40E+07,3.40E+16,1.38E+08,1.90E+05,1.58E+11,1.66E+08
5.66E-06,3.93E-01,4.51E+07,4.51E+16,1.10E+08,7.59E+04,5.24E+09,1.50E+07
8.61E-11,5.61E-05,1.57E+07,1.57E+16,2.23E+08,1.43E+05,9.30E+10,1.16E+08
2.13E-05,9.52E+00,4.81E+07,4.81E+16,2.70E+08,4.35E+06,1.94E+12,3.17E+08
3.34E-03,3.83E+03,1.18E+07,1.18E+16,4.30E+07,6.22E+07,7.13E+13,7.45E+08
1.56E-03,4.93E+02,3.38E+07,3.38E+16,2.06E+08,1.05E+07,3.34E+12,4.20E+08
7.66E-05,5.42E+01,1.31E+07,1.31E+16,2.97E+08,1.32E+06,9.34E+11,3.72E+08
2.61E-05,1.35E+02,7.24E+06,7.24E+15,1.26E+08,2.17E+06,1.12E+13,6.52E+08
1.40E-17,5.32E-12,8.16E+06,8.16E+15,8.00E+07,0.00E+00,0.00E+00,0.00E+00
1.60E-05,1.82E+01,1.79E+07,1.79E+16,1.26E+08,2.80E+06,3.17E+12,3.46E+08
2.00E-15,2.57E-09,1.17E+07,1.17E+16,1.94E+08,2.15E+03,2.74E+09,5.00E+06
7.50E-05,2.06E+01,5.92E+07,5.92E+16,1.58E+08,2.43E+06,6.67E+11,1.85E+08
3.75E-12,5.53E-06,1.84E+07,1.84E+16,1.80E+07,4.00E+07,5.88E+13,1.86E+08
2.03E-07,3.58E-01,1.08E+07,1.08E+16,2.30E+08,1.16E+05,2.05E+11,2.18E+08
5.33E-08,4.36E-02,1.58E+07,1.58E+16,6.50E+07,1.07E+06,8.71E+11,8.90E+07
2.91E-02,4.12E+03,4.39E+07,4.39E+16,1.89E+08,3.71E+07,5.26E+12,7.83E+08
4.71E-09,3.81E-04,1.82E+07,1.82E+16,1.03E+08,1.26E+06,1.02E+11,9.20E+07
5.52E-05,2.42E+02,8.99E+06,8.99E+15,5.60E+07,7.56E+06,3.32E+13,7.50E+08
1.11E-07,1.45E-01,5.07E+07,5.07E+16,2.82E+08,2.32E+07,3.02E+13,3.16E+08
5.10E-18,2.07E-12,3.14E+07,3.14E+16,1.65E+08,3.43E+05,1.38E+11,5.60E+07
5.76E-07,2.30E-01,9.34E+06,9.34E+15,2.21E+08,3.83E+05,1.52E+11,1.38E+08
3.98E-06,1.81E+01,8.31E+06,8.31E+15,5.70E+07,8.60E+05,3.90E+12,2.13E+08
5.32E-17,5.99E-12,1.12E+07,1.12E+16,2.90E+07,4.32E+06,4.84E+11,2.10E+07
8.22E-33,1.09E-26,1.01E+07,1.01E+16,1.20E+08,2.83E+05,3.74E+11,4.80E+07
1.61E-06,3.55E-01,2.80E+07,2.80E+16,1.89E+08,7.67E+06,1.69E+12,2.12E+08
3.01E-11,1.93E-04,1.22E+07,1.22E+16,1.58E+08,4.09E+02,2.61E+09,1.20E+07
5.17E-04,2.75E+01,7.15E+07,7.15E+16,2.08E+08,1.32E+06,6.98E+10,8.90E+07
9.76E-08,9.34E-03,2.49E+07,2.49E+16,1.81E+08,5.51E+03,5.25E+08,3.00E+06
3.01E-21,6.92E-16,1.72E+07,1.72E+16,1.26E+08,0.00E+00,0.00E+00,0.00E+00
8.27E-07,1.40E-01,1.70E+07,1.70E+16,1.65E+08,5.16E+06,8.70E+11,1.31E+08
4.91E-16,9.56E-11,3.03E+07,3.03E+16,7.70E+07,3.77E+05,7.30E+10,1.30E+07
7.44E-11,8.53E-05,1.19E+07,1.19E+16,2.45E+08,7.85E+06,8.97E+12,2.48E+08
9.34E-17,1.13E-10,1.35E+07,1.35E+16,1.75E+08,0.00E+00,0.00E+00,0.00E+00
5.10E-06,1.44E+00,1.14E+07,1.14E+16,2.18E+08,5.06E+05,1.42E+11,1.34E+08
1.62E-19,8.51E-14,5.95E+06,5.95E+15,2.02E+08,2.67E+06,1.39E+12,1.46E+08
4.51E-07,2.40E-01,1.27E+07,1.27E+16,1.66E+08,9.32E+04,4.93E+10,3.40E+07
1.02E-09,2.98E-03,2.69E+07,2.69E+16,2.88E+08,1.99E+05,5.79E+11,2.04E+08
5.86E-07,1.48E-02,5.64E+07,5.63E+16,6.00E+07,7.87E+06,1.99E+11,1.48E+08
2.22E-10,1.37E-04,1.79E+07,1.79E+16,2.65E+08,2.08E+04,1.27E+10,3.60E+07
1.37E-10,1.29E-05,1.47E+07,1.47E+16,8.10E+07,2.04E+06,1.91E+11,1.05E+08
2.34E-09,9.00E-04,1.86E+07,1.86E+16,5.70E+07,1.37E+07,5.27E+12,2.50E+08
9.14E-04,4.44E+02,2.09E+07,2.09E+16,1.07E+08,2.16E+06,1.05E+12,3.19E+08
6.23E-11,1.15E-04,2.19E+07,2.19E+16,1.67E+08,1.57E+04,2.88E+10,4.30E+07
5.21E-07,3.50E-01,6.62E+07,6.62E+16,1.46E+08,1.89E+05,1.26E+11,1.37E+08
2.57E-07,7.23E-01,1.65E+07,1.65E+16,3.23E+08,3.19E+05,8.94E+11,2.25E+08
6.44E-05,7.79E+01,1.13E+07,1.13E+16,1.63E+08,1.67E+06,2.02E+12,3.81E+08
3.26E-15,7.40E-11,5.28E+07,5.28E+16,3.30E+07,5.57E+06,1.26E+11,4.30E+07
2.00E-05,1.82E+01,6.27E+07,6.27E+16,1.72E+08,7.32E+06,6.64E+12,3.42E+08
3.62E-07,4.39E-02,3.82E+07,3.82E+16,1.99E+08,8.64E+06,1.05E+12,2.86E+08
1.18E-13,2.52E-07,3.11E+07,3.11E+16,2.16E+08,3.49E+05,7.41E+11,6.00E+07
1.59E-06,4.20E-01,5.46E+07,5.46E+16,2.02E+08,4.08E+05,1.08E+11,5.10E+07
2.74E-08,1.10E-03,6.77E+07,6.77E+16,5.70E+07,3.99E+05,1.60E+10,1.70E+07
1.46E-03,1.06E+02,1.67E+07,1.67E+16,8.80E+07,6.79E+06,4.92E+11,2.46E+08
2.17E-04,2.86E+02,5.93E+07,5.93E+16,9.20E+07,1.39E+06,1.82E+12,2.86E+08

1.03E-21,8.76E-15,1.02E+07,1.02E+16,1.70E+08,3.27E+04,2.77E+11,4.80E+07
3.65E-08,1.76E-02,4.46E+07,4.46E+16,1.38E+08,4.40E+06,2.11E+12,1.47E+08
8.58E-09,1.02E-02,3.61E+07,3.61E+16,2.68E+08,4.14E+05,4.89E+11,1.14E+08
1.01E-20,2.48E-14,8.48E+06,8.48E+15,1.39E+08,5.20E+05,1.27E+12,6.70E+07
8.03E-05,3.55E+01,9.44E+06,9.44E+15,6.90E+07,6.06E+05,2.67E+11,8.80E+07
1.49E-43,2.36E-38,8.39E+06,8.39E+15,9.10E+07,0.00E+00,0.00E+00,0.00E+00
8.53E-17,5.00E-11,6.17E+07,6.17E+16,2.38E+08,1.39E+05,8.07E+10,8.30E+07
1.18E-17,7.80E-12,2.18E+07,2.18E+16,1.39E+08,0.00E+00,0.00E+00,0.00E+00
5.45E-06,6.84E-01,3.03E+07,3.03E+16,1.25E+08,2.97E+05,3.72E+10,5.20E+07
3.63E-05,2.80E+02,1.00E+07,1.00E+16,1.83E+08,2.73E+06,2.10E+13,9.72E+08
3.37E-06,2.19E+00,5.02E+07,5.02E+16,1.95E+08,3.14E+05,2.03E+11,1.49E+08
4.67E-06,1.83E+01,8.82E+06,8.82E+15,2.21E+08,7.09E+05,2.77E+12,5.07E+08
3.46E-11,6.56E-05,3.39E+07,3.39E+16,2.77E+08,7.05E+06,1.33E+13,3.11E+08
7.50E-17,9.26E-12,1.38E+07,1.38E+16,1.94E+08,0.00E+00,0.00E+00,0.00E+00
3.99E-06,7.00E-01,1.40E+07,1.40E+16,1.53E+08,1.05E+06,1.83E+11,1.74E+08
8.83E-05,2.40E+00,3.80E+07,3.80E+16,1.09E+08,1.00E+07,2.72E+11,3.17E+08
3.07E-20,1.19E-14,2.13E+07,2.13E+16,1.34E+08,2.44E+05,9.37E+10,5.60E+07
3.51E-11,2.81E-05,5.11E+07,5.11E+16,2.73E+08,3.31E+06,2.65E+12,3.19E+08
2.04E-16,1.38E-10,3.83E+07,3.83E+16,1.44E+08,4.21E+04,2.83E+10,5.10E+07
8.61E-56,6.24E-51,1.47E+07,1.47E+16,1.10E+08,0.00E+00,0.00E+00,0.00E+00
1.49E-07,1.67E-02,1.68E+07,1.68E+16,1.72E+08,4.64E+06,5.18E+11,9.30E+07
6.79E-22,2.56E-15,9.25E+06,9.25E+15,1.78E+08,0.00E+00,0.00E+00,0.00E+00
2.67E-07,2.09E-01,2.31E+07,2.31E+16,1.25E+08,8.15E+06,6.36E+12,1.86E+08
4.26E-09,2.06E-02,9.04E+06,9.04E+15,1.26E+08,2.91E+05,1.40E+12,2.17E+08
4.87E-03,2.79E+04,1.16E+07,1.16E+16,8.20E+07,8.50E+06,4.86E+13,1.19E+09
3.67E-06,4.98E-01,1.29E+07,1.29E+16,4.50E+07,3.60E+05,4.87E+10,3.10E+07
3.44E-04,8.85E+01,1.24E+07,1.24E+16,8.90E+07,8.11E+06,2.09E+12,5.52E+08
1.00E-31,6.50E-27,1.61E+07,1.61E+16,1.46E+08,0.00E+00,0.00E+00,0.00E+00
5.54E-26,2.14E-19,2.26E+07,2.26E+16,2.24E+08,6.24E+05,2.39E+12,6.40E+07
1.75E-05,3.36E+01,4.63E+06,4.63E+15,6.40E+07,4.88E+06,9.35E+12,3.63E+08
5.41E-26,1.14E-19,2.94E+07,2.94E+16,1.50E+08,0.00E+00,0.00E+00,0.00E+00
2.51E-10,4.26E-05,4.02E+07,4.02E+16,2.26E+08,2.13E+04,3.59E+09,8.00E+06
1.36E-10,1.80E-03,8.08E+06,8.08E+15,8.00E+07,5.26E+04,6.93E+11,1.96E+08
6.08E-08,2.17E-02,8.39E+06,8.39E+15,9.50E+07,1.68E+06,5.97E+11,6.40E+07
1.00E-10,1.32E-04,6.38E+07,6.38E+16,1.50E+08,5.28E+05,6.92E+11,6.10E+07
6.61E-26,1.27E-20,2.33E+07,2.33E+16,1.04E+08,0.00E+00,0.00E+00,0.00E+00
2.35E-19,8.90E-15,3.31E+07,3.31E+16,1.00E+08,0.00E+00,0.00E+00,0.00E+00
5.71E-08,2.24E-01,1.33E+07,1.32E+16,1.99E+08,2.59E+06,1.01E+13,3.12E+08
2.95E-10,1.75E-03,1.33E+07,1.33E+16,2.90E+07,2.29E+06,1.35E+13,1.95E+08
3.65E-12,3.63E-06,2.82E+07,2.81E+16,1.99E+08,5.12E+03,5.06E+09,9.00E+06
1.57E-03,8.47E+03,6.35E+06,6.35E+15,8.50E+07,3.36E+06,1.81E+13,1.16E+09
1.30E-08,2.23E-02,2.21E+07,2.21E+16,1.15E+08,1.01E+03,1.72E+09,8.00E+06
5.20E-32,3.21E-26,4.24E+07,4.24E+16,1.04E+08,0.00E+00,0.00E+00,0.00E+00
1.39E-04,3.37E+02,1.58E+07,1.57E+16,1.91E+08,3.98E+05,9.65E+11,3.07E+08
2.24E-11,6.88E-07,4.42E+07,4.42E+16,1.20E+07,1.33E+07,4.06E+11,4.30E+07
1.68E-06,4.79E+00,1.55E+06,1.55E+15,3.90E+07,9.21E+06,2.62E+13,4.29E+08
2.21E-03,1.85E+03,2.71E+07,2.71E+16,7.20E+07,6.31E+06,5.26E+12,4.32E+08
1.66E-09,1.15E-04,4.71E+07,4.71E+16,6.40E+07,1.26E+05,8.70E+09,1.30E+07
8.42E-14,5.48E-08,1.54E+07,1.54E+16,2.00E+08,4.26E+05,2.76E+11,1.42E+08
4.38E-07,1.96E-01,3.71E+07,3.71E+16,2.13E+08,1.18E+07,5.25E+12,2.33E+08
1.77E-05,2.03E+01,5.64E+07,5.64E+16,1.21E+08,1.85E+07,2.12E+13,8.33E+08
1.25E-05,3.96E+00,4.03E+07,4.03E+16,1.60E+08,6.33E+06,2.01E+12,2.92E+08
1.92E-10,1.37E-04,1.35E+07,1.35E+16,2.53E+08,3.52E+05,2.49E+11,1.13E+08
3.61E-03,1.87E+04,4.26E+06,4.26E+15,5.70E+07,5.16E+06,2.67E+13,7.84E+08
1.15E-39,4.39E-34,7.36E+06,7.36E+15,4.90E+07,2.99E+05,1.13E+11,5.50E+07
2.71E-09,3.09E-03,2.08E+07,2.08E+16,2.39E+08,1.06E+05,1.20E+11,1.27E+08
1.31E-06,1.67E+00,1.20E+07,1.20E+16,1.88E+08,7.89E+05,1.01E+12,3.33E+08
4.82E-41,1.33E-35,5.26E+07,5.26E+16,1.87E+08,8.99E+05,2.47E+11,2.30E+07
9.46E-07,1.39E+00,5.57E+07,5.57E+16,1.20E+08,7.14E+06,1.05E+13,3.95E+08
6.08E-12,1.07E-05,5.19E+06,5.19E+15,1.38E+08,3.83E+06,6.74E+12,3.20E+08
4.24E-30,3.47E-24,1.65E+07,1.65E+16,1.90E+08,4.02E+04,3.27E+10,2.50E+07
6.09E-48,8.67E-43,4.03E+07,4.03E+16,1.66E+08,0.00E+00,0.00E+00,0.00E+00
1.65E-05,1.33E+00,1.82E+07,1.82E+16,1.18E+08,1.16E+06,9.38E+10,6.60E+07
1.31E-21,5.77E-15,1.58E+07,1.58E+16,1.40E+08,0.00E+00,0.00E+00,0.00E+00
7.11E-10,9.28E-04,7.33E+07,7.33E+16,2.69E+08,3.36E+06,4.38E+12,2.25E+08
1.24E-07,5.00E-02,3.12E+07,3.12E+16,9.70E+07,7.62E+05,3.07E+11,5.20E+07
2.26E-06,9.01E-01,7.76E+06,7.76E+15,1.15E+08,1.12E+06,4.44E+11,1.27E+08
1.49E-17,6.81E-11,9.30E+06,9.30E+15,2.14E+08,1.30E+02,5.89E+08,3.00E+06
5.35E-13,6.02E-08,2.15E+07,2.15E+16,2.06E+08,2.73E+06,3.06E+11,1.66E+08
1.65E-05,2.18E+01,1.05E+07,1.05E+16,1.78E+08,1.09E+05,1.44E+11,8.60E+07
4.08E-05,8.99E+00,2.11E+07,2.10E+16,4.80E+07,1.51E+07,3.32E+12,3.00E+08
9.03E-11,5.77E-04,1.23E+07,1.23E+16,1.36E+08,1.77E+05,1.13E+12,2.56E+08
5.26E-11,2.80E-06,4.54E+07,4.54E+16,1.76E+08,2.33E+07,1.24E+12,1.20E+08
5.18E-08,4.96E-03,2.49E+07,2.49E+16,2.20E+08,4.00E+04,3.82E+09,1.70E+07
4.02E-06,9.20E-01,2.00E+07,2.00E+16,2.42E+08,1.18E+06,2.71E+11,1.20E+08

7.39E-05,1.25E+01,8.84E+06,8.84E+15,2.00E+07,1.39E+07,2.34E+12,2.84E+08
3.07E-05,5.97E+00,2.61E+07,2.61E+16,5.20E+07,5.37E+06,1.04E+12,1.46E+08
7.47E-10,8.54E-04,1.52E+07,1.52E+16,2.52E+08,6.62E+06,7.56E+12,2.83E+08
4.36E-10,5.26E-04,1.41E+07,1.41E+16,2.70E+08,3.01E+03,3.62E+09,1.80E+07
2.52E-03,7.09E+02,8.58E+06,8.58E+15,1.52E+08,3.00E+06,8.44E+11,3.46E+08
2.00E-28,1.05E-22,7.32E+06,7.32E+15,1.67E+08,0.00E+00,0.00E+00,0.00E+00
4.71E-08,2.50E-02,1.20E+07,1.20E+16,4.80E+07,8.44E+05,4.46E+11,9.10E+07
4.07E-39,1.19E-32,2.17E+07,2.16E+16,1.88E+08,2.47E+06,7.19E+12,5.50E+07
6.40E-04,1.62E+01,6.22E+07,6.22E+16,1.12E+08,1.83E+06,4.64E+10,7.80E+07
7.00E-05,4.29E+01,1.25E+07,1.25E+16,9.70E+07,5.56E+06,3.41E+12,3.23E+08
3.42E-14,3.23E-09,1.70E+07,1.70E+16,1.56E+08,8.21E+04,7.71E+09,2.90E+07
1.88E-07,7.25E-02,3.19E+07,3.19E+16,1.88E+08,2.29E+06,8.80E+11,1.65E+08
2.05E-22,9.99E-17,1.79E+07,1.79E+16,1.29E+08,0.00E+00,0.00E+00,0.00E+00
4.78E-05,8.76E+01,2.26E+07,2.26E+16,1.12E+08,4.05E+05,7.41E+11,1.24E+08
5.57E-09,3.74E-03,2.17E+07,2.17E+16,1.20E+07,4.35E+07,2.91E+13,1.66E+08
2.78E-08,7.83E-02,9.41E+06,9.40E+15,2.74E+08,6.81E+06,1.91E+13,3.51E+08
7.99E-08,9.70E-02,1.19E+07,1.19E+16,3.13E+08,5.69E+05,6.88E+11,1.19E+08
9.00E-05,2.03E+00,5.92E+07,5.92E+16,6.20E+07,7.14E+05,1.61E+10,4.00E+07
1.94E-11,1.76E-05,1.15E+06,1.15E+15,1.00E+07,6.77E+07,6.14E+13,2.98E+08
2.50E-28,3.04E-23,3.60E+07,3.60E+16,2.06E+08,4.29E+06,5.20E+11,4.10E+07
3.45E-13,7.37E-07,2.72E+07,2.72E+16,1.54E+08,4.30E+06,9.14E+12,2.22E+08
4.69E-05,1.24E+01,5.50E+07,5.50E+16,1.79E+08,5.86E+05,1.55E+11,8.20E+07
3.72E-09,1.49E-04,7.65E+07,7.65E+16,2.60E+07,5.64E+05,2.26E+10,2.00E+07
1.04E-06,7.54E-02,1.25E+07,1.25E+16,7.00E+07,1.11E+07,8.01E+11,1.75E+08
4.72E-08,6.24E-02,6.04E+07,6.04E+16,2.89E+08,9.74E+04,1.28E+11,1.28E+08
4.26E-12,3.63E-05,1.09E+07,1.09E+16,2.71E+08,3.33E+05,2.83E+12,1.83E+08
1.31E-08,6.31E-03,4.47E+07,4.47E+16,1.91E+08,4.16E+06,1.99E+12,2.00E+08
6.98E-05,8.26E+01,3.54E+07,3.53E+16,1.28E+08,1.72E+06,2.04E+12,4.71E+08
4.74E-06,1.16E+01,6.16E+06,6.16E+15,6.90E+07,4.72E+06,1.16E+13,3.91E+08
1.41E-16,6.25E-11,8.50E+06,8.50E+15,3.80E+07,1.29E+06,5.68E+11,1.35E+08
5.50E-09,8.74E-04,8.98E+06,8.98E+15,5.50E+07,2.68E+05,4.24E+10,3.90E+07
1.26E-31,7.41E-26,6.02E+07,6.02E+16,1.96E+08,1.80E+05,1.05E+11,1.50E+07
3.12E-16,2.06E-10,3.12E+07,3.12E+16,2.17E+08,3.45E+04,2.26E+10,2.20E+07
2.44E-18,3.07E-13,2.82E+07,2.82E+16,1.30E+08,2.26E+06,2.83E+11,1.40E+08
1.33E-02,1.03E+05,3.62E+06,3.62E+15,6.50E+07,9.09E+06,7.01E+13,1.25E+09
1.69E-07,1.10E-01,5.02E+07,5.02E+16,2.04E+08,1.64E+04,1.06E+10,3.80E+07
2.16E-09,8.47E-03,8.90E+06,8.90E+15,2.66E+08,5.85E+05,2.29E+12,2.49E+08
1.38E-04,2.60E+02,4.12E+07,4.12E+16,3.17E+08,1.74E+06,3.29E+12,4.95E+08
1.72E-04,2.12E+01,1.25E+07,1.25E+16,8.70E+07,2.64E+06,3.24E+11,2.30E+08
2.27E-08,3.98E-03,1.24E+07,1.24E+16,1.49E+08,2.61E+06,4.57E+11,2.83E+08
4.39E-20,1.20E-15,1.90E+07,1.90E+16,1.23E+08,1.42E+07,3.86E+11,7.30E+07
8.71E-07,3.36E-01,2.21E+07,2.21E+16,2.03E+08,2.42E+05,9.29E+10,1.47E+08
3.69E-09,2.96E-03,5.46E+07,5.46E+16,2.82E+08,4.31E+05,3.45E+11,1.54E+08
1.16E-04,7.78E+01,4.28E+07,4.28E+16,1.44E+08,8.96E+05,6.02E+11,9.00E+07
1.42E-08,1.02E-03,1.73E+07,1.73E+16,1.29E+08,5.24E+05,3.78E+10,7.80E+07
2.02E-10,2.26E-05,1.98E+07,1.98E+16,1.54E+08,1.79E+06,2.00E+11,1.94E+08
2.01E-06,7.52E+00,9.23E+06,9.23E+15,2.73E+08,4.86E+05,1.82E+12,3.58E+08
9.59E-34,7.53E-28,2.90E+07,2.90E+16,1.82E+08,6.89E+05,5.37E+11,4.40E+07
2.86E-25,1.39E-18,8.93E+06,8.93E+15,1.13E+08,2.98E+05,1.44E+12,1.31E+08
1.43E-27,8.22E-21,1.82E+07,1.82E+16,2.08E+08,7.13E+04,4.07E+11,3.30E+07
5.15E-14,7.00E-09,1.30E+07,1.30E+16,4.10E+07,2.71E+04,3.66E+09,9.00E+06
7.16E-10,1.84E-04,3.18E+05,3.18E+14,7.00E+06,1.76E+07,4.53E+12,1.52E+08
2.09E-07,1.36E-02,1.85E+07,1.85E+16,9.50E+07,4.34E+04,2.81E+09,9.00E+06
4.90E-10,1.88E-03,2.41E+07,2.41E+16,2.72E+08,1.08E+06,4.13E+12,2.25E+08
7.01E-15,1.35E-08,8.77E+06,8.77E+15,2.36E+08,6.88E+04,1.32E+11,7.00E+07
6.71E-11,1.42E-04,3.33E+07,3.33E+16,5.00E+07,5.00E+05,1.05E+12,8.90E+07
3.51E-33,5.97E-28,3.23E+07,3.23E+16,1.33E+08,0.00E+00,0.00E+00,0.00E+00
5.27E-55,6.98E-48,8.10E+06,8.10E+15,2.08E+08,2.04E+03,2.68E+10,1.70E+07
1.63E-08,5.83E-03,1.03E+07,1.03E+16,7.40E+07,1.63E+03,5.79E+08,4.00E+06
5.30E-08,6.98E-02,7.35E+07,7.35E+16,2.73E+08,1.24E+06,1.63E+12,1.74E+08
7.97E-12,1.53E-06,2.24E+07,2.24E+16,5.20E+07,7.00E+05,1.33E+11,8.40E+07
3.88E-18,1.47E-13,3.28E+07,3.28E+16,1.16E+08,0.00E+00,0.00E+00,0.00E+00
4.15E-06,1.62E+01,6.33E+06,6.33E+15,6.50E+07,1.08E+07,4.23E+13,4.41E+08
1.46E-16,8.65E-10,1.58E+07,1.58E+16,1.59E+08,1.03E+05,6.07E+11,1.60E+08
9.52E-19,9.46E-13,2.67E+07,2.67E+16,7.30E+07,1.39E+05,1.38E+11,1.60E+07
1.46E-46,7.92E-40,7.62E+06,7.62E+15,1.96E+08,8.18E+03,4.41E+10,6.00E+06
9.23E-19,1.58E-12,2.14E+07,2.14E+16,7.80E+07,5.55E+04,9.46E+10,3.50E+07
9.72E-09,6.01E-03,4.45E+07,4.45E+16,8.50E+07,6.76E+04,4.16E+10,2.50E+07
6.93E-21,1.69E-14,1.53E+07,1.53E+16,2.27E+08,6.86E+05,1.66E+12,1.43E+08
1.35E-12,4.16E-08,5.73E+07,5.73E+16,6.90E+07,2.48E+05,7.60E+09,1.00E+07
1.99E-03,5.66E+03,7.70E+06,7.70E+15,1.51E+08,3.27E+06,9.30E+12,1.04E+09
8.41E-06,7.03E+00,2.45E+07,2.45E+16,3.20E+07,8.88E+06,7.40E+12,2.07E+08
2.06E-35,1.43E-30,4.32E+07,4.32E+16,1.10E+08,0.00E+00,0.00E+00,0.00E+00
1.54E-07,9.99E-02,1.45E+07,1.45E+16,1.18E+08,1.30E+06,8.41E+11,2.32E+08
4.61E-15,2.07E-09,4.05E+07,4.05E+16,2.38E+08,8.73E+06,3.89E+12,1.31E+08

2.09E-06,2.39E+00,3.54E+07,3.54E+16,3.00E+08,3.93E+07,4.50E+13,4.14E+08
3.67E-04,1.16E+02,4.29E+07,4.29E+16,1.21E+08,4.84E+06,1.53E+12,4.24E+08
4.66E-14,3.31E-08,1.15E+07,1.15E+16,2.25E+08,5.55E+05,3.93E+11,5.80E+07
1.91E-07,9.91E-01,8.39E+06,8.39E+15,3.04E+08,1.12E+06,5.78E+12,4.86E+08
1.03E-08,3.91E-03,8.91E+06,8.91E+15,5.70E+07,6.39E+04,2.42E+10,2.00E+07
9.94E-05,1.13E+02,1.92E+07,1.92E+16,1.05E+08,1.75E+06,1.99E+12,4.63E+08
4.19E-06,5.36E+00,1.25E+07,1.25E+16,1.58E+08,2.67E+05,3.41E+11,2.35E+08
1.01E-05,2.78E+00,6.09E+07,6.09E+16,1.40E+08,8.37E+05,2.30E+11,1.21E+08
8.76E-08,1.29E-01,5.15E+07,5.15E+16,1.16E+08,1.15E+07,1.69E+13,2.48E+08
3.93E-05,6.92E+01,1.01E+07,1.01E+16,2.20E+08,7.61E+05,1.34E+12,4.59E+08
5.39E-14,4.42E-08,1.67E+07,1.67E+16,9.70E+07,1.31E+05,1.06E+11,1.08E+08
8.52E-05,1.21E+01,7.89E+07,7.89E+16,1.67E+08,2.35E+06,3.32E+11,2.68E+08
7.37E-06,5.97E-01,1.21E+07,1.21E+16,6.90E+07,7.53E+06,6.09E+11,1.27E+08
2.43E-10,1.07E-03,1.64E+07,1.64E+16,2.18E+08,1.47E+04,6.47E+10,4.40E+07
1.20E-07,1.57E-01,7.68E+07,7.68E+16,3.16E+08,2.41E+05,3.13E+11,1.81E+08
1.60E-19,6.49E-14,3.15E+07,3.15E+16,1.60E+08,0.00E+00,0.00E+00,0.00E+00
1.59E-10,6.37E-05,9.61E+06,9.61E+15,2.30E+08,3.03E+03,1.21E+09,7.00E+06
3.43E-08,1.56E-01,9.22E+06,9.22E+15,1.10E+08,2.03E+05,9.19E+11,2.58E+08
6.00E-12,6.75E-07,2.19E+07,2.19E+16,1.36E+08,2.32E+06,2.60E+11,1.18E+08
3.46E-09,4.59E-03,1.05E+07,1.05E+16,1.07E+08,3.69E+05,4.87E+11,2.12E+08
1.18E-02,2.59E+03,1.72E+07,1.72E+16,9.30E+07,2.02E+06,4.44E+11,2.13E+08
9.74E-10,6.25E-03,1.32E+07,1.32E+16,1.23E+08,2.27E+04,1.45E+11,5.50E+07
1.19E-13,6.37E-09,1.24E+07,1.24E+16,1.50E+07,2.89E+07,1.54E+12,9.90E+07
1.21E-16,1.16E-11,2.46E+07,2.46E+16,1.53E+08,0.00E+00,0.00E+00,0.00E+00
1.36E-11,3.14E-06,2.09E+07,2.09E+16,2.39E+08,2.73E+05,6.26E+10,7.80E+07
2.87E-06,4.85E-01,1.99E+07,1.99E+16,1.76E+08,2.92E+06,4.93E+11,1.34E+08
9.79E-07,1.90E-01,2.85E+07,2.85E+16,8.90E+07,2.62E+06,5.07E+11,1.94E+08
2.27E-04,2.59E+02,1.78E+06,1.78E+15,1.60E+07,2.03E+07,2.32E+13,5.67E+08
9.73E-24,1.17E-17,7.54E+02,7.54E+11,3.00E+06,1.22E+07,1.46E+13,3.93E+08
8.30E-11,2.35E-05,1.15E+07,1.15E+16,2.13E+08,2.77E+05,7.78E+10,5.90E+07
4.87E-07,2.55E-01,5.71E+06,5.71E+15,6.10E+07,4.03E+06,2.10E+12,2.11E+08
1.91E-08,1.02E-02,1.27E+07,1.27E+16,5.10E+07,4.14E+05,2.19E+11,5.80E+07
2.48E-08,7.25E-02,2.47E+07,2.47E+16,2.69E+08,2.77E+06,8.07E+12,1.76E+08
2.73E-03,6.91E+01,5.27E+07,5.27E+16,7.20E+07,5.20E+06,1.32E+11,8.90E+07
3.52E-11,2.17E-05,1.41E+07,1.41E+16,2.31E+08,3.38E+06,2.07E+12,2.33E+08
1.79E-06,1.68E-01,1.60E+07,1.60E+16,1.37E+08,9.94E+05,9.35E+10,5.30E+07
4.73E-07,1.82E-01,3.40E+07,3.40E+16,3.13E+08,9.04E+04,3.47E+10,7.30E+07
1.92E-09,9.37E-04,2.28E+07,2.28E+16,2.63E+08,1.05E+05,5.07E+10,8.90E+07
3.34E-10,6.15E-04,2.47E+07,2.47E+16,6.90E+07,5.36E+05,9.81E+11,5.40E+07
7.32E-05,4.91E+01,6.66E+07,6.66E+16,2.33E+08,1.03E+06,6.87E+11,2.31E+08
9.31E-05,2.62E+02,1.25E+07,1.25E+16,2.22E+08,4.70E+06,1.32E+13,5.07E+08
3.45E-18,4.20E-12,1.16E+07,1.16E+16,2.20E+08,1.91E+04,2.32E+10,2.00E+07
1.23E-09,2.79E-05,5.85E+07,5.85E+16,5.40E+07,4.15E+05,9.37E+09,1.60E+07
2.28E-05,2.07E+01,2.14E+07,2.14E+16,1.93E+08,4.03E+07,3.66E+13,5.38E+08
6.11E-06,7.41E-01,4.71E+07,4.71E+16,3.08E+08,1.79E+05,2.17E+10,7.30E+07
2.31E-03,4.91E+03,2.82E+07,2.82E+16,1.16E+08,2.05E+06,4.35E+12,2.65E+08
1.26E-05,3.33E+00,5.44E+07,5.44E+16,2.11E+08,9.51E+05,2.51E+11,7.60E+07
2.63E-05,1.05E+00,6.77E+07,6.77E+16,5.70E+07,6.51E+05,2.60E+10,4.20E+07
1.71E-46,1.25E-41,1.72E+07,1.72E+16,1.15E+08,0.00E+00,0.00E+00,0.00E+00
4.88E-08,6.45E-02,5.99E+07,5.99E+16,2.12E+08,2.14E+05,2.81E+11,1.69E+08
2.06E-10,1.76E-03,1.01E+07,1.01E+16,2.74E+08,1.00E+06,8.48E+12,1.46E+08
1.82E-03,8.72E+02,4.25E+07,4.25E+16,2.41E+08,3.95E+06,1.89E+12,2.18E+08
4.38E-06,5.19E+00,3.55E+07,3.55E+16,1.89E+08,1.46E+06,1.73E+12,3.53E+08
2.48E-10,6.10E-04,2.45E+05,2.45E+14,1.00E+07,9.65E+06,2.37E+13,1.81E+08
5.08E-10,2.25E-04,9.73E+06,9.72E+15,1.27E+08,2.71E+04,1.20E+10,3.90E+07
8.55E-06,1.36E+00,7.99E+06,7.99E+15,2.90E+07,1.16E+06,1.83E+11,6.00E+07
5.65E-13,3.31E-07,6.08E+07,6.08E+16,1.40E+08,6.42E+05,3.74E+11,9.30E+07
3.21E-06,2.11E+00,2.85E+07,2.85E+16,2.68E+08,3.17E+06,2.08E+12,1.80E+08
3.07E-56,3.86E-51,2.69E+07,2.69E+16,9.40E+07,0.00E+00,0.00E+00,0.00E+00
1.56E-21,1.21E-14,1.08E+07,1.08E+16,2.19E+08,1.96E+05,1.52E+12,6.20E+07
3.25E-09,2.12E-03,4.76E+07,4.76E+16,1.39E+08,3.11E+06,2.02E+12,1.16E+08
1.05E-06,4.10E+00,7.60E+06,7.60E+15,2.16E+08,1.91E+06,7.47E+12,3.73E+08
5.99E-18,1.14E-11,4.00E+07,4.00E+16,2.27E+08,9.23E+05,1.74E+12,9.00E+07
2.96E-06,3.64E-01,1.37E+07,1.37E+16,1.11E+08,1.44E+06,1.77E+11,1.52E+08
1.56E-03,2.73E+02,8.31E+06,8.31E+15,1.77E+08,5.58E+06,9.78E+11,2.62E+08
6.10E-11,1.67E-06,3.31E+07,3.31E+16,8.20E+07,1.00E+07,2.72E+11,1.15E+08
2.19E-04,8.41E+01,2.15E+07,2.15E+16,1.26E+08,7.38E+05,2.84E+11,1.81E+08
5.40E-09,4.33E-03,4.40E+07,4.40E+16,2.72E+08,1.26E+06,1.01E+12,3.69E+08
7.07E-19,4.78E-13,3.56E+07,3.56E+16,3.40E+07,2.52E+06,1.69E+12,5.90E+07
1.15E-10,8.29E-06,6.76E+06,6.76E+15,1.00E+07,1.11E+07,8.01E+11,1.28E+08
4.16E-04,4.64E+01,1.67E+07,1.66E+16,5.70E+07,5.02E+06,5.60E+11,1.72E+08
1.74E-08,6.53E-02,9.54E+06,9.54E+15,2.68E+08,2.77E+05,1.04E+12,2.11E+08
6.33E-07,4.95E-01,3.17E+07,3.17E+16,1.66E+08,5.57E+05,4.35E+11,2.15E+08
1.71E-24,8.29E-18,5.92E+06,5.92E+15,3.10E+07,2.36E+06,1.14E+13,9.70E+07
2.00E-06,1.14E+01,2.00E+07,2.00E+16,3.33E+08,2.61E+05,1.49E+12,4.10E+08

7.72E-11,1.05E-05,1.31E+07,1.31E+16,3.90E+07,1.84E+05,2.48E+10,3.40E+07
7.07E-12,1.83E-06,2.02E+07,2.02E+16,2.49E+08,1.62E+05,4.17E+10,8.10E+07
2.19E-08,1.42E-03,1.66E+07,1.66E+16,5.00E+07,1.91E+06,1.24E+11,5.60E+07
1.70E-05,6.53E+01,2.47E+07,2.47E+16,2.15E+08,6.85E+05,2.62E+12,3.68E+08
5.34E-12,1.03E-05,9.09E+06,9.08E+15,2.50E+08,3.31E+05,6.34E+11,1.82E+08
1.90E-08,4.00E-02,3.31E+07,3.31E+16,3.60E+07,7.12E+05,1.50E+12,8.10E+07
2.60E-06,4.41E-01,3.91E+07,3.91E+16,1.91E+08,1.66E+06,2.81E+11,2.10E+08
1.02E-07,1.35E+00,8.37E+06,8.37E+15,1.68E+08,9.58E+03,1.26E+11,7.20E+07
1.09E-09,3.90E-04,1.02E+07,1.02E+16,5.90E+07,2.08E+05,7.39E+10,3.20E+07
1.57E-06,2.06E+00,7.37E+07,7.37E+16,3.26E+08,5.20E+05,6.81E+11,3.03E+08
3.41E-43,6.53E-38,2.30E+07,2.30E+16,1.23E+08,0.00E+00,0.00E+00,0.00E+00
3.03E-07,1.15E-02,3.20E+07,3.20E+16,9.60E+07,0.00E+00,0.00E+00,0.00E+00
1.21E-20,4.76E-14,1.56E+07,1.56E+16,2.12E+08,3.22E+05,1.26E+12,4.90E+07
4.81E-23,2.85E-16,1.55E+07,1.55E+16,1.98E+08,1.69E+04,9.95E+10,1.60E+07
6.46E-04,6.38E+02,2.69E+07,2.68E+16,1.07E+08,1.35E+06,1.33E+12,3.20E+08
1.08E-07,5.85E-01,5.96E+06,5.96E+15,1.78E+08,3.32E+06,1.79E+13,4.51E+08
1.84E-44,3.16E-38,2.06E+07,2.06E+16,1.61E+08,0.00E+00,0.00E+00,0.00E+00
4.20E-28,2.60E-22,4.06E+07,4.06E+16,1.84E+08,2.94E+03,1.81E+09,9.00E+06
2.47E-09,6.00E-03,1.33E+07,1.33E+16,2.16E+08,2.81E+06,6.82E+12,1.91E+08
4.30E-10,1.32E-05,5.73E+07,5.73E+16,5.00E+07,4.50E+05,1.38E+10,9.00E+06
3.16E-04,8.99E+02,7.81E+06,7.81E+15,2.87E+08,8.53E+05,2.42E+12,5.66E+08
5.75E-15,4.82E-09,2.58E+07,2.58E+16,1.74E+08,7.97E+06,6.65E+12,1.32E+08
2.75E-13,1.91E-08,4.51E+07,4.51E+16,9.40E+07,3.82E+05,2.64E+10,6.40E+07
5.35E-06,3.48E+00,1.52E+07,1.52E+16,1.28E+08,5.97E+05,3.87E+11,1.35E+08
2.96E-11,1.33E-05,4.24E+07,4.24E+16,2.30E+08,3.74E+06,1.67E+12,8.90E+07
1.07E-03,1.23E+03,5.39E+07,5.39E+16,1.28E+08,2.14E+07,2.45E+13,8.01E+08
1.64E-06,5.20E-01,2.00E+07,2.00E+16,8.70E+07,2.31E+07,7.31E+12,4.09E+08
1.01E-08,7.16E-03,5.18E+06,5.18E+15,1.00E+08,6.75E+06,4.78E+12,2.61E+08
5.22E-11,2.72E-04,9.12E+06,9.11E+15,2.56E+08,2.55E+05,1.32E+12,1.10E+08
3.07E-11,1.17E-05,8.43E+06,8.43E+15,8.30E+07,3.82E+04,1.45E+10,1.20E+07
1.20E-08,1.37E-02,8.46E+06,8.46E+15,1.41E+08,1.22E+07,1.38E+13,1.84E+08
2.75E-07,3.52E-01,1.23E+07,1.22E+16,2.63E+08,5.45E+04,6.96E+10,1.05E+08
3.41E-08,9.42E-03,5.63E+07,5.62E+16,1.77E+08,5.22E+06,1.44E+12,1.09E+08
1.01E-11,1.49E-05,6.28E+07,6.28E+16,2.59E+08,3.61E+04,5.30E+10,3.90E+07
5.60E-22,9.90E-16,9.78E+06,9.78E+15,1.50E+08,2.22E+04,3.91E+10,3.00E+07
2.93E-29,2.40E-23,1.66E+07,1.66E+16,1.87E+08,2.32E+05,1.89E+11,6.70E+07
4.57E-18,6.51E-13,7.15E+07,7.15E+16,2.10E+08,1.75E+05,2.48E+10,2.10E+07
1.91E-13,1.55E-08,1.66E+07,1.66E+16,1.21E+08,2.64E+06,2.13E+11,1.15E+08
5.24E-10,2.30E-03,1.47E+07,1.46E+16,6.20E+07,1.96E+06,8.58E+12,3.99E+08
6.00E-07,7.81E-01,6.02E+05,6.02E+14,8.00E+06,7.27E+07,9.47E+13,5.59E+08
2.45E-47,9.91E-42,3.10E+07,3.10E+16,1.75E+08,6.77E+03,2.72E+09,3.00E+06
3.43E-22,1.37E-16,8.37E+06,8.37E+15,1.79E+08,3.71E+04,1.48E+10,1.50E+07
3.49E-63,1.59E-56,7.02E+06,7.02E+15,8.60E+07,1.48E+06,6.72E+12,9.70E+07
5.63E-37,6.34E-32,1.46E+07,1.46E+16,1.55E+08,5.11E+06,5.73E+11,9.10E+07
5.05E-07,6.68E-01,9.42E+06,9.42E+15,8.80E+07,1.10E+06,1.46E+12,1.43E+08
1.22E-11,2.70E-06,3.35E+07,3.35E+16,2.29E+08,1.86E+06,4.10E+11,6.90E+07
7.57E-07,4.85E+00,1.17E+07,1.17E+16,1.24E+08,6.97E+03,4.45E+10,7.80E+07
4.64E-04,2.46E+01,6.07E+07,6.07E+16,7.80E+07,1.22E+07,6.47E+11,3.01E+08
1.37E-04,1.31E+01,2.45E+07,2.45E+16,1.07E+08,4.43E+05,4.22E+10,6.50E+07
8.87E-08,2.03E-02,1.94E+07,1.94E+16,2.00E+08,1.47E+06,3.37E+11,6.00E+07
8.37E-05,1.41E+01,2.11E+07,2.11E+16,7.90E+07,1.69E+06,2.85E+11,2.41E+08
2.61E-24,5.09E-19,3.05E+07,3.05E+16,1.69E+08,0.00E+00,0.00E+00,0.00E+00
1.07E-26,1.22E-20,1.87E+07,1.87E+16,1.99E+08,1.54E+04,1.76E+10,1.30E+07
4.29E-10,5.18E-04,1.39E+07,1.39E+16,2.83E+08,2.74E+05,3.30E+11,1.93E+08
2.33E-09,6.58E-04,1.20E+07,1.20E+16,1.99E+08,3.16E+04,8.90E+09,1.90E+07
3.09E-06,1.62E+00,8.93E+06,8.93E+15,1.64E+08,8.48E+05,4.43E+11,1.62E+08
3.90E-10,2.07E-04,9.65E+06,9.65E+15,4.50E+07,2.84E+06,1.50E+12,1.26E+08
1.39E-03,4.04E+03,2.58E+07,2.58E+16,3.38E+08,2.02E+06,5.88E+12,7.61E+08
2.33E-05,5.90E-01,5.02E+07,5.02E+16,6.30E+07,1.40E+07,3.55E+11,1.24E+08
3.10E-16,1.91E-10,1.41E+07,1.41E+16,1.22E+08,7.29E+03,4.47E+09,7.00E+06
8.55E-06,8.04E-01,1.63E+07,1.63E+16,1.19E+08,7.54E+05,7.09E+10,4.60E+07
2.87E-02,1.10E+04,8.78E+06,8.78E+15,6.30E+07,2.52E+07,9.67E+12,9.14E+08
2.68E-05,1.30E+01,1.95E+07,1.95E+16,1.28E+08,3.52E+06,1.71E+12,4.04E+08
2.89E-19,5.32E-13,2.17E+07,2.17E+16,1.16E+08,4.08E+03,7.48E+09,2.30E+07
1.16E-10,7.81E-05,6.65E+07,6.65E+16,2.12E+08,1.53E+05,1.02E+11,1.09E+08
8.05E-17,2.27E-10,1.03E+07,1.03E+16,2.10E+08,4.47E+05,1.25E+12,7.40E+07
1.43E-07,1.73E-01,1.24E+07,1.24E+16,2.27E+08,6.67E+05,8.07E+11,2.39E+08
5.44E-06,1.23E-01,5.29E+07,5.29E+16,2.10E+07,6.83E+06,1.54E+11,4.70E+07
2.19E-08,1.99E-02,6.31E+07,6.31E+16,1.67E+08,5.80E+06,5.26E+12,2.29E+08
2.34E-06,2.84E-01,4.47E+07,4.47E+16,2.29E+08,2.76E+06,3.35E+11,2.51E+08
2.28E-09,4.87E-03,2.73E+07,2.73E+16,1.06E+08,4.33E+06,9.20E+12,2.23E+08
1.00E-05,2.66E+00,5.47E+07,5.47E+16,9.30E+07,5.01E+05,1.32E+11,1.27E+08
1.85E-13,7.44E-09,6.95E+07,6.95E+16,5.20E+07,1.16E+05,4.64E+09,1.40E+07
4.76E-04,3.45E+01,1.58E+07,1.58E+16,1.66E+08,4.17E+06,3.02E+11,1.55E+08
2.16E-04,2.84E+02,1.98E+07,1.98E+16,1.80E+07,3.99E+07,5.24E+13,4.89E+08

8.65E-09,7.36E-02,8.21E+06,8.21E+15,2.49E+08,2.87E+06,2.43E+13,2.84E+08
1.84E-04,8.80E+01,2.95E+07,2.95E+16,7.00E+07,1.98E+07,9.48E+12,3.32E+08
6.42E-07,7.59E-01,2.76E+07,2.76E+16,1.07E+08,8.31E+06,9.82E+12,3.26E+08
1.56E-06,3.84E+00,9.02E+06,9.02E+15,2.07E+08,2.01E+06,4.94E+12,2.61E+08
3.89E-23,1.73E-17,9.83E+06,9.83E+15,1.56E+08,0.00E+00,0.00E+00,0.00E+00
8.23E-09,1.31E-03,8.23E+06,8.23E+15,8.10E+07,9.12E+05,1.44E+11,5.80E+07
2.32E-12,1.36E-06,5.82E+07,5.82E+16,1.99E+08,3.73E+06,2.18E+12,1.57E+08
1.40E-04,9.21E+01,2.99E+07,2.99E+16,1.19E+08,1.90E+06,1.25E+12,3.88E+08
1.91E-04,2.39E+01,1.08E+07,1.08E+16,1.90E+07,2.00E+07,2.51E+12,2.57E+08
7.32E-14,5.67E-07,8.22E+06,8.22E+15,1.98E+08,2.89E+06,2.23E+13,1.41E+08
4.26E-08,2.78E-02,5.08E+07,5.07E+16,1.59E+08,3.15E+05,2.05E+11,6.80E+07
1.37E-07,5.37E-01,5.04E+06,5.03E+15,2.05E+08,3.34E+06,1.31E+13,3.03E+08
6.75E-03,1.28E+04,3.21E+07,3.21E+16,2.29E+08,6.58E+06,1.24E+13,6.19E+08
1.10E-04,1.35E+01,1.05E+07,1.05E+16,9.50E+07,4.60E+06,5.64E+11,3.14E+08
2.02E-33,3.57E-28,1.26E+07,1.26E+16,1.34E+08,0.00E+00,0.00E+00,0.00E+00
3.88E-03,1.05E+02,1.45E+07,1.45E+16,7.20E+07,3.10E+07,8.42E+11,4.94E+08
3.55E-08,1.37E-02,2.07E+07,2.07E+16,1.74E+08,1.50E+06,5.76E+11,2.29E+08
3.84E-08,3.07E-02,3.80E+07,3.80E+16,1.52E+08,1.74E+07,1.39E+13,5.48E+08
2.83E-93,1.91E-87,3.99E+07,3.99E+16,1.38E+08,0.00E+00,0.00E+00,0.00E+00
7.87E-19,5.70E-14,1.64E+07,1.64E+16,1.13E+08,0.00E+00,0.00E+00,0.00E+00
3.83E-08,4.29E-03,2.15E+07,2.15E+16,1.88E+08,9.17E+04,1.02E+10,4.20E+07
6.09E-15,2.29E-08,4.09E+06,4.09E+15,1.74E+08,5.23E+06,1.96E+13,1.90E+08
1.14E-03,8.90E+02,3.02E+07,3.01E+16,8.30E+07,2.03E+06,1.58E+12,2.99E+08
9.48E-10,4.59E-03,7.52E+06,7.52E+15,1.80E+08,1.36E+06,6.56E+12,1.74E+08
7.29E-25,4.19E-18,1.78E+07,1.78E+16,1.88E+08,2.95E+03,1.69E+10,5.00E+06
4.83E-13,6.57E-08,1.35E+07,1.35E+16,5.50E+07,6.29E+04,8.50E+09,2.40E+07
6.32E-10,1.63E-04,2.00E+07,2.00E+16,2.25E+08,1.73E+04,4.44E+09,1.30E+07
2.29E-11,1.48E-06,1.79E+07,1.79E+16,1.29E+08,5.51E+05,3.56E+10,6.00E+07
7.20E-04,2.76E+03,1.47E+07,1.47E+16,9.00E+07,1.05E+07,4.00E+13,1.37E+09
4.26E-06,8.17E+00,9.10E+06,9.10E+15,2.84E+08,3.85E+05,7.37E+11,2.66E+08
2.57E-13,5.42E-07,3.27E+07,3.27E+16,1.22E+08,7.93E+02,1.67E+09,8.00E+06
8.54E-08,1.45E-02,3.68E+07,3.68E+16,1.68E+08,3.90E+06,6.59E+11,9.80E+07
4.77E-11,6.31E-04,8.22E+06,8.22E+15,6.80E+07,7.65E+04,1.01E+12,2.01E+08
7.08E-23,2.54E-17,1.02E+07,1.02E+16,1.56E+08,3.25E+03,1.16E+09,7.00E+06
2.81E-06,3.69E+00,7.45E+07,7.45E+16,3.29E+08,1.90E+05,2.49E+11,2.35E+08
7.07E-33,1.36E-27,2.32E+07,2.32E+16,1.00E+08,0.00E+00,0.00E+00,0.00E+00
1.18E-24,2.09E-18,9.27E+06,9.27E+15,1.66E+08,2.69E+02,4.73E+08,2.00E+06
7.82E-07,7.10E-01,5.92E+07,5.92E+16,9.40E+07,1.07E+07,9.69E+12,3.89E+08
6.70E-11,1.78E-05,5.20E+07,5.20E+16,5.40E+07,2.48E+06,6.53E+11,8.70E+07
1.41E-08,1.29E-02,6.97E+07,6.97E+16,2.28E+08,5.62E+05,5.10E+11,1.90E+08
1.63E-04,4.76E+02,2.66E+07,2.66E+16,1.53E+08,1.35E+06,3.92E+12,4.70E+08
9.35E-05,8.49E+01,6.19E+07,6.19E+16,1.01E+08,8.09E+06,7.34E+12,4.60E+08
1.67E-05,2.64E+00,9.01E+06,9.01E+15,6.50E+07,1.41E+05,2.23E+10,5.50E+07
7.49E-04,5.01E+02,5.90E+07,5.90E+16,1.65E+08,7.04E+06,4.70E+12,2.59E+08
7.07E-03,8.36E+03,1.38E+07,1.38E+16,7.70E+07,2.17E+07,2.56E+13,1.22E+09
6.70E-03,1.72E+03,8.35E+06,8.35E+15,7.00E+07,1.23E+07,3.17E+12,6.37E+08
7.90E-07,4.26E+00,7.56E+06,7.55E+15,2.60E+08,2.12E+06,1.14E+13,3.97E+08
3.50E-08,1.39E-02,9.65E+06,9.65E+15,2.59E+08,6.13E+04,2.44E+10,5.50E+07
1.18E-06,1.00E+01,1.09E+07,1.09E+16,2.56E+08,5.10E+05,4.32E+12,4.02E+08
4.16E-06,2.43E+00,5.87E+07,5.87E+16,1.35E+08,3.61E+06,2.10E+12,1.38E+08
1.33E-08,1.81E-03,8.51E+06,8.51E+15,1.20E+07,3.67E+06,4.96E+11,4.90E+07
1.54E-06,9.08E+00,1.34E+07,1.34E+16,4.40E+07,1.51E+06,8.89E+12,1.97E+08
3.00E-08,1.34E-02,5.17E+07,5.17E+16,2.73E+08,7.05E+05,3.15E+11,1.41E+08
1.04E-05,1.26E+01,1.22E+07,1.22E+16,1.07E+08,1.87E+06,2.25E+12,3.51E+08
2.11E-03,4.09E+02,2.57E+07,2.57E+16,7.60E+07,5.61E+06,1.09E+12,2.40E+08
1.11E-07,1.45E-01,5.07E+07,5.07E+16,2.82E+08,2.32E+07,3.02E+13,3.16E+08
3.99E-06,7.00E-01,1.40E+07,1.40E+16,1.53E+08,1.05E+06,1.83E+11,1.74E+08
1.18E-02,2.59E+03,1.72E+07,1.72E+16,9.30E+07,2.02E+06,4.44E+11,2.13E+08
1.07E-03,1.23E+03,5.39E+07,5.39E+16,1.28E+08,2.14E+07,2.45E+13,8.01E+08
1.10E-04,1.35E+01,1.05E+07,1.05E+16,9.50E+07,4.60E+06,5.64E+11,3.14E+08

Attachment C
Test Plan for TPA SCR#523

Test Plan Name:

Tested By: Jose M. Menchaca | Date: May 04, 2005

Host Machine: SUN Ultra-4 server: Spock | Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.00f | Test Version: TPA 5.00g

Process Level (PL) Tests

PL-1. Name:
Path for run directory: ~jmench/tpa500g/
Path for archive of results: ~jmench/tpa500g/
Environment variables: setenv TPA_TEST ~/tpa500g
setenv TPA_DATA ~/tpa500g
Special input files or modifications to input files required :

Pertinent Lines in the tpa.inp file:

Special diagnostic code modifications required :

Program modes to be used (append flags, scenario/model switches, etc.): Default values

Utility scripts needed to perform the test:

Utility codes needed in the analysis of the test data: Microsoft Excel®

Test Description:

1) The szft module uses alluvium RD values for tuff RD parameters. This occurs in the interface to the *calc_rd* subroutine.

After a single vector mean value run, visual inspection of the sz_kdrd.out file shows the radionuclide specific retardation values for the alluvium are indeed different from the tuff retardation value for the same radionuclide.

PASS

2) The *actinide_kdrd.out* file needs to be recreated to supply intermediate values for alluvium parameters.

The actinide_kdrd.out file is now separated into 4 files:

sz_kdrd.out
Input and calculated values used to calculate KDs & RDs for saturated zone.

uz_kdrd.out
Input and calculated values used to calculate KDs & RDs for unsaturated zone

sz_revers.out
Input and calculated values used to calculate KDs & RDs accounting for reversibles for saturated zone

uz_revers.out
Input and calculated values used to calculate KDs & RDs accounting for reversibles for unsaturated zone

PASS

3) The input file *tpa.inp* does not have most recent values for colloid concentrations or colloid retardation factors (from SCR#484).

FAILED

9th entry for Matrix ColloidConcentration_CHnv[kg/m3] is missing an 'e' as shown below.
This was corrected in SCR552 [TPA version 5.0.0i]

```
/home/jmench{36}>grep -n "3.1[0]*[e]*-[0]*4" ~/../janetzke/tpa500*/tpa.inp
/home/jmench/../janetzke/tpa500g/tpa.inp:5362:3.10-04, 0.75
/home/jmench/../janetzke/tpa500h/tpa.inp:5362:3.10-04, 0.75
/home/jmench/../janetzke/tpa500i/tpa.inp:4232:3.10e-4, 0.75
```

```
/home/jmench/../janetzke/tpa500j/tpa.inp:4232:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500k/tpa.inp:4269:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500l/tpa.inp:4273:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500m/tpa.inp:4205:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500n/tpa.inp:4289:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500o/tpa.inp:4298:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500p/tpa.inp:4298:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500q/tpa.inp:4301:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500r/tpa.inp:4308:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500s/tpa.inp:4314:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500t/tpa.inp:4339:3.10e-4, 0.75
/home/jmench/../janetzke/tpa500u/tpa.inp:4339:3.10e-4, 0.75
>
```

4th entry for Matrix ColloidConcentration_BFw_[kg/m3] is 1.122e-6 in SCR but 1.22e-6 in tpa.inp.

```
/home/jmench{44}>grep -n 1.22e-6 ~/../janetzke/tpa500*/tpa.inp
/home/jmench/../janetzke/tpa500g/tpa.inp:5437:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500h/tpa.inp:5437:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500i/tpa.inp:4307:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500j/tpa.inp:4307:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500k/tpa.inp:4344:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500l/tpa.inp:4348:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500m/tpa.inp:4280:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500n/tpa.inp:4364:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500o/tpa.inp:4373:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500p/tpa.inp:4373:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500q/tpa.inp:4376:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500r/tpa.inp:4383:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500s/tpa.inp:4389:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500t/tpa.inp:4414:1.22e-6, 0.3
/home/jmench/../janetzke/tpa500u/tpa.inp:4414:1.22e-6, 0.3
```

No value for MatrixColloidConcentration_UFZ_ given in SCR

```
constant
MatrixColloidConcentration_UFZ_[kg/m3]
1.0e-3
```

4) The parameter AlluviumMatrixPoreRadius_SAV[m] is no longer used, but there is code in *szft.f* referencing it and it is still in *tpa.inp*.

Visual inspection of the tpa.inp files and szft.f files show that the parameter is commented out in the transition from tpa500f to tpa500g.

PASS

5) Calculations of concentfactoreoli, portionflvh, and portioneolh are incorrect in *ashremob.f*

A visual inspection of concentfactoreoli calculations in ashremob.f from tpa500f and tpa500g revealed that the iashplumerealindex was being used as the numerator instead of as an index to the real numerator, masshlweol but is now correctly implemented.

A visual inspection of portionflvh and portioneolh calculations confirms that the code has been revised according to the descriptions in the SCR.

PASS

6) Update *remob_lut.dat* file.

A visual inspection of the remob_lut.dat file confirms that it adheres to the Appendix B listing in SCR 523.

PASS

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-526	**2. Software Title and Version:** TPA 5.0.0p	**3. Project No:** 20.06002.01.354
4. Affected Software Module(s), Description of Problem(s): *dcags.f* Attachment A shows the TPA Version 4.1 and Version 5.0.1 methods for calculating dose. This corrects *dcags.f* to implement the method of Ver 5.0.1 as intended.		
5. Change Requested by: R. Benke 1-26-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 1-26-05 R. Janetzke	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment B.		
8. Implemented by: A. Lozano Albert S. Lozano	**Date:** March 3, 2005	
9. Description of Acceptance Tests: See ATTACHMENT C.		
10. Tested by: R. Nes	**Date:** April 22, 2005	

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
MODIFY FROM	dcags	AshBulkDensity[g /m3]	No change	No change	No change	No change	RB
MODIFY TO	dcags	AshBulkDensity[g /cm3]	No change	No change	No change	No change	RB

ATTACHMENT A

6.4 Modification to the Inhalation Dose Calculation in the DCAGS Module for the TPA Version 5.0.1 Code

The following change is included as part of SCR-526. A summary of the approach taken in the TPA Version 4.1j code is provided first, which is followed by the proposed change for the TPA Version 5.0.1 code. The proposed change only applies to the calculations invoked when the new flag in the TPA input file, AshEvolutionMode, is set to a value of zero.

TPA Version 4.1j Approach for Calculating the Inhalation Dose in the DCAGS Module
The inhalation dose per year (rem/yr) in DCAGS for the ith radionuclide was calculated as:

$$D_{inh,i}(t) = B \cdot I_i \cdot \eta_i \cdot f_e \cdot f_R(t) \cdot \left[(S_0 - S_\infty) \exp(-\lambda_r t) + S_\infty \right]$$

where

B = breathing rate (m^3/yr),
I_i = Inhalation-to-dose conversion factor for the ith radionuclide (rem/Ci),
f_e = occupancy factor for time fractions the individual is exposed to indoor and outdoor contaminated air (-),
$f_R(t)$ = time-dependent fraction of resuspended mass that emanated from the contaminated volcanic layer (-), equal to the ratio of the ash blanket thickness as a function of time to the thickness of the resuspendable layer, (Note: no code changes were made to this variable, and therefore, it is not described further)
η_i = activity per mass of ash for the ith radionuclide (Ci/g)
S_0 = airborne mass load above fresh ash blanket in the year following deposition (g/m^3) = AirborneMassLoadAboveFreshAshBlanket[g/m3],
S_∞ = airborne mass load at long times after the event (g/m^3) = AirborneMassLoadAboveSoil[g/m3], and
λ_r = rate of reduction of airborne mass load (1/yr) = RateOfReductionOf MassLoadingFactor[1/yr].

TPA Version 5.0.1 Approach for Calculating the Inhalation Dose in the DCAGS Module
The inhalation dose per year (rem/yr) in DCAGS for the ith radionuclide was calculated as:

$$D_{inh,i}(t) = B \cdot I_i \cdot \eta_i \cdot f_R(t) \cdot \left[C_1 \cdot \exp(-\lambda_r t) + C_2 \right]$$

with

$$C_1 = \begin{bmatrix} f_{out-H}\left(S_{ash-H} - S_{out-H}\right) + f_{out-L}\left(S_{ash-L} - S_{out-L}\right) \\ + f_{in-H} S_{in-H} + f_{in-L} S_{in-L} + f_{offsite} S_{offsite} \end{bmatrix}$$

and

$$C_2 = f_{out-H} S_{out-H} + f_{out-L} S_{out-L}$$

where

S_{ash-H} = mass load above fresh ash deposit with heavy disturbance (g/m^3) = AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3],
S_{ash-L} = mass load above fresh ash deposit with light disturbance (g/m^3) = AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3],
S_{out-H} = outdoor mass load for dust with heavy disturbance (g/m^3) = AirborneMassLoadOutsideHeavyDisturbance[g/m3],
S_{out-L} = outdoor mass load for dust with light disturbance (g/m^3) = AirborneMassLoadOutsideLightDisturbance[g/m3],
S_{in-H} = indoor mass load for dust with heavy disturbance (g/m^3) = AirborneMassLoadInsideHeavyDisturbance[g/m3],
S_{in-L} = indoor mass load for dust with light disturbance (g/m^3) = AirborneMassLoadInsideLightDisturbance[g/m3],
$S_{offsite}$ = offsite mass load (g/m^3) = AirborneMassLoadOffsite[g/m3],
f_{out-H} = fraction of time receptor spends outdoors with heavy disturbance = OccupancyFractionOutsideHeavyDisturbance[-],
f_{out-L} = fraction of time receptor spends outdoors with light disturbance = OccupancyFractionOutsideLightDisturbance[-],
f_{in-H} = fraction of time receptor spends indoors with heavy disturbance = OccupancyFractionInsideHeavyDisturbance[-],
f_{in-L} = fraction of time receptor spends indoors with light disturbance = OccupancyFractionInsideLightDisturbance[-], and
$f_{offsite}$ = fraction of time receptor spends offsite = OccupancyFractionOffsite[-].

ATTACHMENT B

6.7 Implementation of the modification to the Inhalation Dose Calculation in the DCAGS Module for the TPA Version 5.0.1 Code

[entry made by A. Lozano on March 03, 2005]

The implementation of this consists of the following changes to dcags.f.
Correction of Input parameter name

from AshBulkDensity[g/m3] to AshBulkDensity[g/cm3]

Correction to previous version. The parenthesis in the multiplication of resuspendiblefraction(it) was moved.

Original `resuspendiblefraction(it) only multiplied tmassload`

```
*(resuspendiblefraction(it)*tmassload(it)
+ massloadoutheavy*occupancyoutheavy
+ massloadoutlight*occupancyoutlight
+ massloadinheavy*occupancyinheavy
+ massloadinlight*occupancyinlight
+ massloadoffsite*occupancyoffsite)
```

Correction `resuspendiblefraction(it)multiplies all terms`

```
* resuspendiblefraction(it)* ( tmassload(it)
+ massloadoutheavy*occupancyoutheavy
+ massloadoutlight*occupancyoutlight
+ massloadinheavy*occupancyinheavy
+ massloadinlight*occupancyinlight
+ massloadoffsite*occupancyoffsite)
```

`This correction occurs in three places.`

Prior to modification moving terms from C2 to C1
C1 in the description is equal to

```
occupancyoutheavy *(massloadashheavy-massloadoutheavy)
+ occupancyoutlight *(massloadashlight-massloadoutlight)
```

and appears in the code in three places.

C2 in the description is equal to

```
massloadoutheavy*occupancyoutheavy + massloadoutlight*occupancyoutlight
+ massloadinheavy*occupancyinheavy + massloadinlight*occupancyinlight
+ massloadoffsite*occupancyoffsite)
```

`and appears in four places.`

After modification moving terms from C2 to C1n
C1 in the description prior to correction is equal to

```
occupancyoutheavy *(massloadashheavy-massloadoutheavy)
+ occupancyoutlight *(massloadashlight-massloadoutlight)+
massloadinheavy*occupancyinheavy + massloadinlight*occupancyinlight
+ massloadoffsite*occupancyoffsite)
```

and appears in the code in three places.

C2 in the description is equal to

```
massloadoutheavy*occupancyoutheavy + massloadoutlight*occupancyoutlight
```

and appears in four places.

ATTACHMENT C

Test Plan for TPA SCR#526

Test Plan Name:

Tested By: Razvan Nes, A. Lozano Date: 04-22-2005

Host Machine: Frisco Host OS: Windows 2000 Professional

Baseline Version: tpa500p Test Version: tpa500q

Process Level (PL) Tests

PL-1. Name: Modification to the inhalation dose calculation in the DCAGS module for the TPA Version 5.0.1 Code, **case 1** (receptor group 18 km from the repository)

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : the following apply to tpa500q:

- input file was set for single-realization runs
- MaximumTime[yr]: 2.0e+04
- DistanceToReceptorGroup[km] : 18
- PluvialSwitchTime[yr]:10000

Special diagnostic code modifications required :

- add print statements in *dcags.f* to print in *tpa.out* intermediate values relevant to determine if equation proposed in ATTACHMENT A was correctly implemented

Program modes to be used (append flags, scenario/model switches, etc.):

- VolcanismDisruptiveScenarioFlag: 1 (Yes)
- DirectReleaseOnlyFlag: 1 (Yes)
- SelectAppendFiles = 12, to append auxilliary output files *ashrmovo.ech* and *ashrmovo.rlt*
- AshEvolutionMode: 0 (no ashremob)

Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data: Mathematica®
Test description:

- objective: ensure that inhalation dose calculations by using dcags module in tpa500q are done as per equations proposed in PA-SCR-526
- assumptions: N/A
- constraints: PluvialSwitch and MaximumTime were chosen so that both pluvial and current climates are represented.
- output files to compare or examine: tpa.out to be compared to Mathematica® output
- step by step test procedure to be used:
  1- add print statements in *dcags.f*
  2- exercise tpa500q in single-realization runs
  3 -examine and compare the above-mentioned output files (see ATTACHMENT D) for two radionuclides.

- pass/fail criteria: pass if inhalation dose calculated by using tpa500q and Mathematica® are the same (up to round-off errors).

TestResults: -See ATTACHMENT D;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A
- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

PL-2. Name: Modification to the inhalation dose calculation in the DCAGS module for the TPA Version 5.0.1 Code, **case 2** (receptor group 5 km from the repository)

Path for run directory:
Path for archive of results:
Environment variables:
Special input files or modifications to input files required : the following apply to tpa500q:
- input file was set for single-realization runs
- MaximumTime[yr]: 2.0e+04
- DistanceToReceptorGroup[km] : 5
- PluvialSwitchTime[yr]:10000

Special diagnostic code modifications required :
- add print statements in *dcags.f* to print in *tpa.out* intermediate values relevant to determine if equation proposed in ATTACHMENT A was correctly implemented

Program modes to be used (append flags, scenario/model switches, etc.):
- VolcanismDisruptiveScenarioFlag: 1 (Yes)
- DirectReleaseOnlyFlag: 1 (Yes)
- SelectAppendFiles = 12, to append auxilliary output files *ashrmovo.ech* and *ashrmovo.rlt*
- AshEvolutionMode: 0 (no ashremob)

Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data: Mathematica®

Test description:
- objective: ensure that inhalation dose calculations by using dcags module in tpa500q are done as per equations proposed in PA-SCR-526
- assumptions: N/A
- constraints: PluvialSwitch and MaximumTime were chosen so that both pluvial and current climates are represented.
- output files to compare or examine: tpa.out to be compared to Mathematica® output
- step by step test procedure to be used:
  1- add print statements in *dcags.f*
  2- exercise tpa500q in single-realization runs
  3 -examine and compare the above-mentioned output files (see ATTACHMENT D) for two radionuclides.
- pass/fail criteria: pass if inhalation dose calculated by using tpa500q and Mathematica® are the same (up to round-off errors).

TestResults: -See ATTACHMENT D;
- disposition of output and supporting files :
- criterion 1 evidence: N/A
- criterion 2 evidence: N/A

- . . . : N/A
- overall test status (PASS/FAIL):**PASS**

ATTACHMENT D

PL-1:

Table D-1. Comparison between inhalation dose due to ^{239}Pu calculated with dcags module in tpa500q, and Mathematica® (selected calculation times between 7038.24yr (= t_{event}) and 20000.00yr)

Tpa Time Index	Time[yr]	Tpa500q Inhalation Dose [rem/yr]	Mathematica® Inhalation Dose [rem/yr]
186	7038.241213454755	6.692448616126340	6.69244861612634
196	8896.572784773836	8.730836061172312E-05	8.73083606117231E-05
206	10500.00000000000	1.638319069098443E-06	1.638319069098443E-06
216	11500.00000000000	1.392797415466986E-07	1.392797415466985E-07
226	12500.00000000000	1.212262816323998E-08	1.212262816323998E-08
236	13500.00000000000	1.100489406442298E-09	1.100489406442297E-09
246	14500.00000000000	1.070306261106676E-10	1.070306261106675E-10
256	15500.00000000000	1.148358384601988E-11	1.148358384601988E-11
266	16500.00000000000	1.383159326639798E-12	1.383159326639798E-12
276	17500.00000000000	1.858543998659552E-13	1.858543998659553E-13
286	18500.00000000000	2.716007945011353E-14	2.716007945011354E-14
296	19500.00000000000	4.191692454755144E-15	4.191692454755144E-15
301	20000.00000000000	1.668217127631820E-15	1.668217127631822E-15

Maximum relative error found after analysis of all data (see electronic files) was 9.5E-16.

Table D-2. Comparison between inhalation dose due to ^{241}Am calculated with dcags module in tpa500q, and Mathematica® (selected calculation times between 7038.24yr (= t_{event}) and 20000.00yr)

Tpa Time Index	Time[yr]	Tpa500q Inhalation Dose [rem/yr]	Mathematica® Inhalation Dose [rem/yr]
186	7038.241213454755	1.011161674645197E-02	1.011161674645197E-02
196	8896.572784773836	5.080231795745620E-07	5.080231795745619E-07
206	10500.00000000000	3.691383097213735E-08	3.691383097213734E-08
216	11500.00000000000	7.244519527902377E-09	7.244519527902376E-09
226	12500.00000000000	1.422604634328070E-09	1.42260463432807E-09
236	13500.00000000000	2.793869219076457E-10	2.793869219076456E-10
246	14500.00000000000	5.487021939861366E-11	5.487021939861366E-11
256	15500.00000000000	1.077628203449278E-11	1.077628203449278E-11
266	16500.00000000000	2.116418279887506E-12	2.116418279887504E-12
276	17500.00000000000	4.156560584023071E-13	4.156560584023072E-13
286	18500.00000000000	8.163318408150671E-14	8.16331840815067E-14
296	19500.00000000000	1.603243027087837E-14	1.603243027087837E-14
301	20000.00000000000	7.105026001055507E-15	7.10502600105551E-15

Maximum relative error found after analysis of all data (see electronic files) was 9.0E-16.

PL-2:

Table D-3. Comparison between inhalation dose due to ^{135}Cs calculated with dcags module in tpa500q, and Mathematica® (selected calculation times between 7038.24yr (= t_{event}) and 20000.00yr)

Tpa Time Index	Time[yr]	Tpa500q Inhalation Dose [rem/yr]	Mathematica® Inhalation Dose [rem/yr]
186	7038.241213454755	1.537767274384305E-06	1.537767274384305E-06
196	8896.572784773836	1.154069282005306E-11	1.154069282005306E-11
206	10500.00000000000	7.126427781277607E-14	7.126427781277609E-14
216	11500.00000000000	2.185281630423956E-15	2.185281630423956E-15
226	12500.00000000000	6.701051285209618E-17	6.701051285209618E-17
236	13500.00000000000	2.054842163218013E-18	2.054842163218013E-18
246	14500.00000000000	6.301065513493379E-20	6.301065513493381E-20
256	15500.00000000000	1.932188628208677E-21	1.932188628208676E-21
266	16500.00000000000	5.924954893714656E-23	5.924954893714652E-23
276	17500.00000000000	1.816856283079308E-24	1.816856283079309E-24
286	18500.00000000000	5.571294317981237E-26	5.57129431798124E-26
296	19500.00000000000	1.708408125983576E-27	1.708408125983577E-27
301	20000.00000000000	2.991640416335118E-28	2.991640416335118E-28

Maximum relative error found after analysis of all data (see electronic files) was 1.1E-15.

Table D-4. Comparison between inhalation dose due to ^{246}Cm calculated with dcags module in tpa500q, and Mathematica® (selected calculation times between 7038.24yr (= t_{event}) and 20000.00yr)

Tpa Time Index	Time[yr]	Tpa500q Inhalation Dose [rem/yr]	Mathematica® Inhalation Dose [rem/yr]
186	7038.241213454755	1.295226843351960E-02	1.29522684335196E-02
196	8896.572784773836	2.716457869159650E-06	2.71645786915965E-06
206	10500.00000000000	2.968725387187380E-07	2.968725387187379E-07
216	11500.00000000000	5.463775643969926E-08	5.463775643969925E-08
226	12500.00000000000	1.005577828669498E-08	1.005577828669498E-08
236	13500.00000000000	1.850710635652937E-09	1.850710635652936E-09
246	14500.00000000000	3.406131041543311E-10	3.406131041543311E-10
256	15500.00000000000	6.268796671215871E-11	6.268796671215867E-11
266	16500.00000000000	1.153737517017001E-11	1.153737517017001E-11
276	17500.00000000000	2.123390385725142E-12	2.123390385725143E-12
286	18500.00000000000	3.907983110272320E-13	3.907983110272322E-13
296	19500.00000000000	7.192427776279215E-14	7.192427776279215E-14
301	20000.00000000000	3.085580812916006E-14	3.085580812916006E-15

Maximum relative error found after analysis of all data (see electronic files) was 9.4E-16.

1. SCR No. (*Software Developer Assigns*): PA-SCR-528	2. Software Title and Version: TPA 5.0.0q	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *gnewdf.dat, dcagw.f, dcags.f, tpa.inp*

NRC has requested implementation of the capability to use an alternate set of dose coefficients from ICRP Publication 72 (International Commission on Radiological Protection, 1996). This change is necessary to allow dose calculations to be conducted using more advanced internal dosimetry modeling (in ICPR Publication 72) than dosimetry methods currently used in the TPA code that are based on Federal Guidance Report 11 (Environmental Protection Agency, 1988) (which, in turn, is consistent with ICRP Publications 26 and 30). This change will allow selection of either the existing Federal Guidance 11 dosimetry approach and or the newer ICRP 72 approach for all TPA dose calculations in DCAGW and DCAGS.

References are included in Attachment 1.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
P. LaPlante 1-20-05	R. Janetzke Date: 1-24-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See Attachment 1.

8. Implemented by:	Date:
Ron Janetzke	4-15-05

9. Description of Acceptance Tests:

See Attachment 2.

Because the dose coefficient changes will be implemented in SCR-552, no testing is done for Item #1.

10. Tested by:	Date:
O. Osidele	4-29-05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description** **1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton** **1. site references (journals, sci. notebooks, publishings)** **2. is uncertainty covered by the distribution / range ?** **3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
MODIFY FROM	dcagw, dcags	ReceptorAgeGroup(1=Nfnt,2Tod, 3PTeen,4Teen,5Adlt,6AdltFGR11)	Flag to select the receptor age group for analysis.	Iconstant	1-6		PL
MODIFY TO	dcagw, dcags	InternalAdultDosimetry(1-4=reserved,5=ICRP72,6=FGR11)	Flag to select dosimetry standard.	Iconstant	5-6	ICRP 72, FGR11	PL

DELETE		DrinkingWaterConsumptionRate1[L/yr]		lognormal	12.0, 670.0	Option removed from code.	PL
DELETE		LeafyVegetableConsumptionRate1[kg/yr]		constant	0.0	Option removed from code.	PL
DELETE		OtherVegetableConsumptionRate1[kg/yr]		constant	0.0	Option removed from code.	PL
DELETE		FruitConsumptionRate1[kg/yr]		constant	0.0	Option removed from code.	PL
DELETE		GrainConsumptionRate1[kg/yr]		constant	0.0	Option removed from code.	PL
DELETE		BeefConsumptionRate1[kg/yr]		constant	0.0	Option removed from code.	PL
DELETE		PoultryConsumptionRate1[kg/yr]		constant	0.0	Option removed from code.	PL
DELETE		MilkConsumptionRate1[kg/yr]		constant	226.0	Option removed from code.	PL
DELETE		EggConsumptionRate1[kg/yr]		constant	0.0	Option removed from code.	PL
DELETE		InhalationExposureTime1[hr]		constant	4563.0	Option removed from code.	PL

DELETE		InhalationRate1[cm3/s]		constant	52.0	Option removed from code.	PL
DELETE		SoilContaminationExposureTime1[hr]		constant	2770.0	Option removed from code.	PL
DELETE		DrinkingWaterConsumptionRate2[L/yr]		lognormal	50.0, 1240.0	Option removed from code.	PL
DELETE		LeafyVegetableConsumptionRate2[kg/yr]		constant	3.5	Option removed from code.	PL
DELETE		OtherVegetableConsumptionRate2[kg/yr]		constant	16.0	Option removed from code.	PL
DELETE		FruitConsumptionRate2[kg/yr]		constant	48.0	Option removed from code.	PL
DELETE		GrainConsumptionRate2[kg/yr]		constant	30.0	Option removed from code.	PL
DELETE		BeefConsumptionRate2[kg/yr]		constant	4.0	Option removed from code.	PL
DELETE		PoultryConsumptionRate2[kg/yr]		constant	3.0	Option removed from code.	PL

DELETE		MilkConsumptionRate2[kg/yr]		constant	127.0	Option removed from code.	PL
DELETE		EggConsumptionRate2[kg/yr]		constant	1.0	Option removed from code.	PL
DELETE		InhalationExposureTime2[hr]		constant	4790.0	Option removed from code.	PL
DELETE		InhalationRate2[cm3/s]		constant	88.0	Option removed from code.	PL
DELETE		SoilContaminationExposureTime2[hr]		constant	2620.0	Option removed from code.	PL
DELETE		DrinkingWaterConsumptionRate3[L/yr]		lognormal	50.0, 1240.0	Option removed from code.	PL
DELETE		LeafyVegetableConsumptionRate3[kg/yr]		constant	4.8	Option removed from code.	PL
DELETE		OtherVegetableConsumptionRate3[kg/yr]		constant	22.0	Option removed from code.	PL
DELETE		FruitConsumptionRate3[kg/yr]		constant	52.0	Option removed from code.	PL

DELETE		GrainConsumptionRate3[kg/yr]		constant	49.0	Option removed from code.	PL
DELETE		BeefConsumptionRate3[kg/yr]		constant	6.0	Option removed from code.	PL
DELETE		PoultryConsumptionRate3[kg/yr]		constant	5.0	Option removed from code.	PL
DELETE		MilkConsumptionRate3[kg/yr]		constant	160.0	Option removed from code.	PL
DELETE		EggConsumptionRate3[kg/yr]		constant	2.0	Option removed from code.	PL
DELETE		InhalationExposureTime3[hr]		constant	4840.0	Option removed from code.	PL
DELETE		InhalationRate3[cm3/s]		constant	139.0	Option removed from code.	PL
DELETE		SoilContaminationExposureTime3[hr]		constant	3500.0	Option removed from code.	PL
DELETE		DrinkingWaterConsumptionRate4[L/yr]		lognormal	55.0, 1850.0	Option removed from code.	PL
DELETE		LeafyVegetableConsumptionRate4[kg/yr]		constant	6.6	Option removed from code.	PL

DELETE		OtherVegetableConsumptionRate4[kg/yr]		constant	30.0	Option removed from code.	PL
DELETE		FruitConsumptionRate4[kg/yr]		constant	58.0	Option removed from code.	PL
DELETE		GrainConsumptionRate4[kg/yr]		constant	56.0	Option removed from code.	PL
DELETE		BeefConsumptionRate4[kg/yr]		constant	10.0	Option removed from code.	PL
DELETE		PoultryConsumptionRate4[kg/yr]		constant	5.0	Option removed from code.	PL
DELETE		MilkConsumptionRate4[kg/yr]		constant	143.0	Option removed from code.	PL
DELETE		EggConsumptionRate4[kg/yr]		constant	2.0	Option removed from code.	PL
DELETE		InhalationExposureTime4[hr]		constant	4690.0	Option removed from code.	PL
DELETE		InhalationRate4[cm3/s]		constant	185.0	Option removed from code.	PL
DELETE		SoilContaminationExposureTime4[hr]		constant	3310.0	Option removed from code.	PL

MODIFY FROM		DrinkingWaterConsumptionRate5[L/yr]		lognormal	95.0, 2380.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY TO		DrinkingWaterConsumptionRate5[L/yr]		constant	730.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY FROM		LeafyVegetableConsumptionRate5[kg/yr]		constant	8.9	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL

MODIFY TO		LeafyVegetableConsumptionRate5[kg/yr]		constant	15.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY FROM		OtherVegetableConsumptionRate5[kg/yr]		constant	41.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY TO		OtherVegetableConsumptionRate5[kg/yr]		constant	7.8	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL

MODIFY FROM		FruitConsumption Rate5[kg/yr]		constant	52.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY TO		FruitConsumption Rate5[kg/yr]		constant	16.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY FROM		GrainConsumption Rate5[kg/yr]		constant	50.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL

MODIFY TO		GrainConsumption Rate5[kg/yr]		constant	0.48	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY FROM		BeefConsumption Rate5[kg/yr]		constant	12.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY TO		BeefConsumptionRate5[kg/yr]		constant	2.9	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL

MODIFY FROM		PoultryConsumptionRate5[kg/yr]		constant	6.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY TO		PoultryConsumptionRate5[kg/yr]		constant	0.8	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY FROM		MilkConsumptionRate5[kg/yr]		constant	74.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL

MODIFY TO		MilkConsumption Rate5[kg/yr]		constant	4.1	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY FROM		EggConsumptionRate5[kg/yr]		constant	2.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY TO		EggConsumptionRate5[kg/yr]		constant	6.7	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL

MODIFY FROM		Inhalation ExposureTime5[hr]		constant	6910.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY TO		Inhalation ExposureTime5[hr]		constant	4200.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY FROM		Inhalation Rate5[cm3/s]		constant	176.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL

MODIFY TO		InhalationRate5[cm3/s]		constant	270.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY FROM		SoilContaminationExposureTime5[hr]		constant	3830.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL
MODIFY TO		SoilContaminationExposureTime5[hr]		constant	1800.0	Convert the existing ICRP 72 dose calculation input parameters to parameters that are more specific to YM-specific adult dose calculations.	PL

Attachment 1
Detailed Description of Changes for SCR-528

1. Change existing data in the ICRP inhalation dose coefficient column of the TPA GENTPA data file gnewdf.dat. The existing column contains maximum values selected from ICRP Publication 72 (International Commission on Radiological Protection, 1996). Supporting documentation for the ICRP 72 coefficients will be reviewed and a new set of dose coefficients for inhalation exposure will be selected. The intent of the data change is to select values that are the most applicable to the expected YM exposure conditions assumed for dose calculations (rather than merely selecting the values that are the most conservative due to large uncertainties). Specific considerations for selection can include chemical form of transported contaminants in the biosphere and the weight of available and applicable data evaluated by ICRP. Also, verify the correct values for ingestion coefficients from ICRP 72 are also included in gnewdf.dat. The new/verified data values are provided in the attached file (gnewdf.dat).

2. Delete all pre-adult age dependent input parameters for GENTPA calculations from tpa.inp. These parameters were used to provide testing capabilities prior to finalization of 10 CFR Part 63. The final regulations in 10 CFR Part 63 specify that adult dosimetry be used for YM calculations. Therefore the capability to conduct age-dependent dose calculations is no longer needed. This change will also allow focusing the code functionality regarding ICRP 72 calculations on selection of the type of dose coefficients (i.e., ICRP vs Federal Guidance Report 11 (Environmental Protection Agency, 1988)) rather than the age of receptor (i.e., age dependent vs adult). Identification of the parameters that should be deleted is included in the comments column of the attached spreadsheet (DOSE3. GENTPA.comments.xls).

3. Change the values for adult:ICRP72 labeled parameters in tpa.inp to match the values for the same parameters identified for adult:FGR11/12. This is necessary to convert the existing ICRP 72 dose calculation input parameters, previously derived from data sources optimized to enhance analysis of age-dependent differences in dosimetry (i.e., most age-dependent parameters selected from the same data source) to parameters that are more specific to YM-specific adult dose calculations. The specific parameter changes are identified in the comments column of the attached spreadsheet (DOSE3. GENTPA.comments.xls).

4. Change the name of the tpa.inp parameter

ReceptorAgeGroup(1=Nfnt,2=Tod,3=PTeen,4=Teen,5=Adlt,6=AdltFGR11)

to

InternalAdultDosimetry(1--4 reserved, 5=ICRP72, 6=FGR11)

This change is related to item 2 above and is necessary to ensure consistency with regulations in 10 CFR Part 63, specifying adult dose calculations, and to thereby to redirect the existing TPA functionality to the selection of the dosimetry approach and data source rather than selection of age-dependent receptor calculations.

5. Correct a parameter transfer problem that was identified during the scoping work for this SCR. Prior implementation of DCAGW calculations using GENTPA relied on an input parameter from tpa.inp called AirborneMassLoadAboveSoil[g/m3]. Although this parameter is specified in tpa.inp under the DCAGS heading, the parameter was also used in DCAGW calculations for inhalation of resuspended soil contaminated by irrigation with groundwater. During execution this parameter is written to the GENTPA ggenii.inp formatted input file (Exposure section, Inhalation subsection, Mass loading factor (g/m3) parameter) prior to its use in executing DCAGW. Prior changes made to DCAGS input parameters has eliminated the need for the AirborneMassLoadAboveSoil[g/m3] parameter in DCAGS, therefore, an alternate means of providing a value for this parameter for use in DCAGW is needed. Because inhalation of resuspended irrigated soil is not considered to be an important pathway in the TPA dose calculations, it is recommended a constant reasonable value of 1.0E-4 g/m3 be used. This value for mass loading is recommended for decommissioning dose analyses by Kennedy and Strenge (1992) based on a review of various field measurements (including arid locations).

The resolution will include editing the GENTPA ggenii.def data file to enter the aforementioned constant value for this parameter 1.0E-4 g/m3 in the Exposure section of the ggenii.def file under Inhalation heading and in the appropriate space for the Mass loading factor (g/m3) input parameter. Similarly, the portion of the TPA code that handles the transfer of the AirborneMassLoadAboveSoil[g/m3] parameter information and overwrites the value to ggenii.inp needs to be rendered inoperable so that the newly entered value in ggenii.def is not overwritten when the code executes (i.e., fixed values in ggenii.def that are not overwritten by tpa.inp parameters remain as valid inputs when the information is transferred to ggenii.inp prior to GENTPA execution).

References:

Kennedy, W.E., and D.L. Strenge. NUREG/CR-5512, Vol. 1, "Residual Radioactive Contamination From Decommissioning: Technical Basis for Translating Contamination Levels to Annual Total Effective Dose Equivalent ." Washington, DC: U.S. Nuclear Regulatory Commission. October, 1992.

International Commission on Radiological Protection. Age-Dependent Doses to Members of the Public from Intake of Radionuclides. Part 5: Compilation of Ingestion and Inhalation Dose Coefficients. ICRP 72. Annals of the ICRP. Tarrytown, NY: Elsevier Science Inc. 1996.

Environmental Protection Agency. Limiting Values of Radionuclide Intakes and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion: Federal Guidance Report No. 11. EPA 520/1-88-020. Washington DC: Environmental Protection Agency. September, 1988.

Attachment 2

Test Plan for TPA SCR#528

Tested by: Olufemi Osidele | Date: April 22, 2005

Host Machine: SUN Ultra-4 server: Spock | Host OS: Sun Solaris 5.9

Baseline Version: 5.0.0r | Test Version: 5.0.0s

General Remarks

Directory path for codes: base version: ~oosidele/tpa500r
test version: ~oosidele/tpa500s

Environment variables: base version: setenv TPA_TEST ~/tpa500r
setenv TPA_DATA ~/tpa500r
test version: setenv TPA_TEST ~/tpa500s
setenv TPA_DATA ~/tpa500s

Special diagnostic code modifications required :

For test item 5, source code file *dcagw.f* was modified to execute the lines of code commented out under change item 5 (see Description of Changes, above). The lines of code to be modified are enclosed with tags `SCR 528 test` in the attached file *dcagw_test.f*. The modified code is in the attached file *dcagw_test5.f*.

Test Description

All referenced test results files are on the attached CD titled: *"Test Results for SCR#528"*.

1. <u>Dose coefficients</u>

   Objective: To update dose coefficients for inhalation exposure based on ICRP Publication 72 (update *gnewdf.dat* file).

   Test status: Not tested because dose coefficient update will be performed as SCR 552.

2. <u>Age-dependent input parameters for GENTPA</u>

   Objective: To delete pre-adult age dependent input parameters for GENTPA calculations from *tpa.inp*.

Affected module(s): DCAGW, DACGS

Assumptions: None

Output files to compare or examine: None.

Test procedure:

(i) Compare contents of *tpa.inp* in the test and base versions using the command:
```
diff tpa500s/tpa.inp tpa500r/tpa.inp
```
(ii) Examine the `gentpa` section of the *tpa.inp* files compared in step (i).

Pass/Fail criterion(ia):

Results should show that the input parameters in the base version are commented in the test version of *tpa.inp*.

Test results:

See screen output of comparison results in file *diff_tpainp.out*, showing lines that differ between the test and base versions of *tpa.inp*. Lines from the test file start with "<", and lines from the base file start with ">". Four pre-adult receptor age group parameters contain index numbers **1** through **4**. Parameters for these age groups are commented out (with "**") in the test file. (See files *tpa_test.inp* and *tpa_base.inp* for the files compared)

Test status: **PASS.**

3. <u>Adult group input parameters for GENTPA</u>

Objective: To change the values of adult parameters derived from ICRP72 in *tpa.inp* to match with corresponding values derived from FGR11/12.

Affected module(s): DCAGW, DACGS

Assumptions: None

Output files to compare or examine: None.

Test procedure:

(i) Compare contents of *tpa.inp* in the test and base versions using the command:
```
diff tpa500s/tpa.inp tpa500r/tpa.inp
```
(ii) Examine the `gentpa` section of the *tpa.inp* files compared in step (i).

Pass/Fail criterion(ia):

Results should show that the adult ICRP72 derived input parameters in the test version of *tpa.inp* are the same as the corresponding FGR11/12 values.

Test results:

See screen output of comparison results in file *diff_tpainp.out*. The adult receptor age group parameters derived from ICRP72 contain index number **5**; corresponding parameters from FGR11/12 contain index number **6**. In the test version (see *tpa_test.inp*), the adult ICRP72 parameters are commented (with "`**`") and redefined with values equal to the FGR11/12 derived values.

Test status: **PASS**

4. Receptor age group parameter

Objective: To rename the receptor age group parameter in *tpa.inp*.

Affected module(s): DCAGW, DACGS

Assumptions: None

Output files to compare or examine: None.

Test procedure:

(i) Compare contents of *tpa.inp* in the test and base versions using the command:

```
diff tpa500s/tpa.inp tpa500r/tpa.inp
```

(ii) Examine the *dcagw.f* and *dcags.f* files for code changes.

Pass/Fail criterion(ia):

Results should show that the receptor age group parameter has been renamed as requested.

Test results:

See screen output of comparison results in file *diff_tpainp.out*. The parameter `ReceptorAgeGroup(...)` in the base version of *tpa.inp* is replaced with `InternalAdultDosimetry(...)` in the test version. Changes also implemented in source codes (see files *dcagw_test.f* and *dcags_test.f*).

Test status: **PASS**

5. Mass loading parameter

Objective: To set a constant value of 1.0E-4 g/m3 for the airborne mass loading parameter for use in DCAGW only.

Affected module(s): DCAGW

Assumptions: None

Output files to compare or examine: *ggenii.inp*

Test procedure:

(i) Examine *ggenii.def* in the test version (`Exposure` section, `Inhalation` subsection, `Mass loading factor (g/m3)` parameter);
(ii) Run the test version (*~oosidele/tpa500s/tpa.e*) for one realization;
(iii) Examine the mass loading factor written to *ggenii.inp*.
(iv) Remove comments used in disabling transfer of mass load parameter from the DCAGS module; re-run the test version;
(v) Compare mass loading factor in *ggenii.inp* with the value obtained in step (iii).

Pass/Fail criterion(ia):

The mass loading parameter in *ggenii.def* should be 1.0E-4 g/m3. This value should be written to *ggenii.inp* in step (ii), but overwritten in step (iv).

Test results:

A value of `.0001` is assigned to the `Mass loading factor (g/m3)` parameter (see `Exposure` section, `Inhalation` subsection in file *ggenii_test5.def*). The same value is written to *ggenii_test5_step2.inp* in step (ii), but overwritten by `0.000000` in *ggenii_test5_step4.inp*.

Test status: **PASS**

1. SCR No. (*Software Developer Assigns*): PA-SCR-529	2. Software Title and Version: TPA 5.0.0v	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *exec.f, szft.f, tpa.inp, subarea.f*

1) *Szft.f* does not permit the running of the saturated zone NEFTRAN run with separate legs for each geologic zone (STFF, SAV).
2) optional - *Uzft.f* does not permit the running of the unsaturated zone NEFTRAN with a composite layer separate from a matrix flow layer. Matrix diffusion should be an option for the multi-NEFTRAN run approach for the UZ.
3) When a subarea has zero waste packages, a divide by zero occurs.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
T. McCartin 3-1-05	R. Janetzke Date: 3-4-05 R. Janetzke

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

1) Parameter **SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)** was added to the *tpa.inp* file to indicate the special running of NEFMKS for the *szft.f* module to run the STFF leg first and then the SAV leg as separate NEFMKS runs. Routines **prenefmksaTUFF** and **prenefmksaALLUV** were added to *szft.f* to prepare the NEFMKS input file for the special runs. A new intermediate array (**ciperyrinsaintoalluv**) is used for this case as a transfer mechanism to supply the output of the STFF leg to the input of the SAV leg. The **prenefmksaTUFF** and **prenefmksaALLUV** routines are copies of the **prenefmksa** routine with some tailoring to make them specific to the associated leg (especially in the areas where leg parameters are indexed in an array and where error statements were made unique to their individual routines). When the separate run mode is selected several new files are created to store the intermediate output values. (*nefiituff.** and *nefiialluv.** with file name extensions of *.cum, .dis, .inp, .out, .src,* and *.vel*).
2) This option was declined.
3) A simple error check was put in *subarea.f* subroutine **ssadba**().

8. Implemented by: R. Janetzke	Date:
T. McCartin / R. Janetzke	5-5-05 / 5-12-05

9. Description of Acceptance Tests:

See Attachment A.

10. Tested by:	Date:
O. Osidele Olu Osidele	11-03-05

SCR529 UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)
ADD	SZFT	**SeparateNEFMKSRunsForSTFFandSAV(0=no, 1=yes)**	Selects one of two operational modes for the saturated zone flow and transport calculations. To run SZFT in the original normal mode, set = 0. To run SZFT in the new mode where each leg uses a separate NEFMKS run then set =1. Under certain combinations of parameter values this mode can run faster than the original mode.	iconstant	0	Normal mode is to be used unless special conditions arise that, in the determination of the analyst, requires separate runs for the saturated zone legs.	TJM

Attachment A

Test Plan for TPA SCR 529

Test Plan Name:

Tested By: Olufemi Osidele

Date: November 3, 2005

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.9

Baseline Version: 5.0.0v

Test Version: 5.0.0w

Tests

1. Include options to run NEFTRAN once for the entire saturated zone combining tuff (STFF) and alluvium (SAV) legs, or twice with separate runs for STFF and SAV. The input parameter `SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)` is set in *tpa.inp* to indicate the desired option.

Paths for run directory: home/oosidele/runSCR529sep0
home/oosidele/runSCR529sep1

Path for archive of results: home/oosidele/runSCR529sep0
home/oosidele/runSCR529sep1
Results also archived on CD titled "*Test Plan for SCR 529*" in sub-directories ~/runSCR529sep0 and ~/runSCR529sep1 respectively

Environment variables: TPA_TEST=/home/oosidele/tpa500w
TPA_DATA=/home/oosidele/tpa500w

Special input files or modifications to input files required: None

Special diagnostic code modifications required: None

Program modes to be used (append flags, scenario/model switches, etc.):
Output Print Options set in *tpa.inp* to append all output files.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: - objective: To test the implementation of option set in *tpa.inp* by the parameter `SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)`.
- assumptions: None
- constraints: None
- output files to compare or examine: *nefii*.cum, nefii*.dis, nefii*.inp, nefii*.out, nefii*.src, nefii*.vel*

- step by step test procedure to be used

1) Examine code modifications in */home/oosidele/tpa500w/szft.f*
2) Run the test version (*/home/oosidele/tpa500w/tpa.e*) with the `SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)` parameter set to `0`, for a single NEFTRAN run comprising both STFF and SAV legs
3) Set `SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)` to `1`, indicating two separate NEFTRAN runs, one for STFF and the other for SAV parameter set. Rerun the test version.
4) Examine the run directories and compare the NEFTRAN output files for the saturated zone created by steps 2) and 3) above.

- pass fail criteria

1) NEFTRAN output files created in step 2) should be *nefiisz.cum*, *nefiisz.dis*, *nefiisz.inp*, *nefiisz.out*, *nefiisz.src*, and *nefiisz.vel*.
2) NEFTRAN output files in step 3) should be *nefiituff.cum*, *nefiituff.dis*, *nefiituff.inp*, *nefiituff.out*, *nefiituff.src*, *nefiituff.vel* for STFF, and *nefiialluv.cum*, *nefiialluv.dis*, *nefiialluv.inp*, *nefiialluv.out*, *nefiialluv.src*, *nefiialluv.vel* for SAV.

Test Results:

Test results are archived in the CD titled "*Test Plan for SCR 529*". Sub-directories ~/runSCR529sep0 and ~/runSCR529sep1 contain the run directories and results for steps 2) and 3) respectively. The run directories show that the appropriate NEFTRAN output files were created for the selected options.

Overall test status: **PASS**

2. Error check to prevent division by zero when a subarea has no waste packages.

Paths for run directory: home/oosidele/runSCR529zeroWP

Path for archive of results: home/oosidele/runSCR529zeroWP
Results also archived on CD titled "*Test Plan for SCR 529*" in sub-directory ~/runSCR529zeroWP

Environment variables: TPA_TEST=/home/oosidele/tpa500w
TPA_DATA=/home/oosidele/tpa500w

Special input files or modifications to input files required: None

Special diagnostic code modifications required:
Subroutine ssadba() in *subarea.f* modified as follows to force zero waste package in subarea 5

```
c       SCR 529 test O.Osidele Oct 31 2005
        nwppersa(5) = 0.0d0
c       end SCR 529 test
```

This diagnostic modification is archived in *~/runSCR529zeroWP/subarea_mod.f* on the CD titled "*Test Plan for SCR 529*" .

Program modes to be used (append flags, scenario/model switches, etc.): None.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: - objective: To test the error check that prevents division by zero when a subarea has no waste packages..
- assumptions: None
- constraints: None
- output files to compare or examine: None
- step by step test procedure to be used
  1) Examine code modifications in */home/oosidele/tpa500w/subarea.f.*
  2) Activate the special diagnostic code modifications and recompile.
  3) Run the recompiled test version.
  4) Observe the output to screen.
- pass fail criterion
  The program should abort with an error message indicating that the subarea has zero waste packages.

Test Results:

Test results are archived in the CD titled "*Test Plan for SCR 529*". Sub-directory ~/runSCR529zeroWP contains the run directory and results for step 3). The run stopped appropriately at the point of error. The error message in the screen dump file *tpa.out* reports that subarea 5 (set to zero waste package by the diagnostic code modification) has zero waste.

Overall test status: **PASS**

1. SCR No. (*Software Developer Assigns*): PA-SCR-530	2. Software Title and Version: TPA 5.0.0m	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *reader.f, maxntime.i, nintv.i, reflux2.i, seisadj.i, uz_parms.i, wpflow.def, climato2.dat, failtadj.i, SIZES.INC, nefmks.f.exec.f, nfenv.f, uzft.f, tpa.inp, and tpanames.dbs*

TPA simulation times are not accepted beyond 100,000 years.

5. Change Requested by: S. Mohanty 1-19-05	6. Change Authorized by (*Software Developer*): R. Janetzke Date: 2-4-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The TPA Version 5.0.0m code was modified to enable long simulations. That is code modifications allowed, simulation times greater than 100,000 years and 301 time steps, which are the TPA Version 5.0.0m code maximum time and number of time steps.

See Attachment 1for a complete description of these modifications.

8. Implemented by: R. Rice	Date: 3-11-05

9. Description of Acceptance Tests:

SCR # 530 was tested in accordance with the Test Plan described in Attachment 2. Three out of six tests failed. All original/modified source code files, all executables, and all input/output files from testing are contained on the CD(s) titled TPA SCR # 530 - Test Directories.

10. Tested by: C. Scherer	Date: 5-2-2005

CNWRA Form TOP-5 (05/2000)

SCR530 UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
20 to 22	General	aqueousnuclides	number of aqueous (groundwater) nuclides	-	-		
3 Cm245 Am241 Np237 to 5 Cm245 Am241 Np237 U233 Th229	General	** chain 2	added U233 and Th229 because they may be important at times greater than 100,000 years	-	-		

11 to 13	General	colloidalnuclides	number of colloidal aqueous (groundwater) nuclides	-	-		
3 Jc245 Ja241 Np237 to 5 Jc245 Ja241 Np237 U233 Jt229	General	** colloidal chain 2	because U233 and Th229 were added, needed to add the colloid Jt229, and then its parent, U233, to this chain	-	-		
1.0e4 to 1.0e6	General	MaximumTime[yr]	maximum simulation time	-	-		
100 to 4800	General	NumberOfTimeStepsAfterCompliancePeriod	number of time steps after 10,000 year compliance period	-	-		
NEW	EBSREL	GapFractionForU233	percent of U233 inventory contained in the gap (i.e., instant fraction released)	CONSTANT	0.0		

NEW	EBSREL	GapFractionForTH229	percent of Th229 inventory contained in the gap (i.e., instant fraction released)	CONSTANT	0.0		
NEW	EBSREL	ColloidReleaseFactor_Jt229[]	fraction of Jt229 in the colloid (rest is in the aqueous phase)	CONSTANT	0.9		
MODIFIED FROM CONSTANT = 0.0 VALUES	UZFT	MatrixKD_TSw_Cm[m3/kg]	Matrix KD for Cm in the TSw unit	LOGNORMAL	1760., 73663.	Per email from P. Bertetti that stated Cm values/ distributions for matrix Kds should be equal to Am values/ distributions from TPA 4.1jpd	
MODIFIED FROM CONSTANT = 0.0 VALUES	UZFT	MatrixKD_CHnv Cm[m3/kg]	Matrix KD for Cm in the CHnv unit	LOGNORMAL	5340., 223529.	Per email from P. Bertetti that stated Cm values/ distributions for matrix Kds should be equal to Am values/ distributions from TPA 4.1jpd	
MODIFIED FROM CONSTANT = 0.0 VALUES	UZFT	MatrixKD_CHnz Cm[m3/kg]	Matrix KD for Cm in the CHnz unit	LOGNORMAL	4855., 203209.	Per email from P. Bertetti that stated Cm values/ distributions for matrix Kds should be equal to Am values/ distributions from TPA 4.1jpd	

MODIFIED FROM CONSTANT = 0.0 VALUES	UZFT	MatrixKD_PPw_ Cm[m3/kg]	Matrix KD for Cm in the PPw unit	LOGNOR MAL	4005., 16764 7.	Per email from P. Bertetti that stated Cm values/ distributions for matrix Kds should be equal to Am values/ distributions from TPA 4.1jpd	
MODIFIED FROM CONSTANT = 0.0 VALUES	UZFT	MatrixKD_UCF_ Cm[m3/kg]	Matrix KD for Cm in the UCF unit	LOGNOR MAL	4187., 17526 7.	Per email from P. Bertetti that stated Cm values/ distributions for matrix Kds should be equal to Am values/ distributions from TPA 4.1jpd	
MODIFIED FROM CONSTANT = 0.0 VALUES	UZFT	MatrixKD_BFw_ Cm[m3/kg]	Matrix KD for Cm in the BFw unit	LOGNOR MAL	1699., 71123.	Per email from P. Bertetti that stated Cm values/ distributions for matrix Kds should be equal to Am values/ distributions from TPA 4.1jpd	
MODIFIED FROM CONSTANT = 0.0 VALUES	UZFT	MatrixKD_UFZ_ Cm[m3/kg]	Matrix KD for Cm in the UFZ unit	LOGNOR MAL	1638., 68583.	Per email from P. Bertetti that stated Cm values/ distributions for matrix Kds should be equal to Am values/ distributions from TPA 4.1jpd	

Attachment 1

Description of Changes
SCR 530

1. The "maxseismicevents" parameter in the seisadj.i file was modified by increasing "maxseismicevents" from 1500 to 10000.

2. Modified the exec.f screenprint for the disk space requirements with the increased number of time steps. The added coding was:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc (note: values used to determine xmegs above may need to be re-evaluated)
cc        xmegs = xmegs / 1.0d6
cc        if (xmegs .lt. 1.0d0) then
cc          nxmegs = 1
cc          print '(a,i5,a)',' By selecting this option, files are '//
cc    &       'written which may require',nxmegs,' meg of disk space.'
cc        else
cc          nxmegs = int(xmegs)
cc          print '(a,i5,a)',' By selecting this option, files are '//
cc    &       'written which may require',nxmegs,' megs of disk space.'
cc        endif
cc       print *,'(more disk space could be needed)'
cc       print *, ' '
      nxmegs=dint(90.0d0+(xnumber-1.0d0)*2.0d0+(xnumber*130.0d0))
      print '(a,i7,a)',' By selecting this option, files are '//
    &     'written which may require',nxmegs,' megs of disk space.'
      print *,'(NOTE: more disk space could be needed)'
      print *, ' '
```

(Note that these values may need to be re-evaluated given the changes in the file sizes with the increased time steps.)

3. In exec.f, modified the number of time steps for "kMaxTimeSteps" as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc     parameter (kMaxTimeSteps = 501)
     parameter (kMaxTimeSteps = 5001)
```

4. Modified the maximum number of time steps in maxntime.i as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc     parameter (maxntime  = 401 )
     parameter (maxntime  = 5001 )
```

5. Added the following to the reflux2 and reflux3 subroutines in the nfenv.f module, so that

the reflux period ends at 20,000 years instead of 10,000 years.

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc (remove 10,000 years reflux condition and use
cc  20,000 years which is consistent with Fig. 3-3
cc  in the March 2004 TPA 4.1 Sensitivity Analysis Report)
cc      refluxend = 1.0E4
      refluxend = 2.0E4
```

6. Modified the variable "nintv" in nintv.i as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc      parameter (nintv = 2000)
      parameter (nintv = 5001)
```

7. Increased the value for the variable "n3" in reflux2.i as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc      parameter (n3 = 100000)
      parameter (n3 = 1000000)
```

8. Added two aqeuousnuclides to the tpa.inp file (U233 and Th229) at the end of the decay chain with Cm245 -> Am241 -> Np237 and increased the number of aqueousnuclides from 20 to 22 (and the subject decay chain lenghth from 3 to 5). Also needed add parameters to the tpa.inp file for "GapFractionForU233" and "GapFractionForTH299".

9. Made the MatrixKd values for Cm and Am the same in tpa.inp (i.e., same distribution and minimum/maximum values). Note that Am MatrixKds are not sampled in TPA Version 5.0.0.f.

10. Increased the value for the variable "mnCliTS" in uz_parms.i as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc      parameter (mnCliTS     = 1001)
      parameter (mnCliTS     = 2001)
```

11. Modified the parameter "maxnumdis" in uzft.f as follows to allow for a larger NEFTRAN output file:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc      PARAMETER (maxnumdis=99999)
      PARAMETER (maxnumdis=999999)
```

12. Accompanying the modification in #23 above (i.e., there may be up to one more order of magnitude increase in the number of time steps in the NEFTRAN output file), the dimensions specified in the uzft.f read statement needs to be increased from an "I5" to an "I6" (to cover the potential order of magnitude increase) as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc      read(i3,'(7x, i2, 11x, i2, 8x, i5)',err=100)
      read(i3,'(7x, i2, 11x, i2, 8x, i6)',err=100)
```

13. In examining failt.f, noted that the file failtadj.i had been added to the TPA code during modifications from Version 4.1jpd to 5.0.0.f. This file contains the variable "nintv" whose value was increased as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc      PARAMETER (nintv = 2000)
      PARAMETER (nintv = 5001)
```

14. Similar to #23and #24 above, needed to modify nefmks.f to write the number of NEFTRAN discharge rates with up to 6 (instead of 5) digits as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc 9080    FORMAT(' CHAIN#',I2,', #ISOTOPES',I2,', #RATES',I5)
 9080    FORMAT(' CHAIN#',I2,', #ISOTOPES',I2,', #RATES',I6)
```

15. With the addition of U233 and Th229, needed to increase the array dimension parameter "NDBF" used in NEFTRAN and set in SIZES.INC. The SIZES.INC file was modified as follows:

```
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc (needed to increase after adding U233 and Th229)
cc     PARAMETER (NDJPN=20000, NDBF=300000, MXELEM=30)
     PARAMETER (NDJPN=20000, NDBF=1500000, MXELEM=30)
```

16. Modified the climato2.dat file to enable long simulations by repeating the 100,000 year cycles 10 times (allowing a maximum time of 1,000,000 years). This file is named "climato2.dat_cycles". Also, created a file named "climato2.dat_no_cycles" which will be the basecase "climato2.dat" file at this time. The "climato2.dat_no_cycles" file includes data from 0 years through 50,000 years; then, from 50,000 years through the maximum time (1,000,000 years), the values in this file are kept constant at 1.0. (Note that the "climato2.dat" file was modified from TPA Version 4.1jpdls_beta4 during development toward the TPA Version 5.0.0.f code according to values supplied by R. Fedors; also, R. Fedors was consulted about long simulations and recommended the implemented approach - [i.e., repeating the 100,000 year cycles.]) See below for a listing of one of these files ("climato2.dat_no_cycles").

0	0	0
1000	0.364364174	0.364364174
2000	0.50775941	0.50775941
3000	0.586599682	0.586599682
4000	0.632253812	0.632253812
5000	0.655878738	0.655878738
6000	0.655878738	0.655878738
7000	0.655878738	0.655878738
8000	0.655878738	0.655878738
9000	0.655878738	0.655878738
10000	0.655878738	0.655878738
11000	0.66734938	0.66734938
12000	0.678820022	0.678820022
13000	0.690290664	0.690290664
14000	0.701761306	0.701761306
15000	0.713231949	0.713231949
16000	0.724702591	0.724702591
17000	0.736173233	0.736173233
18000	0.747643875	0.747643875
19000	0.759114517	0.759114517
20000	0.770585159	0.770585159
21000	0.782055801	0.782055801
22000	0.793526443	0.793526443
23000	0.804997085	0.804997085
24000	0.816467727	0.816467727
25000	0.827938369	0.827938369
26000	0.839409011	0.839409011
27000	0.850879653	0.850879653
28000	0.862350295	0.862350295
29000	0.873820937	0.873820937
30000	0.885291579	0.885291579
31000	0.896762221	0.896762221
32000	0.908232864	0.908232864
33000	0.919703506	0.919703506
34000	0.931174148	0.931174148
35000	0.94264479	0.94264479
36000	0.954115432	0.954115432
37000	0.965586074	0.965586074
38000	0.977056716	0.977056716
39000	0.988527358	0.988527358
40000	0.999998	0.999998
41000	1	1
50000	1	1
1000000	1	1

17. Modified the tpanames.dbs file by adding information for the two new U233 and Th229 gap fraction parameters inserted into the tpa.inp file when U233 and Th229 were added (see #17). The following two lines were inserted into the tpanames.dbs file between the two lines provided below. (Note: there is no comment in this file because of formatting requirements.)

(line before insertion point)

GapFractionForNP237 G%-Np237

(the 2 lines inserted)

GapFractionForU233 G%-U233
GapFractionForTH229 G%-Th229

(line after insertion point)
GapFractionForAM243 G%-Am243

18. Modified the wpflow.def file to increase the maximum time (i.e., increased from 100,000 years to 1,000,000 years). The line added at the end of this file follows. (Note: there is no comment in this file because of formatting requirements.)

1000000.0000 0.044721 0.173205

19. In the tpa.inp file, needed to modify the UZFT Matrix Kds for Cm from "constant=0.0" to distributions that matched the TPA 4.1jpd for Am. This is consistent with the email from P. Bertetti's recommendation. That is,

```
lognormal
MatrixKD_TSw_Cm[m3/kg]
1760., 73663.
***
lognormal
MatrixKD_CHnvCm[m3/kg]
5340., 223529.
***
lognormal
MatrixKD_CHnzCm[m3/kg]
4855., 203209.
***
lognormal
MatrixKD_PPw_Cm[m3/kg]
4005., 167647.
***
lognormal
MatrixKD_UCF_Cm[m3/kg]
4187., 175267.
***
lognormal
MatrixKD_BFw_Cm[m3/kg]
1699., 71123.
***
lognormal
MatrixKD_UFZ_Cm[m3/kg]
1638., 68583.
```

20. Ran the TPA code and found NEFTRAN execution stopped in the UZ and SZ a number of times. After a number of NEFTRAN execution stoppages, ended up modifying parameters in the file SIZES.INC to the following values:

"NDJPN" set equal 100000
"NDDF" set equal to 200000
"NDBF" set equal to 2000000

21. Ran the TPA code and noted that the number of ejected WPs is listed as 2012602235 (a bogus number). Communicated with R. Janetzke who stated this needed change will be accomplished through SCR 519.

22. In the tpa.inp file, added U233 and Jt229 to the second colloid chain (also increased the length of this chain from 3 to 5 and increased the number of colloidalnuclides from 11 to 13). Also, added the following parameter to the tpa.inp file.

```
**
constant
ColloidReleaseFactor_Jt229[]
0.9
**
```

23. After running the TPA code, noted that there was a screenprint error that stated that in a colloid chain, there could not be a colloidalnuclide that followed an aqueousnuclide. Modified the reader.f file to remove this error trap. Next, testing will be conducted to determine if the TPA code is correctly handling this situation. The following lines of the error trap were commented out for this testing.

```
cc rwr 2-11-05; SCR530
cc modified for long TPA simulations
cc        if ( lSoluteFound .and. indexofnucs .eq. 0) then
cc          print *, ' '
cc          print *, '  ***>>> Error in Reader <<<*** '
cc          print *, ' Do not understand name of nuclide.'
cc          print *, ' Needs to be one of the solute nuclides'
cc          print *, ' already delcared in tpa.inp since a solute '
cc          print *, ' nuclide has already appeared in this chain.'
cc          print *, ' name = ', cldnames(kkcount)
cc          print *, ' Look on line = ', iline
cc          print *, ' '
cc          print *, ' solute nuclide names appearing in a colloid'
cc          print *, ' chain need to be one of the following:'
cc          do i = 1, nnucl
cc            print *, names(i)
cc          end do
cc          print *, ' '
cc          CALL QUERYSTOP()
cc        end if
```

24. In running the TPA code, noted SZ NEFTRAN execution stopped with a cryptic system error message that stated there was abnormal termination of a process (i.e., SZ NEFTRAN). After a preliminary investigation, determined that the SZ NEFTRAN velocity file (NEFII.VEL) had what appeared to be a relatively large flow rate for the first of the three SZ legs (e.g., 309, 584, and 42 for the 1st, 2nd, and 3rd legs, respectively).

Decreasing the velocity of the 1st leg from 309 to 209 yielded a successful SZ NEFTRAN execution. Passed this information on to R. Janetzke.

25. Added the new parameter for "ColloidReleaseFactor_Jt229[]" to the tpanames.dbs file. That is, the following line was inserted into this file following the line that corresponds to the same parameter for "Jt230".

```
ColloidReleaseFactor_Jt229[]                    CRFJt229
```

26. Ran the TPA code for 50 realizations and found UZ NEFTRAN execution stops on realization #4 and subarea #4 because the "discharge array" dimensions were exceeded. Increased "NDDF" in SIZES.INC from 20000 to 30000 and re-ran the TPA code. (Note that this increase in "NDDF" did result in successful execution of the UZ NEFTRAN code for this realization and subarea.)

27. Conducted two TPA code simulations each using the TPA Version 5.0.0f code from Vermont and the TPA Version 5.0.0f_ ls2 code developed as noted above. Using the same "tpa.inp" file in both simulations, and the cyclical data in the "climato2.dat" file for the "long simulation" run, found using the MS DOS Prompt command line "fc", that the output is identical (except, as expected, for the time stamp of the run) for 10,000 yr and 100,000 yr simulations. Therefore, the changes introduced in creating the TPA Version 5.0.0f_ls2 code have been verified as not affecting TPA code output.

28. Needed to test whether adding U233 and Jt229 to the end of colloid chain 2 yielded correct values - since there is an error check in reader.f, which was disabled as described above, that does not allow a colloid chain [which always begins with a colloid] to switch from an aqueousnuclide [U233] back to a colloid [Jt229]). To conduct this testing, performed TPA code simulations using the TPA Version 5.0.0f_ls2 code for subarea 1 at 10,000, 100,000, and 1,000,000 yrs on GRYPHON with the APPEND option active for all files, and using (1) TPA Version 5.0.0f aqueous and colloid radionuclides only; (2) #1 with U233 and Th229 added to aqueousnuclide chain 2; (3) #2 with U233 and Jt229 added to colloid chain 2. By examining *.ech and *.rlt files from EBSREL, UZFT, SZFT, and DCAGW, the treatment of U233 and Jt229 can be checked for correctness. From this testing found the following:

29. NOTE: During testing described above, noted that the partitioning of aqueousnuclides that are entering the UZ into colloids and aqueousnuclides assumes the aqueousnuclides are not decreased. In fact, set (1) the colloid loss to zero and (2) 100% of the aqueousnuclide to colloids. Found equal amounts, at the same time, of an aqueousnuclide and its corresponding colloid at same time being passed into UZ NEFTRAN. This, obviously, does not conserve mass - comments in "ebsrel.f" note the following.

(Note the purpose for this EBSREL subroutine:)

```
c=====================================================================
    subroutine releasecolloids( iebsnefdat, nnucl, numclnuc, cldnames)
```

```
c=====================================================================
c
c   NAME: releasecolloids - Release irrversible colloids.
c
c   PURPOSE:
c         This module adjusts the release values in ebsnef.dat file to
c         create releases from colloidal radionuclides by reducing
c         the releases of aqueous nuclides by a factor and assigning
c         the remaining portion to the colloidal nuclide.
c
```

(Note the comment below when assigning release rates to the colloids:)

```
c  Do not diminish solute nuclides when releasing colloids.
```

After consultation with R. Janetzke, found that these changes were made by T. McCartin

30. Starting with the TPA Version 5.0.0m code, incorporated the TPA Version 5.0.0f_ls2 code modifications and performed test runs. The files copied directly from the TPA Version 5.0.0f_ls2 code into the TPA Version 5.0.0m code were reader.f, maxntime.i, nintv.i, reflux2.i, seisadj.i, uz_parms.i, wpflow.def, climato2.dat, failtadj.i, SIZES.INC, and nefmks.f. The TPA Version 5.0.0f_ls2 code files that needed to be merged with the TPA Version 5.0.0m code files were exec.f, nfenv.f, uzft.f, tpa.inp, and tpanames.dbs.

31. This code was compiled and executed in a Toshiba Laptop computer (512 MB RAM). The code was not able to execute RELEASET during a TPA code run, but was able to do so in standalone mode.

32. Executed the above code on GRYPHON (d:\rrice\tpa500m_ls\run) successfully for the basecase (execution time was 5 minutes). Then, ran this code (d:\rrice\tpa500m_ls\run250) for 250 realizations with the APPEND OPTION activated. Code execution stopped on realization 36, subarea 3, because of an array out of bounds (discharge array) in UZ NEFTRAN. Noted in these runs a SATK message and WP corrosion failure times of either about 100 years or 900,000 years (or none in 1e6 years).

33. In addition to tpa.inp file modifications for the number of time steps (for the maximum and compliance period time steps), the files which must be modified to increase/decrease the number of time steps are: exec.f, maxntime.i, nintv.i, reflux2.i, seisadj.i, uz_parms.i, and failtadj.i. Comment #30 above lists all files modified and inserted into the TPA Version 5.0.0m code.(NOTE: a search for "rwr" in comments for SCR 530 will find the changes in these files; also, in this code development effort, values were set at "5001" - which can be increased/decreased depending in the project and computer resources.)

34. Passed the modified files on to R. Janetzke together with this SCR and accompanying documentation.

Attachment 2

Test Plan/Report for TPA SCR #530

Test Plan Name: Test Changes to Actinide Kd/Rd Calculations

Tested By: Carol S. Scherer **Date:** May 2, 2005

Host Machine: SUN Ultra-4 server: Spock **Host OS:** Sun Solaris 5.8

Baseline Version: TPA 5.0.0m **Test Version: TPA** 5.0.0o

Testing Setup:

Directories/paths used for testing:
$HOME = spock/home/cscherer
Path for run directory: ***$HOME/scr530***

Environment variables:

TPA_TEST = $HOME /
TPA_DATA = $HOME /

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 530 - Test Directories*" (attached).

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***scr530***, ***scr530/tpa500m***

2. Copy **TPA** version 5.0.0o to ***$HOME/scr530***. Compile *tpa.e*.

3. Copy **TPA** version 5.0.0m to ***$HOME/scr530/tpa500m***. Compile *tpa.e*.

Function Level Tests:

These tests are designed to demonstrate the functionality of the specified module.

1. Name: Visual Inspection of Source Code and *tpa.inp* for **TPA**5.0.0o.

Paths for archives of results: ***$HOME /scr530/test-report/flt1*-inspect**

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: base case *tpa.inp* for each version; set OutputMode to 1.

Utility scripts needed to perform the test: command file *compare_allfiles-10K* (copy attached to this document)

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to verify that specified changes have been made to **TPA**
- assumptions: all setup instructions have been carried out.
- constraints: none.
- output files to compare or examine: none.
- step by step test procedure to be used:
  1. look at *scr_530.wpd*, *tpa.inp*, and **TPA** source code for version 5.0.0o and verify that the changes specified in the scr document have been made.
- pass/fail criteria: the test passes if:
  1. Specified changes have been made.

Results of running test:

FAILED. Colloidal nuclide chain 2 is missing two nuclides. SCR # 527 has been generated to correct this problem. Changes were made to the values for Matrix Kds for Cm but are commented out with the previous values still in place.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

1. Name: Compare Output from **TPA5.0.0o** and **TPA5.0.0m** at 10,000 Years.

   Paths for archives of results: ***$HOME /scr530/test-report/slt1***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: The same *climato2.dat* file was used for both runs. For **TPA**5.0.0m, the following changes were made to source code file *seisadj.i* and nfenv.f to match **TPA**5.0.0o:

maxseismicevents = 7100
refluxend = 2.0e4

Program modes to be used: use base case *tpa.inp* for each version and make the following changes:

set OutputMode to 1

Utility scripts needed to perform the test: command file *compare_allfiles-10K* (copy attached to this document)

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code generates the same results as the modified code at 10,000 years.

- assumptions: all setup instructions have been carried out.

- constraints: the files *tpa_allfiles-10K-500m.out* and *tpa_allfiles-10K-500m.out* do not exist in the run directory.

- output files to compare or examine: *compallfiles-10K.out*, *tpa_allfiles-10K-500m.out* and *tpa_allfiles-10K-500m.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>***/tpa500m***
  2. run *tpa.e* using command "***tpa.e > tpa_allfiles-10K-500m.out***"
  3. —> change directory to <<run directory>>
  4. run *tpa.e* using command "***tpa.e > tpa_allfiles-10K-500o.out***"
  5. run compare_allfiles-10K
  6. compare the two captured display output files

- pass/fail criteria: the test passes if:

  1. Both **TPA** runs complete successfully.

2. There are no differences in the values listed in the ASCII text output files (not binary files), except for time/date stamps, version differences, number of time steps, the addition of the 2 new Gap Fractions, extra spaces in output, comment lines (starting with ** in *tpa.inp*, *tpameans.out*, *tpamax.out*, & *tpamin.out*), or small rounding errors. There should also be a difference in the amount of space estimated for the "append all files" option between the two versions.

Results of running test:

PASSED.

2. Name: Compare Output from **TPA5.0.0o** and **TPA5.0.0m** at 100,000 Years.

Paths for archives of results: ***$HOME /scr530/test-report/slt2-100Kbase***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: The same *climato2.dat* file was used for both runs. For **TPA**5.0.0m, the following changes were made to source code file *seisadj.i* and nfenv.f to match **TPA**5.0.0o:

maxseismicevents = 7100
refluxend = 2.0e4

Program modes to be used: use base case *tpa.inp* for each version and make the following changes:

set OutputMode to 1
set MaximumTime to 1.0e5

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code generates the same results as the modified code at 100,000 years.

- assumptions: all setup instructions have been carried out.

- constraints: the files *tpa_allfiles-100K-500m.out* and *tpa_allfiles-100K-500m.out* do not exist in the run directory.

- output files to compare or examine: *rgwna_o-m.xls, rgwna.tpa (both runs), compallfiles-100K.out*, *tpa_allfiles-100K-500m.out* and *tpa_allfiles-100K-500m.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>***/tpa500m***
  2. run *tpa.e* using command "***tpa.e > tpa_allfiles-100K-500m.out***"
  3. —> change directory to <<run directory>>
  4. run *tpa.e* using command "***tpa.e > tpa_allfiles-100K-500o.out***"
  5. run compare_allfiles-100K
  6. create the spreadsheet *rgwna_o-m.xls* with containing dose values from rgwna.tpa from both TPA runs for the nuclides Pu239, I129, and Tc99. Calculate the percentage difference in values from both runs.
  7. compare the two captured display output files

- pass/fail criteria: the test passes if:

  1. Both **TPA** runs complete successfully.

  2. There are no differences in the values listed in the ASCII text output files (not binary files), except for time/date stamps, version differences, number of time steps, the addition of the 2 new Gap Fractions, extra spaces in output, comment lines (starting with ** in *tpa.inp*, *tpameans.out*, *tpamax.out*, & *tpamin.out*), or small rounding errors. There should also be a difference in the amount of space estimated for the "append all files" option between the two versions.

  3. In the spreadsheet *rgwna_o-m.xls*, differences in values for doses for Pu239, I129, and Tc99 differ by less than 0.1%.

Results of running test:

PASSED.

3. Name: Compare Output From Mean Case Runs At 10,000, 100,000, and 1,000,000 Years

Paths for archives of results: ***$HOME /scr530/test-report/slt3-mean***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use tpameans.out from a **TPA**5.0.0o base case run as *tpa.inp* for each version and make the following changes:

set OutputMode to 1

leave MaximumTime at 1.0e4 for 1st run
set MaximumTime to 1.0e5 for 2nd run
set MaximumTime to 1.0e6 for 3rd run

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code generates the reasonable results at 1,000,000 when compared with the results from 10,000- and 100,000-year runs.

- assumptions: all setup instructions have been carried out.

- constraints: the files *tpa_10K.out, tpa_100K.out,* and *tpa_1M.out* do not exist in the run directory.

- output files to compare or examine: *climato2.dat*, *ebsflo.dat, rgwna.tpa* (from each run), *ebsrel.rlt* (from 1,000,000-year run), *szft.rlt* (from 1,000,000-year run), *uzft.rlt* (from 1,000,000-year run), *tpa_10K*, *tpa_100K.out,* and *tpa_1M.out*; spreadsheet *rgwna-mean-alltimes.xls*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. run1: run *tpa.e* using command "***tpa.e > tpa_10K.out***"
  3. run2: run *tpa.e* using command "***tpa.e > tpa_100K.out***"
  4. run3: run *tpa.e* using command "***tpa.e > tpa_1M.out***"
  5. create spreadsheet (*rgwna-mean-alltimes.xls*) containing *rgwna.tpa* from all three runs; add *climato2.dat*, *ebsflo.dat* and U233, U234, & U238 results from subarea 7 from *ebsrel.rlt*, *uzft.rlt*, and *szft.rlt*. Graph each nuclide with 10,000-, 100,000-, and 1,000,000-year dose results on the same graph. Graph U233, U234, and U238 with the climate and flow data on the same graph.
  6. look at graphs

- pass/fail criteria: the test passes if:

  1. All TPA runs complete successfully.

  2. Doses from the million-year runs appear reasonable and seem to continue on from the doses reported for the ten thousand and hundred thousand year runs. Hundred thousand year runs tend to overlay ten thousand year runs, and million year runs tend to overlay hundred thousand year runs, with minor differences.

3. The cycles that appear in the doses for the nuclides (e.g., U233, U234, and U238) in the million-year runs follow the climate and flow cycles. Releases for these nuclides from EBS, UZ and SZ show some delay from retardation and spreading due to dispersion as water flows through the layers.

Results of running test:

PASSED.

4. Name: Test Multiple Realization Run (430 realizations chosen because there are 429 sampled parameters).

Paths for archives of results: ***$HOME /scr530/test-report/slt4-430r***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: base case *tpa.inp* for each **TPA**5.0.0o; set OutputMode to 1.

Utility scripts needed to perform the test: command file *compare_allfiles-10K* (copy attached to this document)

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code functions correctly for multiple realizations

- assumptions: all setup instructions have been carried out.

- constraints: the file *tpa_base-1M-430r.out* does not exist in the run directory.

- output files to compare or examine: *tpa_base-1M-430r.out*

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>
  2. run *tpa.e* using command "***tpa.e > tpa_base-1M-430r.out***"
  3. examine the two captured display output files

- pass/fail criteria: the test passes if:

  1. The **TPA** run completes successfully.

Results of running test:

FAILED. The **TPA** run aborts in realization 5. SCR # 525 was generated to resolve this problem.

5. Name: Test 1,000,000-Year Run w/ All Append Files and Generate Restart Turned On For 4 Realizations.

   Paths for archives of results: ***$HOME /scr530/test-report/slt5*-restart**

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: base case *tpa.inp* for **TPA**5.0.0o and make the following changes:

   set OutputMode to 1
   set MaximumTime to 1.0e6
   set NumberOfRealizations to 4

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to demonstrate that the restart option functions correctly at 1,000,000 years and to show that there are enough system resources to handle the maximum number of files expanded to accommodate 1,000,000-year realizations.

   - assumptions: all setup instructions have been carried out.

   - constraints: the files *tpa_4r-nostop.out. tpa_4r-stop1.out,* and *tpa_4r-resumed.out* do not exist in the run directory.

   - output files to compare or examine: *tpa_4r-resumed.out* and *tpa_4r-nostop.out*

   - step by step test procedure to be used:
     1. —> change directory to <<run directory>
     2. run *tpa.e* using command "***tpa.e > tpa_4r-nostop.out***"
     3. run *tpa.e* using command "***tpa.e > tpa_4r-stop1.out***"
     4. abort the TPA run after the 1st realization is completed (before the 2nd realization is completed)
     5. run *tpa.e* using command "***tpa.e > tpa_4r-resumed.out***"
     6. compare the two captured display output files

- pass/fail criteria: the test passes if:

  1. Both **TPA** runs complete successfully.

  2. The output from the aborted/restarted **TPA** run match the output from the non-aborted run.

Results of running test:

FAILED. Output from the two runs don't match. This discrepancy will be addressed in SCR580.

NOTES:

ATTACHMENT A

Compare_allfiles-10K Command File

```
echo ' 1) diff NEFII.VEL          ../mod500m-10K/NEFII.VEL'
diff NEFII.VEL          ../mod500m-10K/NEFII.VEL
echo ' '
echo ' ************************************************'
echo ' '
echo ' 2) diff airpkdos.res       ../mod500m-10K/airpkdos.res'
diff airpkdos.res       ../mod500m-10K/airpkdos.res
echo ' '
echo ' ************************************************'
echo ' '
echo ' 3) diff arpkds_c.res       ../mod500m-10K/arpkds_c.res'
diff arpkds_c.res       ../mod500m-10K/arpkds_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo ' 4) diff ashout.res         ../mod500m-10K/ashout.res'
diff ashout.res         ../mod500m-10K/ashout.res
echo ' '
echo ' ************************************************'
echo ' '
echo ' 5) diff chlrdmf.dat        ../mod500m-10K/chlrdmf.dat'
diff chlrdmf.dat        ../mod500m-10K/chlrdmf.dat
echo ' '
echo ' ************************************************'
echo ' '
echo ' 6) diff corrode.out        ../mod500m-10K/corrode.out'
diff corrode.out        ../mod500m-10K/corrode.out
echo ' '
echo ' ************************************************'
echo ' '
echo ' 7) diff cp.tpa             ../mod500m-10K/cp.tpa'
diff cp.tpa             ../mod500m-10K/cp.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo ' 8) diff cumrel.res         ../mod500m-10K/cumrel.res'
diff cumrel.res         ../mod500m-10K/cumrel.res
echo ' '
echo ' ************************************************'
echo ' '
echo ' 9) diff cumrel_c.res       ../mod500m-10K/cumrel_c.res'
diff cumrel_c.res       ../mod500m-10K/cumrel_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '10) diff cumrelse.out       ../mod500m-10K/cumrelse.out'
diff cumrelse.out       ../mod500m-10K/cumrelse.out
echo ' '
echo ' ************************************************'
echo ' '
echo '11) diff dcagw.ech          ../mod500m-10K/dcagw.ech'
diff dcagw.ech          ../mod500m-10K/dcagw.ech
echo ' '
echo ' ************************************************'
echo ' '
echo '12) diff dcagw.rlt          ../mod500m-10K/dcagw.rlt'
diff dcagw.rlt          ../mod500m-10K/dcagw.rlt
echo ' '
echo ' ************************************************'
echo ' '
```

```
echo '13) diff dcfgw.cum          ../mod500m-10K/dcfgw.cum'
diff dcfgw.cum          ../mod500m-10K/dcfgw.cum
echo ' '
echo ' ************************************************'
echo ' '
echo '14) diff deltaec.inp        ../mod500m-10K/deltaec.inp'
diff deltaec.inp        ../mod500m-10K/deltaec.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '15) diff diagnose.out       ../mod500m-10K/diagnose.out'
diff diagnose.out       ../mod500m-10K/diagnose.out
echo ' '
echo ' ************************************************'
echo ' '
echo '16) diff drifts.dat         ../mod500m-10K/drifts.dat'
diff drifts.dat         ../mod500m-10K/drifts.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '17) diff dsfail.ech         ../mod500m-10K/dsfail.ech'
diff dsfail.ech         ../mod500m-10K/dsfail.ech
echo ' '
echo ' ************************************************'
echo ' '
echo '18) diff dsfail.res         ../mod500m-10K/dsfail.res'
diff dsfail.res         ../mod500m-10K/dsfail.res
echo ' '
echo ' ************************************************'
echo ' '
echo '19) diff dsfail.rlt         ../mod500m-10K/dsfail.rlt'
diff dsfail.rlt         ../mod500m-10K/dsfail.rlt
echo ' '
echo ' ************************************************'
echo ' '
echo '20) diff dsfailt.dat        ../mod500m-10K/dsfailt.dat'
diff dsfailt.dat        ../mod500m-10K/dsfailt.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '21) diff dsfailt.inp        ../mod500m-10K/dsfailt.inp'
diff dsfailt.inp        ../mod500m-10K/dsfailt.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '22) diff dsfailt.out        ../mod500m-10K/dsfailt.out'
diff dsfailt.out        ../mod500m-10K/dsfailt.out
echo ' '
echo ' ************************************************'
echo ' '
echo '23) diff ebscld.out         ../mod500m-10K/ebscld.out'
diff ebscld.out         ../mod500m-10K/ebscld.out
echo ' '
echo ' ************************************************'
echo ' '
echo '24) diff ebsfail.ech        ../mod500m-10K/ebsfail.ech'
diff ebsfail.ech        ../mod500m-10K/ebsfail.ech
echo ' '
echo ' ************************************************'
echo ' '
echo '25) diff ebsfail.inp        ../mod500m-10K/ebsfail.inp'
diff ebsfail.inp        ../mod500m-10K/ebsfail.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '26) diff ebsfail.rlt        ../mod500m-10K/ebsfail.rlt'
```

```
diff ebsfail.rlt        ../mod500m-10K/ebsfail.rlt
echo ' '
echo ' ***************************************************'
echo ' '
echo '27) diff ebsfilt.inp        ../mod500m-10K/ebsfilt.inp'
diff ebsfilt.inp        ../mod500m-10K/ebsfilt.inp
echo ' '
echo ' ***************************************************'
echo ' '
echo '28) diff ebsfilt.out        ../mod500m-10K/ebsfilt.out'
diff ebsfilt.out        ../mod500m-10K/ebsfilt.out
echo ' '
echo ' ***************************************************'
echo ' '
echo '29) diff ebsflo.dat         ../mod500m-10K/ebsflo.dat'
diff ebsflo.dat         ../mod500m-10K/ebsflo.dat
echo ' '
echo ' ***************************************************'
echo ' '
echo '30) diff ebsnef.dat         ../mod500m-10K/ebsnef.dat'
diff ebsnef.dat         ../mod500m-10K/ebsnef.dat
echo ' '
echo ' ***************************************************'
echo ' '
echo '31) diff ebsnef.out         ../mod500m-10K/ebsnef.out'
diff ebsnef.out         ../mod500m-10K/ebsnef.out
echo ' '
echo ' ***************************************************'
echo ' '
echo '32) diff ebsnef2.dat        ../mod500m-10K/ebsnef2.dat'
diff ebsnef2.dat        ../mod500m-10K/ebsnef2.dat
echo ' '
echo ' ***************************************************'
echo ' '
echo '33) diff ebspac.nuc         ../mod500m-10K/ebspac.nuc'
diff ebspac.nuc         ../mod500m-10K/ebspac.nuc
echo ' '
echo ' ***************************************************'
echo ' '
echo '34) diff ebsrel.cum         ../mod500m-10K/ebsrel.cum'
diff ebsrel.cum         ../mod500m-10K/ebsrel.cum
echo ' '
echo ' ***************************************************'
echo ' '
echo '36) diff ebsrel.ech         ../mod500m-10K/ebsrel.ech'
diff ebsrel.ech         ../mod500m-10K/ebsrel.ech
echo ' '
echo ' ***************************************************'
echo ' '
echo '37) diff ebsrel.inp         ../mod500m-10K/ebsrel.inp'
diff ebsrel.inp         ../mod500m-10K/ebsrel.inp
echo ' '
echo ' ***************************************************'
echo ' '
echo '38) diff ebsrel.rlt         ../mod500m-10K/ebsrel.rlt'
diff ebsrel.rlt         ../mod500m-10K/ebsrel.rlt
echo ' '
echo ' ***************************************************'
echo ' '
echo '39) diff ebssf.dat          ../mod500m-10K/ebssf.dat'
diff ebssf.dat          ../mod500m-10K/ebssf.dat
echo ' '
echo ' ***************************************************'
echo ' '
echo '40) diff ebstrh.dat         ../mod500m-10K/ebstrh.dat'
diff ebstrh.dat         ../mod500m-10K/ebstrh.dat
```

```
echo ' '
echo ' ************************************************'
echo ' '
echo '41) diff ebstrhc.inp        ../mod500m-10K/ebstrhc.inp'
diff ebstrhc.inp        ../mod500m-10K/ebstrhc.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '42) diff echofail.dat       ../mod500m-10K/echofail.dat'
diff echofail.dat       ../mod500m-10K/echofail.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '43) diff echofilt.dat       ../mod500m-10K/echofilt.dat'
diff echofilt.dat       ../mod500m-10K/echofilt.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '44) diff epa_ave.out        ../mod500m-10K/epa_ave.out'
diff epa_ave.out        ../mod500m-10K/epa_ave.out
echo ' '
echo ' ************************************************'
echo ' '
echo '45) diff epapktim.out       ../mod500m-10K/epapktim.out'
diff epapktim.out       ../mod500m-10K/epapktim.out
echo ' '
echo ' ************************************************'
echo ' '
echo '46) diff eqvdia.ech         ../mod500m-10K/eqvdia.ech'
diff eqvdia.ech         ../mod500m-10K/eqvdia.ech
echo ' '
echo ' ************************************************'
echo ' '
echo '47) diff eqvdia.rlt         ../mod500m-10K/eqvdia.rlt'
diff eqvdia.rlt         ../mod500m-10K/eqvdia.rlt
echo ' '
echo ' ************************************************'
echo ' '
echo '48) diff failt.cum          ../mod500m-10K/failt.cum'
diff failt.cum          ../mod500m-10K/failt.cum
echo ' '
echo ' ************************************************'
echo ' '
echo '49) diff failt.out          ../mod500m-10K/failt.out'
diff failt.out          ../mod500m-10K/failt.out
echo ' '
echo ' ************************************************'
echo ' '
echo '50) diff fluoride.dat       ../mod500m-10K/fluoride.dat'
diff fluoride.dat       ../mod500m-10K/fluoride.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '51) diff frac_rel.out       ../mod500m-10K/frac_rel.out'
diff frac_rel.out       ../mod500m-10K/frac_rel.out
echo ' '
echo ' ************************************************'
echo ' '
echo '52) diff gdefault.inp       ../mod500m-10K/gdefault.inp'
diff gdefault.inp       ../mod500m-10K/gdefault.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '53) diff gentoo.out         ../mod500m-10K/gentoo.out'
diff gentoo.out         ../mod500m-10K/gentoo.out
echo ' '
```

```
echo ' ************************************************'
echo ' '
echo '54) diff genv.cum          ../mod500m-10K/genv.cum'
diff genv.cum          ../mod500m-10K/genv.cum
echo ' '
echo ' ************************************************'
echo ' '
echo '55) diff genv.in           ../mod500m-10K/genv.in'
diff genv.in           ../mod500m-10K/genv.in
echo ' '
echo ' ************************************************'
echo ' '
echo '56) diff genv.out          ../mod500m-10K/genv.out'
diff genv.out          ../mod500m-10K/genv.out
echo ' '
echo ' ************************************************'
echo ' '
echo '57) diff gftrans.inp       ../mod500m-10K/gftrans.inp'
diff gftrans.inp       ../mod500m-10K/gftrans.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '58) diff ggenii.cum        ../mod500m-10K/ggenii.cum'
diff ggenii.cum        ../mod500m-10K/ggenii.cum
echo ' '
echo ' ************************************************'
echo ' '
echo '59) diff ggenii.inp        ../mod500m-10K/ggenii.inp'
diff ggenii.inp        ../mod500m-10K/ggenii.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '60) diff ggenii.out        ../mod500m-10K/ggenii.out'
diff ggenii.out        ../mod500m-10K/ggenii.out
echo ' '
echo ' ************************************************'
echo ' '
echo '61) diff gmedia.out        ../mod500m-10K/gmedia.out'
diff gmedia.out        ../mod500m-10K/gmedia.out
echo ' '
echo ' ************************************************'
echo ' '
echo '62) diff gsccdf.res        ../mod500m-10K/gsccdf.res'
diff gsccdf.res        ../mod500m-10K/gsccdf.res
echo ' '
echo ' ************************************************'
echo ' '
echo '63) diff gsccdf_c.res      ../mod500m-10K/gsccdf_c.res'
diff gsccdf_c.res      ../mod500m-10K/gsccdf_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '64) diff gw_cb_ad.dat      ../mod500m-10K/gw_cb_ad.dat'
diff gw_cb_ad.dat      ../mod500m-10K/gw_cb_ad.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '65) diff gw_cb_ci.dat      ../mod500m-10K/gw_cb_ci.dat'
diff gw_cb_ci.dat      ../mod500m-10K/gw_cb_ci.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '66) diff gw_pb_ad.dat      ../mod500m-10K/gw_pb_ad.dat'
diff gw_pb_ad.dat      ../mod500m-10K/gw_pb_ad.dat
echo ' '
echo ' ************************************************'
```

```
echo ' '
echo '67) diff gw_pb_ci.dat       ../mod500m-10K/gw_pb_ci.dat'
diff gw_pb_ci.dat       ../mod500m-10K/gw_pb_ci.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '68) diff gwccdf.res         ../mod500m-10K/gwccdf.res'
diff gwccdf.res         ../mod500m-10K/gwccdf.res
echo ' '
echo ' ************************************************'
echo ' '
echo '69) diff gwccdf_c.res       ../mod500m-10K/gwccdf_c.res'
diff gwccdf_c.res       ../mod500m-10K/gwccdf_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '70) diff gwork.buf          ../mod500m-10K/gwork.buf'
diff gwork.buf          ../mod500m-10K/gwork.buf
echo ' '
echo ' ************************************************'
echo ' '
echo '71) diff gwpkdos.res        ../mod500m-10K/gwpkdos.res'
diff gwpkdos.res        ../mod500m-10K/gwpkdos.res
echo ' '
echo ' ************************************************'
echo ' '
echo '72) diff gwpkds_c.res       ../mod500m-10K/gwpkds_c.res'
diff gwpkds_c.res       ../mod500m-10K/gwpkds_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '73) diff gwttuzsz.res       ../mod500m-10K/gwttuzsz.res'
diff gwttuzsz.res       ../mod500m-10K/gwttuzsz.res
echo ' '
echo ' ************************************************'
echo ' '
echo '74) diff infilper.res       ../mod500m-10K/infilper.res'
diff infilper.res       ../mod500m-10K/infilper.res
echo ' '
echo ' ************************************************'
echo ' '
echo '75) diff inv1000.out        ../mod500m-10K/inv1000.out'
diff inv1000.out        ../mod500m-10K/inv1000.out
echo ' '
echo ' ************************************************'
echo ' '
echo '76) diff lhs.csv            ../mod500m-10K/lhs.csv'
diff lhs.csv            ../mod500m-10K/lhs.csv
echo ' '
echo ' ************************************************'
echo ' '
echo '77) diff lhs.inp            ../mod500m-10K/lhs.inp'
diff lhs.inp            ../mod500m-10K/lhs.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '78) diff lhs.out            ../mod500m-10K/lhs.out'
diff lhs.out            ../mod500m-10K/lhs.out
echo ' '
echo ' ************************************************'
echo ' '
echo '79) diff lhse.out           ../mod500m-10K/lhse.out'
diff lhse.out           ../mod500m-10K/lhse.out
echo ' '
echo ' ************************************************'
echo ' '
```

```
echo '80) diff maxrel.dat        ../mod500m-10K/maxrel.dat'
diff maxrel.dat        ../mod500m-10K/maxrel.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '81) diff mechfail.dat      ../mod500m-10K/mechfail.dat'
diff mechfail.dat      ../mod500m-10K/mechfail.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '82) diff mechfail.inp      ../mod500m-10K/mechfail.inp'
diff mechfail.inp      ../mod500m-10K/mechfail.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '83) diff mechfail.out      ../mod500m-10K/mechfail.out'
diff mechfail.out      ../mod500m-10K/mechfail.out
echo ' '
echo ' ************************************************'
echo ' '
echo '84) diff mv.tpa            ../mod500m-10K/mv.tpa'
diff mv.tpa            ../mod500m-10K/mv.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '85) diff nearfld.res       ../mod500m-10K/nearfld.res'
diff nearfld.res       ../mod500m-10K/nearfld.res
echo ' '
echo ' ************************************************'
echo ' '
echo '86) diff nefii.dis         ../mod500m-10K/nefii.dis'
diff nefii.dis         ../mod500m-10K/nefii.dis
echo ' '
echo ' ************************************************'
echo ' '
echo '87) diff nefii.inp         ../mod500m-10K/nefii.inp'
diff nefii.inp         ../mod500m-10K/nefii.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '88) diff nefii.out         ../mod500m-10K/nefii.out'
diff nefii.out         ../mod500m-10K/nefii.out
echo ' '
echo ' ************************************************'
echo ' '
echo '89) diff nefii.rel         ../mod500m-10K/nefii.rel'
diff nefii.rel         ../mod500m-10K/nefii.rel
echo ' '
echo ' ************************************************'
echo ' '
echo '90) diff nefiisz.cum       ../mod500m-10K/nefiisz.cum'
diff nefiisz.cum       ../mod500m-10K/nefiisz.cum
echo ' '
echo ' ************************************************'
echo ' '
echo '91) diff nefiisz.dis       ../mod500m-10K/nefiisz.dis'
diff nefiisz.dis       ../mod500m-10K/nefiisz.dis
echo ' '
echo ' ************************************************'
echo ' '
echo '92) diff nefiisz.inp       ../mod500m-10K/nefiisz.inp'
diff nefiisz.inp       ../mod500m-10K/nefiisz.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '93) diff nefiisz.out       ../mod500m-10K/nefiisz.out'
```

```
diff nefiisz.out        ../mod500m-10K/nefiisz.out
echo ' '
echo ' ************************************************'
echo ' '
echo '94) diff nefiisz.src        ../mod500m-10K/nefiisz.src'
diff nefiisz.src        ../mod500m-10K/nefiisz.src
echo ' '
echo ' ************************************************'
echo ' '
echo '95) diff nefiisz.vel        ../mod500m-10K/nefiisz.vel'
diff nefiisz.vel        ../mod500m-10K/nefiisz.vel
echo ' '
echo ' ************************************************'
echo ' '
echo '96) diff nefiiuz.cum        ../mod500m-10K/nefiiuz.cum'
diff nefiiuz.cum        ../mod500m-10K/nefiiuz.cum
echo ' '
echo ' ************************************************'
echo ' '
echo '97) diff nefiiuz.dis        ../mod500m-10K/nefiiuz.dis'
diff nefiiuz.dis        ../mod500m-10K/nefiiuz.dis
echo ' '
echo ' ************************************************'
echo ' '
echo '98) diff nefiiuz.inp        ../mod500m-10K/nefiiuz.inp'
diff nefiiuz.inp        ../mod500m-10K/nefiiuz.inp
echo ' '
echo ' ************************************************'
echo ' '
echo '99) diff nefiiuz.out        ../mod500m-10K/nefiiuz.out'
diff nefiiuz.out        ../mod500m-10K/nefiiuz.out
echo ' '
echo ' ************************************************'
echo ' '
echo '100) diff nefiiuz.src        ../mod500m-10K/nefiiuz.src'
diff nefiiuz.src        ../mod500m-10K/nefiiuz.src
echo ' '
echo ' ************************************************'
echo ' '
echo '101) diff nefiiuz.vel        ../mod500m-10K/nefiiuz.vel'
diff nefiiuz.vel        ../mod500m-10K/nefiiuz.vel
echo ' '
echo ' ************************************************'
echo ' '
echo '102) diff nfenv.ech          ../mod500m-10K/nfenv.ech'
diff nfenv.ech          ../mod500m-10K/nfenv.ech
echo ' '
echo ' ************************************************'
echo ' '
echo '103) diff nfenv.rlt          ../mod500m-10K/nfenv.rlt'
diff nfenv.rlt          ../mod500m-10K/nfenv.rlt
echo ' '
echo ' ************************************************'
echo ' '
echo '104) diff npkdoset.res       ../mod500m-10K/npkdoset.res'
diff npkdoset.res       ../mod500m-10K/npkdoset.res
echo ' '
echo ' ************************************************'
echo ' '
echo '105) diff npkdst_c.res       ../mod500m-10K/npkdst_c.res'
diff npkdst_c.res       ../mod500m-10K/npkdst_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '106) diff pkmndose.res       ../mod500m-10K/pkmndose.res'
diff pkmndose.res       ../mod500m-10K/pkmndose.res
```

```
echo ' '
echo ' ************************************************'
echo ' '
echo '107) diff pkreltim.res       ../mod500m-10K/pkreltim.res'
diff pkreltim.res       ../mod500m-10K/pkreltim.res
echo ' '
echo ' ************************************************'
echo ' '
echo '108) diff pkrltm_c.res       ../mod500m-10K/pkrltm_c.res'
diff pkrltm_c.res       ../mod500m-10K/pkrltm_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '109) diff rel_flow.out       ../mod500m-10K/rel_flow.out'
diff rel_flow.out       ../mod500m-10K/rel_flow.out
echo ' '
echo ' ************************************************'
echo ' '
echo '110) diff relccdf.res        ../mod500m-10K/relccdf.res'
diff relccdf.res        ../mod500m-10K/relccdf.res
echo ' '
echo ' ************************************************'
echo ' '
echo '111) diff relcum.out         ../mod500m-10K/relcum.out'
diff relcum.out         ../mod500m-10K/relcum.out
echo ' '
echo ' ************************************************'
echo ' '
echo '112) diff releaset.cum       ../mod500m-10K/releaset.cum'
diff releaset.cum       ../mod500m-10K/releaset.cum
echo ' '
echo ' ************************************************'
echo ' '
echo '113) diff releaset.out       ../mod500m-10K/releaset.out'
diff releaset.out       ../mod500m-10K/releaset.out
echo ' '
echo ' ************************************************'
echo ' '
echo '114) diff relfrac.out        ../mod500m-10K/relfrac.out'
diff relfrac.out        ../mod500m-10K/relfrac.out
echo ' '
echo ' ************************************************'
echo ' '
echo '115) diff relgwgs.res        ../mod500m-10K/relgwgs.res'
diff relgwgs.res        ../mod500m-10K/relgwgs.res
echo ' '
echo ' ************************************************'
echo ' '
echo '116) diff rgwna.tpa          ../mod500m-10K/rgwna.tpa'
diff rgwna.tpa          ../mod500m-10K/rgwna.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '117) diff rgwnapani.tpa      ../mod500m-10K/rgwnapani.tpa'
diff rgwnapani.tpa      ../mod500m-10K/rgwnapani.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '118) diff rgwnapdw.tpa       ../mod500m-10K/rgwnapdw.tpa'
diff rgwnapdw.tpa       ../mod500m-10K/rgwnapdw.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '119) diff rgwnapext.tpa      ../mod500m-10K/rgwnapext.tpa'
diff rgwnapext.tpa      ../mod500m-10K/rgwnapext.tpa
echo ' '
```

```
echo ' ************************************************'
echo ' '
echo '120) diff rgwnapinh.tpa      ../mod500m-10K/rgwnapinh.tpa'
diff rgwnapinh.tpa      ../mod500m-10K/rgwnapinh.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '121) diff rgwnapmlk.tpa      ../mod500m-10K/rgwnapmlk.tpa'
diff rgwnapmlk.tpa      ../mod500m-10K/rgwnapmlk.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '122) diff rgwnappla.tpa      ../mod500m-10K/rgwnappla.tpa'
diff rgwnappla.tpa      ../mod500m-10K/rgwnappla.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '123) diff rgwnr.tpa          ../mod500m-10K/rgwnr.tpa'
diff rgwnr.tpa          ../mod500m-10K/rgwnr.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '124) diff rgwsa.tpa          ../mod500m-10K/rgwsa.tpa'
diff rgwsa.tpa          ../mod500m-10K/rgwsa.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '125) diff rgwsap.tpa         ../mod500m-10K/rgwsap.tpa'
diff rgwsap.tpa         ../mod500m-10K/rgwsap.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '126) diff rgwsr.tpa          ../mod500m-10K/rgwsr.tpa'
diff rgwsr.tpa          ../mod500m-10K/rgwsr.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '127) diff rlccdf_c.res       ../mod500m-10K/rlccdf_c.res'
diff rlccdf_c.res       ../mod500m-10K/rlccdf_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '128) diff rlgwgs_c.res       ../mod500m-10K/rlgwgs_c.res'
diff rlgwgs_c.res       ../mod500m-10K/rlgwgs_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '129) diff samplpar.abb       ../mod500m-10K/samplpar.abb'
diff samplpar.abb       ../mod500m-10K/samplpar.abb
echo ' '
echo ' ************************************************'
echo ' '
echo '130) diff samplpar.hdr       ../mod500m-10K/samplpar.hdr'
diff samplpar.hdr       ../mod500m-10K/samplpar.hdr
echo ' '
echo ' ************************************************'
echo ' '
echo '131) diff samplpar.res       ../mod500m-10K/samplpar.res'
diff samplpar.res       ../mod500m-10K/samplpar.res
echo ' '
echo ' ************************************************'
echo ' '
echo '132) diff seismo.ech         ../mod500m-10K/seismo.ech'
diff seismo.ech         ../mod500m-10K/seismo.ech
echo ' '
echo ' ************************************************'
```

```
echo ' '
echo '133) diff seismo.rlt        ../mod500m-10K/seismo.rlt'
diff seismo.rlt        ../mod500m-10K/seismo.rlt
echo ' '
echo ' ************************************************'
echo ' '
echo '134) diff sotnef.dat        ../mod500m-10K/sotnef.dat'
diff sotnef.dat        ../mod500m-10K/sotnef.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '135) diff sp.tpa            ../mod500m-10K/sp.tpa'
diff sp.tpa            ../mod500m-10K/sp.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '136) diff spquery.tpa       ../mod500m-10K/spquery.tpa'
diff spquery.tpa       ../mod500m-10K/spquery.tpa
echo ' '
echo ' ************************************************'
echo ' '
echo '137) diff sz_kdrd.out       ../mod500m-10K/sz_kdrd.out'
diff sz_kdrd.out       ../mod500m-10K/sz_kdrd.out
echo ' '
echo ' ************************************************'
echo ' '
echo '138) diff sz_revers.out     ../mod500m-10K/sz_revers.out'
diff sz_revers.out     ../mod500m-10K/sz_revers.out
echo ' '
echo ' ************************************************'
echo ' '
echo '139) diff szft.ech          ../mod500m-10K/szft.ech'
diff szft.ech          ../mod500m-10K/szft.ech
echo ' '
echo ' ************************************************'
echo ' '
echo '140) diff szft.rlt          ../mod500m-10K/szft.rlt'
diff szft.rlt          ../mod500m-10K/szft.rlt
echo ' '
echo ' ************************************************'
echo ' '
echo '141) diff thermal.dat       ../mod500m-10K/thermal.dat'
diff thermal.dat       ../mod500m-10K/thermal.dat
echo ' '
echo ' ************************************************'
echo ' '
echo '142) diff totdos_c.res      ../mod500m-10K/totdos_c.res'
diff totdos_c.res      ../mod500m-10K/totdos_c.res
echo ' '
echo ' ************************************************'
echo ' '
echo '143) diff totdose.res       ../mod500m-10K/totdose.res'
diff totdose.res       ../mod500m-10K/totdose.res
echo ' '
echo ' ************************************************'
echo ' '
echo '144) diff tpamax.out        ../mod500m-10K/tpamax.out'
diff tpamax.out        ../mod500m-10K/tpamax.out
echo ' '
echo ' ************************************************'
echo ' '
echo '145) diff tpameans.out      ../mod500m-10K/tpameans.out'
diff tpameans.out      ../mod500m-10K/tpameans.out
echo ' '
echo ' ************************************************'
echo ' '
```

```
echo '146) diff tpamin.out        ../mod500m-10K/tpamin.out'
diff tpamin.out        ../mod500m-10K/tpamin.out
echo ' '
echo ' ************************************************'
echo ' '
echo '147) diff trelease.out      ../mod500m-10K/trelease.out'
diff trelease.out      ../mod500m-10K/trelease.out
echo ' '
echo ' ************************************************'
echo ' '
echo '148) diff uz_kdrd.out       ../mod500m-10K/uz_kdrd.out'
diff uz_kdrd.out       ../mod500m-10K/uz_kdrd.out
echo ' '
echo ' ************************************************'
echo ' '
echo '149) diff uz_revers.out     ../mod500m-10K/uz_revers.out'
diff uz_revers.out     ../mod500m-10K/uz_revers.out
echo ' '
echo ' ************************************************'
echo ' '
echo '150) diff uzflow.ech        ../mod500m-10K/uzflow.ech'
diff uzflow.ech        ../mod500m-10K/uzflow.ech
echo ' '
echo ' ************************************************'
echo ' '
echo '151) diff uzflow.rlt        ../mod500m-10K/uzflow.rlt'
diff uzflow.rlt        ../mod500m-10K/uzflow.rlt
echo ' '
echo ' ************************************************'
echo ' '
echo '152) diff uzft.ech          ../mod500m-10K/uzft.ech'
diff uzft.ech          ../mod500m-10K/uzft.ech
echo ' '
echo ' ************************************************'
echo ' '
echo '153) diff uzft.rlt          ../mod500m-10K/uzft.rlt'
diff uzft.rlt          ../mod500m-10K/uzft.rlt
echo ' '
echo ' ************************************************'
echo ' '
echo '154) diff weldfail.out      ../mod500m-10K/weldfail.out'
diff weldfail.out      ../mod500m-10K/weldfail.out
echo ' '
echo ' ************************************************'
echo ' '
echo '155) diff wpfillstats.out   ../mod500m-10K/wpfillstats.out'
diff wpfillstats.out   ../mod500m-10K/wpfillstats.out
echo ' '
echo ' ************************************************'
echo ' '
echo '156) diff wpflow.dat        ../mod500m-10K/wpflow.dat'
diff wpflow.dat        ../mod500m-10K/wpflow.dat
```

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-546	2. Software Title and Version: TPA 5.0.0g	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): releaset.f

Releaset has long run times for long simulation times.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
R. Codell Date: 2-2-2005	R. Janetzke Date: 2-4-2005

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): A note from R. Codell:

```
I fixed the problem of long run times I think by modifying the minimum volumes in the
waste package to be artificially large. The changes are in 'liqrel()' after line 1329.
The new minimum volume is 100 times bigger than the maximum flow rate though the waste
package per year. This seems to have no effect on the results for long times even
though it is physically the wrong volume. The large volume assures that the time step
can be large when things change slowly. I would think the effects of the change would
be more noticeable for 10,000 year runs, but cannot be seen for a million year run.
For the one run I did, it reduced the number of calls to the derivative routine from
880,000 to about 47,000, which is about 20 time faster.
```

See attachment A for changes.

8. Implemented by:	Date:
R. Codell	2-12-05

9. Description of Acceptance Tests:

See attachment B for description of acceptance tests.

10. Tested by:	Date:
R. Rice	5/12/05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)

Attachment A

```
c
C  note: solubility is in kg/m^3 = mg/l to be input in radionuclide
C        data file
C-----------------------------------------------------------------------
CCCCCC
C     Start here.
CCCCCC

        pi = 4.*atan(1.)
        iflaga = 0
c        set minimum volume in stirred tank for numerical purposes
        qtmp=0.0
        do i=1,ntemp
crbc99 check only up to first 10,000 years
c       if(qin(i).gt.qtmp.and.tflo(i).lt.10000.d0)qtmp=qin(i)
crbc2/7/05 for long time runs, go beyond 10000 years
c       if(qin(i).gt.qtmp)qtmp=qin(i)
c
        end do
c        prevent division by zero
        if(qtmp.le.0.0d0) qtmp=1.0d-20
        if ( vtmp/qtmp.lt.100. ) then
          vmax = 100.*qtmp
        else
          vmax = vtmp
        end if
crbc1-5-98 caculate the vfull factor for flow through model based on
c           the time constant
        vfullflow=100.*qtmp

cc rwj 3-29-00  Per telecon with R. Codell, keep volume large enough for
cc              efficient integration stepping 10 liters min rbc5/10/00.
c       if (vfullflow .lt. 0.01)vfullflow = 0.01
crbc2/10/05 increase minimum to 100 years
        if (vfullflow .lt. 100.0)vfullflow = 100.0
c

c        write (1, *) 'above:vmax,vtmp,qtmp=', vmax, vtmp, qtmp

C calculate uo2 matrix leachng time

        tmass0 = amass0*xfrac
        tftc = max(tfail, tcool)

c        write (1, *) 'amass0=', amass0
```

Attachment B

Test Plan for TPA SCR#546

Test Plan Name: Releaset modifications to decrease run time for long simulation times

Tested By: R. Rice **Date:** May 12, 2005

Host Machine: Toshiba Laptop **Host OS:** XP Professional

Baseline Version: 5.0.0g **Test Version:** 5.0.0h

(Note that Version 5.0.0o was also used as a test version since it is the first version that allows long simulations)

System Level (SL) Tests

SL-1. Name: Versions 5.0.0g and 5.0.0h comparison

Path for run directory: c:\SCR546_working\tpa500g\basecase and
c:\SCR546_working\tpa500h\basecase
(see 100k and meanvalue subdirectories)

Path for archive of results: \SCR546_working\tpa500g\basecase and
\SCR546_working\tpa500h\basecase (archived on CD 1 of 3)

Environment variables: TPA_DATA=c:\SCR546_working\tpa500g\
TPA_TEST=c:\SCR546_working\tpa500g\

and

TPA_DATA=c:\SCR546_working\tpa500h\
TPA_TEST=c:\SCR546_working\tpa500h\

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Using the basecase TPA code for Versions 5.0.0g and 5.0.0h, compare TPA code output to check the impact of modifications made to the RELEASET

source code to decrease run time

- Objective: Verify RELEASET modifications have an acceptable impact on the calculated peak mean dose for 10kyr and 100kyr runs (basecase) and for 10kyr and 100kyr runs (mean values).

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: screenprint (i.e., *tpa.out*)

- Step by step test procedure to be used:

Execute the TPA Versions 5.0.0g and 5.0.0h code using the basecase *tpa.inp* file and the mean value *tpa.inp* file for both 10kyr and 100 kyr runs. Then, perform the following:

1. Examine the peak mean dose and the time of the peak mean dose from these runs in the screenprint
2. Compare the values in #1 from corresponding TPA Versions 5.0.0g and 5.0.0h code runs
3. Determine the percent differences between values in #2 and compare this with the PASS/FAIL criteria for the test

- Pass/Fail criteria:

Criteria 1: Peak mean dose and the time of the peak mean dose percent differences should be less than 20% (note that the author of the SCR expected differences in results as run time decreased)

Criteria 2: Peak mean dose percent differences should decrease for corresponding10kyr and 100kyr TPA code runs in the basecase and meanvalue runs (see the note above for Criteria 1)

Test Results: The screenprint (*tpa.out*) in the run subdirectories for this test is includes on the CD attached to this test plan (see on CD 1 of 3). The test results are provided in the table below.

	Peak Mean Dose in rem/yr (Time of the Peak Mean Dose in yr)		
Max. Time (yr)	**TPA Version 5.0.0g**	**TPA Version 5.0.0h**	**Percent Difference**
10,000 - basecase	1.9726E-4 (8,690.8)	2.2177E-4 (8,896.6)	12.4% (2.4%)
100,000 - basecase	1.9649E-4 (8,690.8)	2.1241E-4 (8,690.8)	8.1% (0.0%)
10,000 - meanvalue	1.2789E-4 (8,101.3)	1.3474E-4 (8,101.3)	5.4% (0.0%)
100,000 - meanvalue	1.2915E-4 (8,101.3)	1.2703E-4 (8,293.4)	-1.6% (2.4%)

- Overall test status: <u>PASS</u>

SL-2. Name: Version 5.0.0o comparison with and without RELEASET modifications

Path for run directory: c:\SCR546_working\tpa500o_preSCR546\ and
c:\SCR546_working\tpa500o_postSCR546\

Path for archive of results: \SCR546_working\tpa500o_preSCR546\ (archived on CD 2 of 3) and
\SCR546_working\tpa500o_postSCR546\ (archived on CD 3 of 3)

Environment variables: TPA_DATA=d:\rrice\SCR546_working\tpa500o_preSCR546\
TPA_TEST=d:\rrice\SCR546_working\tpa500o_preSCR546\

and

TPA_DATA=d:\rrice\SCR546_working\tpa500o_postSCR546\
TPA_TEST=d:\rrice\SCR546_working\tpa500o_postSCR546\

Special input files or modifications to input files required: Compile Version 5.0.0h *releaset.f* using the *maxntime.i* file from Version 5.0.0o which has increased number of time steps

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Compare results from the basecase TPA code for Version 5.0.0o with RELEASET executables from (1) 5.0.0o, called "postSCR546", and (2) 5.0.0h compiled using the increased number of time steps from *maxntime.i* in Version 5.0.0o, called "preSCR546)".

- **Objective:** For long simulations (1,000,000 years or 1e6 yr) and for 10kyr (1e4 yr) and 100kyr (1e5 yr) simulations with basecase Version 5.0.0o, verify that *releaset.f* output, peak mean dose, and time of the peak mean dose are consistent with and without the *releaset.f* modifications. Also, verify that the run time for the long simulations is reduced.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** screenprint (i.e., *tpa.out*) and

- Step by step test procedure to be used:

Execute the TPA Version 5.0.0o coded with and without the *releaset.f* modifications for (1) meanvalues (1e6 yr), (2) multiple realizations (1e6 yr; use the first 4 realizations out of 500), and (3) single subarea (1e6, 1e5, and 1e4 yr; subarea 1 for realization 1 out of 500). Then, perform the following:

1. For the meanvalues (1e6 yr), examine the peak mean dose and the time of the peak mean dose in the screenprint
2. Compare the values in #1 from preSCR5456 and postSCR546 TPA code runs
3. Determine the percent differences between values in #2 and compare this with the PASS/FAIL criteria for the test
4. Repeat steps #1-3 for the multiple realization run (1e6 yr)
5. Repeat steps #1-3 for the single subarea run and 1e6, 1e4, and 1e4 yr runs
6. For the 1e6 yr runs above, examine the number of times derivs is called (refer to the contents of the *releaset.out* file) for the preSCR546 and postSCR546 cases

- Pass/Fail criteria:

Criteria 1: Peak mean dose and the time of the peak mean dose percent differences should be less than 20% (note that the author of the SCR expected differences in results as run time decreased)

Criteria 2: Peak mean dose percent differences should decrease for corresponding 1e4, 1e5, and 1e6 yr TPA code runs in the single subarea run (see the note above for Criteria 1)

Criteria 3: Number of times derivs is called should decrease or stay the same for preSCR546 and postSCR546 results

Test Results: The screenprint (*tpa.out*) in the run subdirectories for this test is includes on the CDs attached to this test plan. In the "preSCR546" (CD 2 of 3) and "postSCR546" (CD 3 of 3) subdirectories, see subdirectories named "meanvalue", "4real", and "sa1_real1". The later subdirectory also contains "10k" and "100k" subdirectories.

For the meanvalue runs, test results are provided in the table below.

	Peak Mean Dose in rem/yr (Time of the Peak Mean Dose in yr)		
Max. Time (yr)	**preSCR546**	**postSCR546**	**Percent Difference**
1,000,000	8.5141E-6 (98,481.0)	8.5075E-6 (98,481.0)	-0.078% (0.0%)

For the multiple (i.e., 4) realization runs, test results are provided in the table below.

Peak Mean Dose in rem/yr (Time of the Peak Mean Dose in yr)

Max. Time (yr)	preSCR546	postSCR546	Percent Difference
1,000,000	1.3475E-2 (200,580.0)	1.3461E-2 (201,190.0)	-0.10% (0.30%)

For the single subarea runs, test results are provided in the table below.

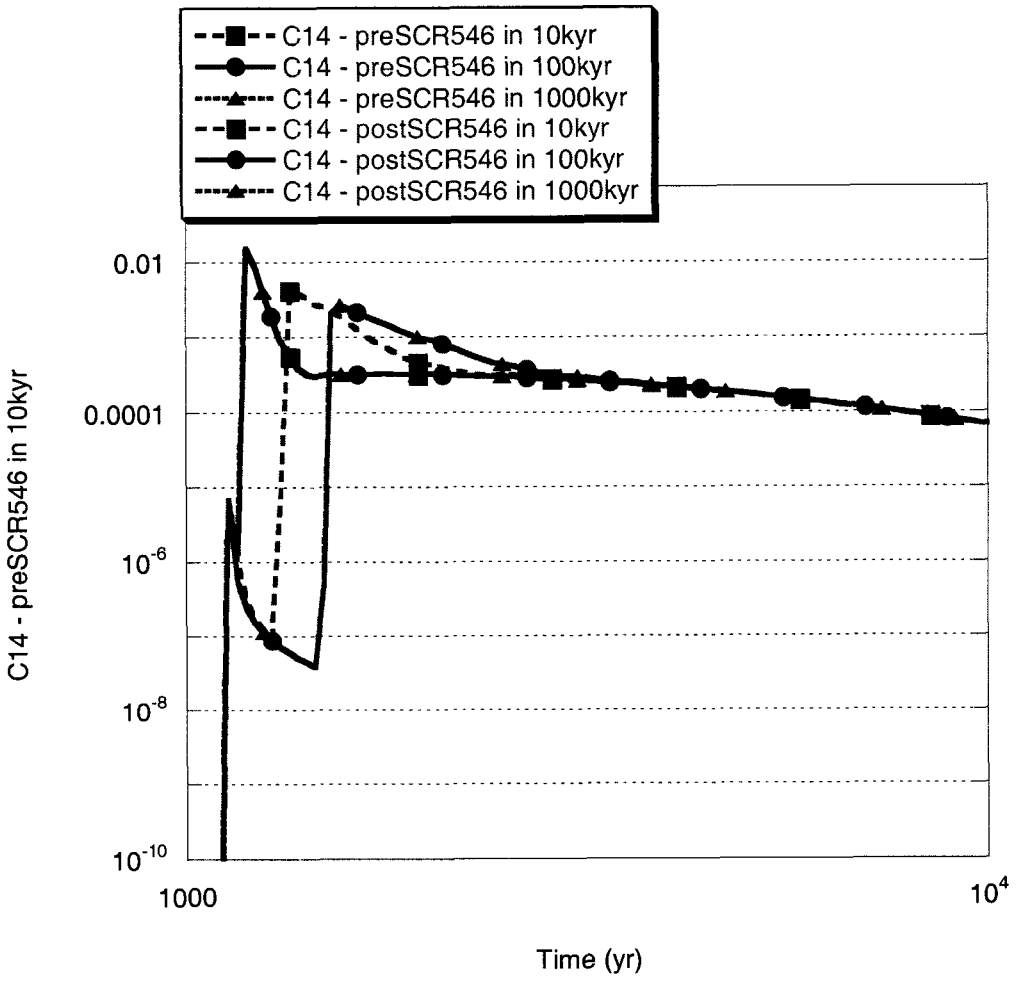
	Peak Mean Dose in rem/yr (Time of the Peak Mean Dose in yr)		
Max. Time (yr)	**preSCR546**	**postSCR546**	**Percent Difference**
10,000	1.0065E-5 (1,994.7)	9.7353E-6 (1,994.7)	-3.3% (0.0%)
100,000	1.4637E-4 (100,000.0)	1.4689E-4 (100,000.0)	0.36% (0.0%)
1,000,000	1.5378E-4 (101,990.0)	1.5382E-4 (101,990.0)	0.026% (0.0%)

For the number of times derivs called for 1e6 yr runs, test results are provided in the table below.

	Number of Times "derivs" called in RELEASET (from *releaset.out)*		
Run	**preSCR546**	**postSCR546**	**Factor Decrease**
meanvalue*	92,203	88,312	1.04
multiple realizations*	87,829	87,829	1.00
single subarea	196,921	88,300	2.23

* from subarea 7 (i.e., the last subarea analyzed in that particular TPA code simulation)

A plot of the results from the single subarea case for C14 release rates in preSCR546 and postSCR546 provides an illustration of an example of these satisfactory test results. The plot is provided below.



- Overall test status: <u>PASS</u>

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-547	2. Software Title and Version: TPA 5.0.0p	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *tpa.inp*

Based on the e-mail from D. Pickett presented in Attachment A.

5. Change Requested by: R. Codell Date: 2-1-05	6. Change Authorized by (*Software Developer*): R. Janetzke Date: 2-1-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The *tpa.inp* was changed from:

```
logtriangular
SolubilityNp[kg/m3]
1.2e-3, 3.4e-2, 2.4
```

To:

```
loguniform
SolubilityNp[kg/m3]
1.1e-4, 5.9e-1
```

8. Implemented by: R. Janetzke	Date: 4-9-05

9. Description of Acceptance Tests: Examined the p and q versions for change.

```
** ( From p version)
logtriangular
SolubilityNp[kg/m3]
1.2e-3,  3.4e-2,  2.4

** ( From q version )
** rwj 4-9-05; SCR547
**logtriangular
loguniform
SolubilityNp[kg/m3]
1.1e-4,  5.9e-1
**1.2e-3,  3.4e-2,  2.4
**
```

```
Expected mean value from Att. A
8.1e-3 kg/m3

Value from q ver of tpameans.out file
constant
SolubilityNp[kg/m3]
8.0560536244491D-03
```

PASS

10. Tested by: A. Lozano	Date: 4-11-05

CNWRA Form TOP-5 (05/2000

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
MODIFY FROM	ebsrel	`Solubility Np[kg/m3]`	Spent fuel Neptunium solubility.	Logtriangular	`1.2e-3, 3.4e-2, 2.4`	See Attachment A	DP
MODIFY TO	ebsrel	`Solubility Np[kg/m3]`	Spent fuel Neptunium solubility	Loguniform	`1.1e-4, 5.9e-1`	See Attachment A	DP

Attachment A

Here's where my thinking stands on Np solubility limit. Feel free to forward to interested parties. (Note: calculations and analyses recorded in Scientific Notebook 172. DOE reports used were mainly TBDoc 7, ANL-WIS-MD-00010 Rev 2, and ANL-EBS-MD-000033 Rev 2.)

First, as you probably heard at the latest team meeting, DOE told the NWTRB that they are currently revising the Np solubility limit abstraction. I'll keep looking for the slides at the NWTRB website, but Bret seemed to say that they will be lowering their values. It would be nice if this were a topic in a future NWTRB meeting, but we'll have to wait and see. One of the documents I used - "Dissolved Concentration Limits of Radioactive Elements," ANL-WIS-MD-000010 - has been revised but the revision has not been released.

As I've mentioned, in the most recent DOE documents, they concluded that the basis for a secondary retention model for Np concentration limit was insufficient. For instance, one recent set of experiments showed little to no Np incorporation into schoepite, which DOE considers to be the dominant secondary U phase. I'm sure they're still looking at this, and perhaps new data will be coming out. (Note that Bill Murphy agrees that the data and model are not good enough at this point.)

For now, what I've done is to come up with a new proposed distribution based on the DOE solubility models and in-package chemistry models. We don't have independent models at this point, but I hope to before the end of the year. The DOE abstraction is a function of pH and f(CO2), so I used the most current TSPA abstracted ranges of those parameters and looked to see what Np solubility limits they would predict for those ranges. For instance, the DOE in-package chemistry model for CSNF after 600 years samples pH from a uniform distribution from 4.5 to 7.0. I've examined the bases for this distribution, and it seems sound, though pH up to 8 can be attained if water flux rates are higher than 50 L/yr per waste package. Because pH is sampled uniformly, the log of Np solubility is linear with pH, and f(CO2) has little effect in this pH range, the resulting [Np] distribution is log-uniform.

DOE considers two solubility-controlling Np pure phase solids: Np2O5 and NpO2. The former is observed in low-temperature solubility experiments, while the latter is only observed in higher-temperature experiments. Thermodynamic data suggest that NpO2 should be the more stable phase, but it may be kinetically disfavored at laboratory time scales.

Therefore, DOE uses Np2O5 because it gives higher Np concentrations and the lab data are not compelling enough to go with NpO2. I've incorporated the uncertainty in solid phase by using the Np2O5 maximum and the NpO2 minimum for my distribution. (The lower minimum for NpO2 also indirectly accounts for the unrelated possibility of pH up to 8 at higher fluxes leading to lower concentrations.)

The resulting log-uniform distribution, with [Np] in kg/m3:

minimum = -3.95 (1.1e-4 kg/m3)
mean = -2.09 (8.1e-3 kg/m3)
maximum = -0.23 (5.9e-1 kg/m3)

Compared to the current log-triangular TPA distribution, the new maximum is about twice as high, the new minimum is an order of magnitude lower, and the new mean is about one-third. So, overall, the distribution is lower, but because it's uniform instead of triangular, there's the possibility of greater influence of high values.

For comparison to that Figure 6-12 in TBDoc 7 (note units change), this proposed range is from 0.1 to 590 mg/L. So even though the minimum is an order of magnitude lower than the existing TPA minimum, the numbers are still above the majority of the leach test results. But, as I've said before, that's not unexpected for a solubility limit.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-548	**2. Software Title and Version:** TPA 5.0s	**3. Project No:** 20.06002.01.354
4. Affected Software Module(s), Description of Problem(s): Update to Software Validation Test Plan (SVTP).		
5. Change Requested by: R. Folck Date: 4-8-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 4-8-05	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment A for updated SVTP.		
8. Implemented by: R. Janetzke	**Date:** 4-9-05	
9. Description of Acceptance Tests: **None.**		
10. Tested by:	**Date:**	

CNWRA Form TOP-5 (05/2000)

Attachment A

1 SCOPE OF VALIDATION

1.1 INTRODUCTION

This report is a software validation plan for the Total-System Performance Assessment (TPA) Version 5.0.1 as outlined in Appendix F of the CNWRA Technical Operating Procedure 18 (TOP-18). This version of the code is an update to the TPA version 5.0q. It is assumed that the reader is familiar with the function and operation of the TPA code.

The purpose of software validation is to improve the software product and ensure its proper operation via a systematic process of testing and review. There has been much inconsistency in the use of the terms 'validation' and 'verification is the software industry. The American National Standard ANSI/ANS-10.4-1987 refers to 'program validation' as testing each requirement and simply noting if the test was successful. This is a very high level approach that may be suitable for simple business applications that access a data base, perform a few calculations and display the results. In this case, simply checking that the correct data was retrieved from the data base and that the calculation returned the correct result by visual inspection may constitute validation. However, modeling complex physical processes that have not been modeled before does not lend itself to such a scheme, and a more comprehensive approach may be required.

Software verification has a similar purpose, but usually addresses the mechanics of the inter-operation among the modules. On the surface, validation is very similar to the verification process, since both involve testing and review. However for the purposes of this report and the use of CNWRA Technical Operating Procedure 18, software verification is thought of as checking the process by which the software was developed (demonstrating credibility), whereas validation is the process of ensuring that the software performs the required functions (demonstrating capability).

This software validation test plan documents the tests to be executed on the Total-System Performance Assessment (TPA) code version 5.0.1. Two general categories of tests will be performed, system level and process level. Only the TPA executive and its associated modules that have been modified since Version 5.0q will undergo both system level and process level tests, and only the auxiliary codes modified since Version 5.0 will undergo system level tests.

1.2 SYSTEM LEVEL TESTS

System level tests evaluate the main results of the system taken as whole. This usually involves the review of the major output files as well as any screen output. For this, contrived cases will be developed for the TPA and auxiliary codes, such that the results can be easily checked against, existing studies, hand calculations or a spreadsheet. The TPA code uses 10 auxiliary codes.

1.3 PROCESS LEVEL TESTS

Process level tests evaluate the results of an individual subroutine or function subprogram. This usually involves the generation of what is called scaffolding software that supports the module and aids in the display of input and output parameters as it is tested in a standalone environment separate from the rest of the system.

2 REFERENCES

CNWRA Technical Operating Procedure 18, revision 9, 12-20-2004.

CRWMS M&O. "Total System Performance Assessment for the Site Recommendation." TDR–WIS–PA–000001. Revision 00 ICN 01. Las Vegas, Nevada: TRW Environmental Safety Systems, Inc. 2000.

———. "Supplemental Science and Performance Analyses." TDR–MGR–MD–000001. Revision 00. Las Vegas, Nevada: CRWMS M&O . 2001.

Stothoff, S. NUREG/CR–6333. "BREATH Version 1.1—Coupled Flow and Energy Transport in Porous Media, Simulator Description and User Guide." CNWRA 94-020. San Antonio, Texas: CNWRA. 1995.

3 ENVIRONMENT

3.1 Software

The software to be used for this validation process is the TPA version 5.0.1 code. The TPA code can be obtained locally from host machines \\Vermont (PC version) or Spock (UNIX version). A complete listing of the executive subprograms appears in Appendix A. The programs will be compiled using the SUNWspro Fortran compiler version 5.0 or Lahey LF95 version 7.1.

The subprograms of the executive are to be tested via a method that permits the input parameters to be set without the use of any intervening software from the original system. This usually requires scaffold software to be developed to provide an environment that can exercise the module as it would be used in the executive module. The scaffold software should present a known set of input parameters to the module and record the state of all of the output parameters upon completion. Possible test cases to consider are text book examples, case studies previously documented in the literature, and mathematical limits or singularities of the input parameters. An effort should be made to exercise all of the possible error paths in order to check that the error messages are meaningful and correct, and that all error conditions are handled appropriately.

3.2 Hardware

The validation tests will be performed on a SUN/sparc processor using the SUN OS version

5.8 operating system or a PC using the Microsoft/Windows XP operating system. All test results should be archived on a CD or the DVD storage facility at the CNWRA.

4 PREREQUISITES

The execution of the TPA code requires the setting of two environment variables, TPA_TEST and TPA_DATA. These should point to the parent directory for the *codes* and *data* subdirectories.

5 ASSUMPTIONS AND CONSTRAINTS

It is assumed that the tests performed on the UNIX system will have the same results if performed on a Windows/XP system. It is also assumed that the scaffold software produces the same behavior of the module under test as it exhibits in the TPA code. The TPA code also uses output from external codes ITYM and MULTIFLO, and it is assumed that their validation will be provided elsewhere.

6 TEST CASES

6.1 Test Cadre

The exact compliment of tests for each tested module will be determined by the test lead, co-lead and the PI for TPA code development. As a minimum, tests shall stress the module in several ways including neutralizing the barrier under consideration, and then neutralizing all barriers except the one under consideration to the extent possible. Other stress tests should consider extremes of input parameters used by the module.

7 NOTES

7.1 Testing

As stated in TOP-18, tests shall provide evidence of correct and successful implementation of the underlying theory and algorithms, and evidence of benchmarking or comparative testing against results from other software. Also tests shall describe comparisons of test results to research papers, laboratory experiments, existing test cases, or previously published sources of data, when available.

As a way to establish confidence in the software, test cases may consist of comparison with known solutions, hand calculations, or to computations obtained with commercial mathematical software, such as MathCad, Mathematica or Matlab. Each test case should have a clear and concise description of the theory and/or algorithm involved, test method, and expected results. Section 4.2

of TOP-18 covers these and other topics related to software validation.

The test plan, documentation, and results for each tested module will be contained in a Software Validation Test Report (SVTR) as shown in Appendix B.

Appendix A

```
tpa500o/array.f:      subroutine zero( n, v )
tpa500o/array.f:      subroutine zeroi( n, iv )
tpa500o/array.f:      subroutine clearchar( n, name )
tpa500o/array.f:      subroutine initr( val, n, v )
tpa500o/array.f:      subroutine scale(c, n, v )
tpa500o/array.f:      subroutine scopy(c, n, vin, vout )
tpa500o/array.f:      subroutine acopy(c, n, vin, vout )
tpa500o/array.f:      subroutine addto(n, vin1, vin2 )
tpa500o/array.f:      subroutine isoneofset( iquery, nset, iset, index )
tpa500o/array.f:      subroutine checkinorder( n, x, icheck )
tpa500o/array.f:      subroutine checkforduplicates( n, x, icheck )
tpa500o/array.f:      subroutine icheckforduplicates( n, ix, icheck )
tpa500o/array.f:      subroutine sortqr(n, v, ipt)
tpa500o/array.f:      subroutine maplist(n1, x1, y1, n2, x2, y2)
tpa500o/array.f:      subroutine maptimeofevent(timeofevent, valueinitial, valueinput,
tpa500o/ashplumo.f:     subroutine ashplumo(ir,amtuejected,gramsashpercm2,gramsfpercm2)
tpa500o/ashplumo.f:     subroutine ashplume(ir,xmin,xmax,numptsx,ymin,ymax,numptsy,
tpa500o/ashremob.f:     subroutine ashremob( irl, mxntime, mxnnucldr, ntim, tim, nnucldr,
tpa500o/ashrmovo.f:       subroutine ashrmovo(gramsfpercm2,
tpa500o/ashrmovo.f:       subroutine leachrate(dkd,fpe,fpsat,fie,fisat,precip,dirr,
tpa500o/condxyzt.f:     subroutine cond3dxyzt(  aLin, aBin, aHin,
tpa500o/condxyzt.f:     subroutine xgauleg(func,a,b,n,ss)
tpa500o/dcags.f:      subroutine dcags( irl, mxntime, mxnnucldr,
tpa500o/dcags.f:      subroutine checkvalues( massloadashheavy,  massloadashlight,
tpa500o/dcags.f:      subroutine gentpags( irl, gset )
tpa500o/dcags.f:      subroutine copylinesgs(ifromlun, itolun, nlines)
tpa500o/dcags.f:      subroutine gentodcfgs(climate,age,rir)
tpa500o/dcagw.f:      subroutine dcagw( irl, mxntime, mxnnucl,
tpa500o/dcagw.f:      subroutine gentpa( irl )
tpa500o/dcagw.f:      subroutine copylines(ifromlun, itolun, nlines)
tpa500o/dcagw.f:      subroutine gentodcf(climate,age)
tpa500o/dsfail.f:     SUBROUTINE DSFAIL(numberOfTimeSteps, timeValue,
tpa500o/dsfail.f:     SUBROUTINE buildInputFiles(iUnitFile, iUnitFluoride,
tpa500o/dsfail.f:     SUBROUTINE setupCommons(iUnitInput, dataFile)
tpa500o/ebsfail.f:      subroutine ebsfail(seismicFailDS, ir, isa, ntim, tim,
tpa500o/ebsfail.f:      SUBROUTINE getDSFailure(timeMark, seismicFailDS, time,
tpa500o/ebsrel.f:      subroutine ebsrel( seismicFailDS, ir, isa, mxntime,
tpa500o/ebsrel.f:      subroutine addebsnef( iebssfdat, iebsglassdat, iebsnefdat)
tpa500o/ebsrel.f:      subroutine releasecolloids( iebsnefdat, nnucl, numclnuc, cldnames)
tpa500o/exec.f:      subroutine writehead( iunit, title1, title2, datetim, m1, m2,
tpa500o/exec.f:      subroutine writehead2( iunit, title1, title2, datetim, m1, m2,
tpa500o/exec.f:      subroutine writedata( iunit, maxntime, ntim, nd2,
tpa500o/exec.f:      subroutine writeepaccdf(mxntime, mxnnucl, ntim, tim, nnucl, names,
tpa500o/exec.f:      subroutine cumfail( isa, ntim, tim,
tpa500o/exec.f:      subroutine putfailwp (isa, initialonly, corrosiononly,
tpa500o/exec.f:      subroutine setfiles(iflagsetfiles, mylastcheck)
tpa500o/exec.f:        subroutine EpaCCDF(mylastcheck)
tpa500o/exec.f:        subroutine EpaCCDF_c(mylastcheck)
tpa500o/exec.f:        subroutine CcdfIndexed( n, value, prob, nret, ccdf, ind)
tpa500o/exec.f:      subroutine checknr(nr, istartreal, istopreal)
tpa500o/exec.f:      subroutine checknsa(nsa, istartsuba, istopsuba)
tpa500o/exec.f:      subroutine cleanupwd ()
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tpa500o/exec.f:      subroutine findPkMnDose( inunit, outunit )
tpa500o/exec.f:      subroutine setup_kdrd_files()
tpa500o/faulto.f:      subroutine faulto( nsa, mxntim, ntim, tim, pfail )
tpa500o/fileunit.f:     subroutine printfun( )
tpa500o/fileutil.f:     SUBROUTINE getIntegerValue(iUnit, valueInteger, valueName,
tpa500o/fileutil.f:     SUBROUTINE getRealArray(iUnit, numValues, valueReal, valueName,
tpa500o/fileutil.f:     SUBROUTINE setIntegerArray(outFile, numValues, integerValue,
tpa500o/fileutil.f:     SUBROUTINE setIntegerValue(outFile, iValue, fileComment)
tpa500o/fileutil.f:     SUBROUTINE setRealArray(outFile, numValues, realValue,
tpa500o/fileutil.f:     SUBROUTINE setRealValue(outFile, rValue, fileComment)
tpa500o/fileutil.f:     SUBROUTINE setStringValue(outFile, valueString, fileComment)
tpa500o/iareader.f:       subroutine iasetup()
tpa500o/iareader.f:       subroutine iafile(iaunit)
tpa500o/iareader.f:       subroutine iabarrier(iaunit)
tpa500o/iareader.f:       subroutine iacomponent(iaunit)
tpa500o/iareader.f:       subroutine iaparameter(iaunit)
tpa500o/iareader.f:       subroutine checkforduplicate( cnamearray, index, maxsize,
tpa500o/iareader.f:       subroutine iavalue(iaunit)
tpa500o/iareader.f:       subroutine nextline(iaunit, clineid, cparamvalue, dparamvalue)
tpa500o/invent.f:      subroutine decay43mol( time, amolepermtu )
tpa500o/invent.f:      subroutine decayremove43mol( dt, dlremove, dnt1, dnt2 )
tpa500o/invent.f:      subroutine chains(maxnt, nt, time, dlt, dlr, dnt1, dn )
tpa500o/invent.f:      subroutine chainsolver(len, maxnt, nt, tim, dnt1, dlt, dlr, dn)
tpa500o/invent.f:      subroutine newinventdb()
tpa500o/invent.f:      subroutine decay43molglass( time, amolepermtuglass )
tpa500o/invent.f:      subroutine allchains(maxnt, nt, time, dlt, dlr, dnt1, dn )
tpa500o/mv.f:     subroutine newmvdb( )
tpa500o/mv.f:     subroutine setconsmv( imv, iowner, consv )
tpa500o/mv.f:     subroutine printtitlesmv( iunit )
tpa500o/mv.f:     subroutine printvaluesmv( iunit, ir )
tpa500o/nfenv.f:      subroutine nfenvFI( isa, ntim, tim, qm3peryrperwpinsa, temprep,
tpa500o/nfenv.f:      subroutine nfenv(seismicFailDS, isa, ntim, tim, relhumwp,
tpa500o/nfenv.f:      subroutine saddscale( n, c1, v1, c2, v2, v3 )
tpa500o/nfenv.f:      subroutine newxyinrotcs( xyi,  theta, xyo )
tpa500o/nfenv.f:        subroutine reflux1( iSA, tclosure, hloss_fact, ntim, tim,
tpa500o/nfenv.f:        subroutine nfdrip( iSA, ntim,
tpa500o/nfenv.f:       SUBROUTINE fill (ntim, tim, thick, xloss_i, xloss_d,
tpa500o/nfenv.f:       subroutine infil_calc (nreflux,xinterp_xmperyrinsa,
tpa500o/nfenv.f:      subroutine rock (thick, porosity, sat_init, sat_resid, boil)
tpa500o/nfenv.f:       subroutine dryout (boil, nreflux, xloss_d, period, reflux_d)
tpa500o/nfenv.f:      subroutine reflux3 (itpa, isa, ntim, tim,
tpa500o/nfenv.f:       subroutine interpolate (newtim, ntim, tim, qm3peryrinsa,
tpa500o/nfenv.f:       subroutine thickness_reader (nreflux,
tpa500o/nfenv.f:       subroutine convertuz (isa, newtim, ntim, qm3peryrinsa,
tpa500o/nfenv.f:       subroutine perched_vol (nreflux, xinterp_xmperyrinsa,
tpa500o/nfenv.f:       subroutine losses (I, nreflux, perchedVol, xinterp_thick, xloss,
tpa500o/nfenv.f:        subroutine phillips_3d (i, nreflux, xinterp_thick, perchedvol,
tpa500o/nfenv.f:      subroutine tabulartemprh(ntim, tim, tempwp,relhumwp)
tpa500o/nfenv.f:      subroutine nearestpointonline ( x1, y1, x2, y2,
tpa500o/nfenv.f:      SUBROUTINE getPeakTimeOfDryout(numTime, time, tempRepository,
tpa500o/nfenv.f:      SUBROUTINE getLastTimeOfDryout(numTime, time,
tpa500o/nfenv.f:      SUBROUTINE getFirstTimeOfDryout(numTime, time,
tpa500o/nfenv.f:      SUBROUTINE assignConcentrations( numTime, time, dsFailTime,
tpa500o/nfenv.f:      SUBROUTINE assignConcentrationsFI( numTime, time,
tpa500o/nfenv.f:      subroutine calcTempsLinear(time, timeClosure,
tpa500o/nfenv.f:      subroutine calcTempsIterative(time, timeClosure, tempRW, tempBF,
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tpa500o/nfenv.f:      subroutine checkValidity()
tpa500o/nfenv.f:      subroutine calculateTemperaturesAbove()
tpa500o/numrecip.f:       subroutine gauleg(x1,x2,x,w,n)
tpa500o/numrecip.f:      subroutine zbrent1(root, func, x1, x2, tol, errorflag)
tpa500o/numrecip.f:      subroutine zbrent(root, func, x1, x2, tol, errorflag)
tpa500o/numrecip.f:      subroutine zbrak1(fx, x1, x2, n, xb1, xb2, nb, nbmax)
tpa500o/numrecip.f:      subroutine zbrak(fx, x1, x2, n, xb1, xb2, nb, nbmax)
tpa500o/peakfind.f:     subroutine peakfinder( mxntime, mxnnucl,
tpa500o/ran.f:     subroutine setran( aseed1 )
tpa500o/ran.f:     subroutine setranseis( aseed1 )
tpa500o/reader.f:     subroutine reader( iunit,
tpa500o/reader.f:     subroutine skipcommentline( iunit )
tpa500o/reader.f:     subroutine readname( iunit, name )
tpa500o/reader.f:     subroutine checknucchains(nnucl, names)
tpa500o/reader.f:     subroutine readabbdb()
tpa500o/reader.f:     subroutine findstringinset(name, max, stringset, index)
tpa500o/reader.f:     subroutine addabb(name, index)
tpa500o/reader.f:     subroutine makeifmt(number, format)
tpa500o/reader.f:     subroutine drifts( nsa, xy, amtusa, nwpsa )
tpa500o/reader.f:       subroutine segmenthitpoly(xw,yw, xe,ye,
tpa500o/reader.f:       subroutine outputWPendpoints( iunit, maxedges, xyhits,
tpa500o/reader.f:     subroutine fillsubareas( nsa, DriftSpacing,
tpa500o/reader.f:     subroutine writemeanvalues( iunit )
tpa500o/reader.f:     subroutine readcolloids( iunit, numclnuc, cldnames, numclchn,
tpa500o/reader.f:     subroutine querystop()
tpa500o/reader.f:     subroutine check_inputs()
tpa500o/reader.f:     subroutine check_timenextevent(eventname)
tpa500o/reader.f:     subroutine check_payload_glass()
tpa500o/sampler.f:      subroutine newspdb()
tpa500o/sampler.f:      subroutine addconstantpdf( name, conval)
tpa500o/sampler.f:      subroutine addiconstantpdf( name, iconval)
tpa500o/sampler.f:      subroutine adduniformpdf( name, xmin, xmax )
tpa500o/sampler.f:      subroutine addiuniformpdf( name, ixmin, ixmax )
tpa500o/sampler.f:      subroutine addloguniformpdf(  name, xmin, xmax )
tpa500o/sampler.f:      subroutine addnormalpdf( name,
tpa500o/sampler.f:      subroutine addlognormalpdf( name,
tpa500o/sampler.f:      subroutine addbetapdf( name,
tpa500o/sampler.f:      subroutine addlogbetapdf( name,
tpa500o/sampler.f:      subroutine addexponentialpdf( name, alam )
tpa500o/sampler.f:      subroutine addfiniteexponentialpdf( name, alam, xmin, xmax )
tpa500o/sampler.f:      subroutine addtriangularpdf( name,
tpa500o/sampler.f:      subroutine addlogtriangularpdf( name,
tpa500o/sampler.f:      subroutine newrealization(iunitsp, iunitcp, restart_flag)
tpa500o/sampler.f:      subroutine newlhssm( nbins )
tpa500o/sampler.f:      subroutine addhazardcurve( name, nbin, amag, period )
tpa500o/sampler.f:      subroutine samplehazardcurve( name, maxevents, timemax,
tpa500o/sampler.f:      subroutine lhsnew( maxnbin, maxnsp, nbin, nsp, x )
tpa500o/sampler.f:      subroutine printtitlessp( iunitcp, iunitsp, restart_flag )
tpa500o/sampler.f:      subroutine printvaluessp( iunit, ir )
tpa500o/sampler.f:      subroutine writesnllhsinp( iunit )
tpa500o/sampler.f:      subroutine checkspname( name )
tpa500o/sampler.f:      subroutine adduserdiscreteempirical( name, n, v )
tpa500o/sampler.f:      subroutine addusersupplieddiscrete( name, n, v, v2 )
tpa500o/sampler.f:      subroutine addusersuppliedpwisecdf( name, n, v, v2 )
tpa500o/sampler.f:      subroutine addcorrel( name1i, name2i, c)
tpa500o/sampler.f:      subroutine printtimesvalue( iunittimesvalue,ir,nr)
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tpa500o/sampler.f:     subroutine updatelhs( )
tpa500o/sampler.f:     subroutine checklhsout( numvec )
tpa500o/sampler.f:     subroutine retrieve_input(pname, ptype, pindex, dp1, dp2, dp3,
tpa500o/sampler.f:     subroutine update_input(pname, ptype, pindex, dp1, dp2, dp3,
tpa500o/seismo2.f:     subroutine eqvdia(numTime, time,
tpa500o/seismo2.f:     subroutine calculateDriftBFParameters(numTime, time,
tpa500o/seismo2.f:     subroutine processDriftHeight(analysisTime, deltaTime,
tpa500o/seismo2.f:     SUBROUTINE MECHDRIVER (numTime, maxNumTime, time,
tpa500o/seismo2.f:     SUBROUTINE buildCharacterString(characterString, lengthString,
tpa500o/seismo2.f:     SUBROUTINE buildMechfailInputFile(inFile, outFile, numTime,
tpa500o/seismo2.f:     subroutine getEquivalentDiameters(numTime, Time, closureTime,
tpa500o/subarea.f:     subroutine ssadb( nsa, xy )
tpa500o/subarea.f:     subroutine gnsa( nsa )
tpa500o/subarea.f:     subroutine gsarea( isa, area )
tpa500o/subarea.f:     subroutine gsaxy( isa, xy )
tpa500o/subarea.f:     subroutine gsaxym( isa, xymiddle )
tpa500o/subarea.f:     subroutine gsamtu( isa, amtupersa )
tpa500o/subarea.f:     subroutine gsanwp( isa, nwppersa )
tpa500o/subarea.f:     subroutine qphitsa( xyp, isa, iflag )
tpa500o/subarea.f:     subroutine qchitsa( xyp, radius, isa, iflag, areainsa )
tpa500o/subarea.f:     subroutine qlhitsa( xyp1, xyp2, isa, iflag, alengthinsa )
tpa500o/subarea.f:     subroutine linehitline( xyp1l1, xyp2l1,
tpa500o/subarea.f:     subroutine solve2x2( a, b, x )
tpa500o/subarea.f:     subroutine checkin( xyp, xy, iflag)
tpa500o/subarea.f:     subroutine root( n, x, eps, ifail, x2, f, df, dat,
tpa500o/subarea.f:     subroutine solvenxn( n, a, b, x )
tpa500o/subarea.f:     subroutine triangle( x1, y1, x2, y2, x3, y3, area)
tpa500o/subarea.f:     subroutine quadrilateral(xysa,quadarea)
tpa500o/subarea.f:     subroutine ssadba( amtupersa, nwppersa )
tpa500o/subarea.f:     subroutine gsanwpglass( isa, nwppersa, nglasspersa )
tpa500o/szft.f:     subroutine szft(ir, isa, mxntime, mxnnucl, ntim_c,
tpa500o/szft.f:     subroutine prenefmksa(isa, mxntime, ntim_c, ntimg, timg, mxnnucl,
tpa500o/szft.f:     subroutine getszunits (isa, disttocg, samixlength, widthmix,
tpa500o/szft.f:     subroutine centroid ( x, y, resultx, resulty )
tpa500o/szft.f:     subroutine distancebetween2points(xl1, yl1, xl2, yl2, dist)
tpa500o/szft.f:     subroutine rangecheck (modulename, variablename, ivaluemin,
tpa500o/szft.f:     subroutine disttoline (x, y, xl1, yl1, xl2, yl2, dist)
tpa500o/szft.f:     subroutine interpolateTAI( distLo,  distHi,  distTAI,
tpa500o/szft.f:     subroutine calc_vel_gwtt(mxntime, ntim, tim, itime_c, maxlyr,
tpa500o/szft.f:     subroutine setvelfile(mxntime, tim, ntim, numlayers, maxlyr,
tpa500o/szft.f:     subroutine mod_rdrdi(elist, maxiso, maxlyr, maxnumelem, numelem,
tpa500o/uzflow.f:     subroutine clidat_init( )
tpa500o/uzflow.f:     subroutine get_climean()
tpa500o/uzflow.f:     subroutine get_clinoise_set(mset)
tpa500o/uzflow.f:     subroutine climate_init( )
tpa500o/uzflow.f:     subroutine climato( )
tpa500o/uzflow.f:     subroutine get_data_file(zroutine, zfile)
tpa500o/uzflow.f:     subroutine DEMij_to_m(DTBLStat, mi, mx, my)
tpa500o/uzflow.f:     subroutine mapDTBL_to_SAs(DTBLStat, imap, imapMN)
tpa500o/uzflow.f:     subroutine load1DTBL(yfirst, iounit, zfile, DTBLStat, array)
tpa500o/uzflow.f:     subroutine loadDTBL(iounit, zfile, mndim1, mndim2, mndim3, ndim,
tpa500o/uzflow.f:     subroutine set_iouzflow()
tpa500o/uzflow.f:     subroutine uzflow_init( )
tpa500o/uzflow.f:     subroutine calc_wp(val, nvec, vec, wgt1, wgt2, mpnt1, mpnt2)
tpa500o/uzflow.f:     subroutine calc_mai(mSA, nTS, ainit, uzhpu)
tpa500o/uzflow.f:     subroutine calc_ainit(mnft, ainit_tab, fmin, fmax)
```

```
tpa500o/uzflow.f:      subroutine uzflow(isFirstSubarea, mSA, ntim, tim, QinSA)
tpa500o/uzft.f:     subroutine uzft( ir, isa, mxntime, mxnnucl,  ntim_c,
tpa500o/uzft.f:     subroutine prenefmks(isa, mxntime, ntim_c, ntimg, timg, nnucl,
tpa500o/uzft.f:     SUBROUTINE opnfil (unit,filnam,status,lplain,errnum,errmsg)
tpa500o/uzft.f:     subroutine runnefmks(istatus)
tpa500o/uzft.f:     subroutine writesource(mxntime, ntim, tim, nnucl, name,
tpa500o/uzft.f:     subroutine aftnefmks( mxntime,ntim,tim,nnucl,names,
tpa500o/uzft.f:     subroutine writevelocities( mxntime, ntim, tim, nefleg,
tpa500o/uzft.f:     subroutine getvertlayers ( maxlayers, salayernam, numsalayers)
tpa500o/uzft.f:     subroutine getelements( numisotopes, chainlist, maxnumelem,
tpa500o/uzft.f:     subroutine putgwtt (isa, zone, gwtt)
tpa500o/uzft.f:     subroutine trapint (n, x, y, result)
tpa500o/uzft.f:     subroutine calc_kd( ssareain, pco2in, phin, kds)
tpa500o/uzft.f:     subroutine calc_rd(matrixorfracture,frac_aperture,
tpa500o/uzft.f:     subroutine mod_kd(lname, ename, media, kd, rd)
tpa500o/volcano.f:     subroutine volcano( nsa, mxntim, ntim, tim,
tpa500o/volcano.f:     subroutine getdrifts(drxy1out, drxy2out, nWPindrift, maxdrifts,
tpa500o/zportunx.f:     SUBROUTINE ZPORTPARSEUNIXFILENAMETODOS(COMMAND,NEWCMD)
tpa500o/zportunx.f:     SUBROUTINE ZPORTFDATE(RetString)

tpa500o/array.f:     function ainterl( n, t, v, tin )
tpa500o/condxyzt.f:     function tempgl( t )
tpa500o/dsfail.f:     FUNCTION getThickness(iUnitFile, numberOfTimeSteps,
tpa500o/fileunit.f:     function igetunitnumber( name )
tpa500o/iareader.f:     function ucljsg(in)
tpa500o/invent.f:     function dmyexp(x)
tpa500o/invent.f:     function indexperiso( name )
tpa500o/invent.f:     function indexperisonostop( name )
tpa500o/invent.f:     function nameelem( index )
tpa500o/invent.f:     function nameiso( index )
tpa500o/invent.f:     function epalimperiso( index )
tpa500o/invent.f:     function activityperiso( index )
tpa500o/invent.f:     function wmoleperiso( index )
tpa500o/invent.f:     function halflifeperiso( index )
tpa500o/invent.f:     function qpermtu( time )
tpa500o/invent.f:     function indexofcolloidparent( cldname )
tpa500o/mv.f:     function iaddconsmv( name )
tpa500o/mv.f:     function imvquery( name )
tpa500o/mv.f:     function valueconsmv( imv )
tpa500o/nfenv.f:     function pvap( t )
tpa500o/nfenv.f:     function enormsq0_2d ( x0, y0, x1, y1 )
tpa500o/nfenv.f:     function enorm0_2d ( x0, y0, x1, y1 )
tpa500o/nrutil.f:     function fTargetBackfillOuter(temperatureBFO)
tpa500o/nrutil.f:     function fTargetThermalLoad(thermalLoad)
tpa500o/nrutil.f:     function fTargetDripShieldOuter(temperatureDSO)
tpa500o/nrutil.f:     function fTargetDripShieldOuterNoBackfill(temperatureDSO)
tpa500o/nrutil.f:     function fTargetWastePackage(temperatureWP)
tpa500o/nrutil.f:     function fTargetWastePackageEarly(temperatureWP)
tpa500o/ran.f:     function ran1( )
tpa500o/ran.f:     function ran1seis( )
tpa500o/ran.f:     function raneseis(alam)
tpa500o/ran.f:     function iranu(ilow, ihigh)
tpa500o/reader.f:     function trimlen(string)
tpa500o/sampler.f:     function ispquery( namin )
tpa500o/sampler.f:     function ispquerynostop( namin )
tpa500o/sampler.f:     function isconstant( index )
```

```
tpa500o/sampler.f:      function valuesp( ipdf )
tpa500o/sampler.f:      function ivaluesp( ipdf)
tpa500o/sampler.f:      function mget_from_name(zname)
tpa500o/sampler.f:      function iget_from_name(zname)
tpa500o/sampler.f:      function dget_from_name(zname)
tpa500o/subarea.f:      function fcn( n, i, c, xy )
tpa500o/uzflow.f:     function kstr2tok_and_val(zstr, mnstr, ztok, mntok, val)
tpa500o/uzflow.f:     function yutok_in_ustr(ztok, zstr, mntok)
tpa500o/uzflow.f:     function locadd_vector(val, ndim, vec, flagempty)
tpa500o/uzft.f:     function ucljs(in)
tpa500o/uzft.f:     function ljs(in)
tpa500o/uzft.f:     function ljs2(in)
tpa500o/zportunx.f:     FUNCTION ZPORTDERF(X)
tpa500o/zportunx.f:     FUNCTION ZPORTSH(COMMAND)
tpa500o/zportunx.f:     FUNCTION ZPORTTIME()
tpa500o/zportunx.f:     FUNCTION ZPORTCTIME(SYSTIME)
tpa500o/zportunx.f:     FUNCTION ZPORTIEEE_FLAGS(MYACTION,MODE,ININ,OUTOUT)
tpa500o/zportunx.f:     FUNCTION ZPORTFDATEFUN()
```

APPENDIX B

SOFTWARE VALIDATION TEST REPORT (SVTR)

SVTR#:	Project#:
Software Name:	Version:
Test ID:	Test Series Name:

Test Method

- ☐ code inspection
- ☐ output inspection
- ☐ hand calculation
- ☐ spreadsheet
- ☐ graphical
- ☐ comparison with external code results

Test Objective:

Test Environment Setup

Hardware (platform, peripherals):

Software (OS, compiler, libraries, auxiliary codes or scripts):

Input Data (files, data base, mode settings):

Assumptions, constraints, and/or scope of test:

Test Procedure:

Test Results

Location:

Test Criterion or Expected Results:

Test Evaluation (Pass/Fail):

Notes:

Tester:	Date:

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-549	**2. Software Title and Version:** TPA 5.0.0o	**3. Project No:** 20.06002.01.354
4. Affected Software Module(s), Description of Problem(s): *releaset.f, wpflow.def, ebsrel.f, seisadj.i* The subarea **fwet** parameter for *releaset.f* is not correlated to the climate infiltration fluctuations since it is constant for all time.		
5. Change Requested by: R. Codell Date: 2-1-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 2-1-05	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment A for an e-mail description from R. Codell. See Attachment B for a listing of the new *wpflow.def* file from K. Compton.		
8. Implemented by: R. Codell / K. Compton / R. Janetzke	**Date:** 4-4-05	
9. Description of Acceptance Tests: See Attachment C.		
10. Tested by: C. Scherer	**Date:** 4-23-2006	

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)

ATTACHMENT A

It incorporates the following changes:

1. It reads an additional column in file '*ebsflo.dat*' that contains the time dependent value of the parameter in *releaset.f* called '**sawetfrac**', that is the name given to **Fwet**.

2. It maintains the original fixed value of the parameter **sawetfrac** that can be used as a static multiplier or simply set to unity.

...

[It uses subroutines **linearInerpolation()** and **srchpos()** to interpolate values of sawetfrac from the table as a function of time. *(Text added by R. Janetzke 4-9-05)*]

The code has been tested by taking the original file ' *ebsflo.dat*' generated by a tpa run and adding the additional data column that all had the value of 1.0. The results were then visually compared to the original run with *releaset.f* and found to be identical. Curiously, the two runs of *releaset* and *releaset_fw* differed in the number of times the routine **derivs()** was called, but I believe this is due to the way in which I compiled and linked the codes before running.

Note that the attached code version *releaset_fw.f* has been hard-wired to read the file '*hydfiltemp.inp*' instead of the name of the file named in from the ' *ebsrel.inp*' file. I did this to facilitate an easy comparison of the old and the new programs, and leave it to you to change it back to the original way once you are satisfied with it.

ATTACHMENT B

Time history of the factors for flow diversion (Fmult), flow contacting waste packages (Fow), and fraction wetted (Fwet) used in releaset (klc 4/4/05)

time(yr)	Fmult	Fow	Fwet
0	0.11	0.87	0.94
26	0.11	0.87	0.94
58	0.11	0.87	0.94
99	0.11	0.87	0.94
150	0.11	0.87	0.94
215	0.11	0.87	0.94
297	0.11	0.87	0.94
400	0.11	0.87	0.94
530	0.34	0.94	0.98
693	0.34	0.94	0.98
900	0.34	0.94	0.98
1160	0.57	0.96	0.99
1487	0.62	0.96	0.99
1900	0.64	0.97	1.00
2420	0.69	0.97	1.00
3076	0.74	0.97	1.00
3903	0.76	0.97	1.00
4945	0.77	0.98	1.00
6258	0.78	0.98	1.00
7914	0.78	0.98	1.00
10000	0.77	0.97	1.00
34750	0.74	0.97	1.00
59500	0.74	0.97	1.00
84250	0.74	0.97	1.00
109000	0.84	0.98	1.00
133750	0.74	0.97	1.00
158500	0.74	0.97	1.00
183250	0.74	0.97	1.00
208000	0.87	0.99	1.00
232750	0.11	0.87	0.94
257500	0.74	0.97	1.00
282250	0.74	0.97	1.00
307000	0.59	0.96	0.99
331750	0.74	0.97	1.00
356500	0.74	0.97	1.00
381250	0.74	0.97	1.00
406000	0.84	0.98	1.00
430750	0.40	0.95	0.99
455500	0.74	0.97	1.00
480250	0.82	0.98	1.00
505000	0.24	0.94	0.97
529750	0.65	0.97	1.00

554500	0.86	0.99	1.00
579250	0.87	0.99	1.00
604000	0.74	0.97	1.00
628750	0.74	0.97	1.00
653500	0.74	0.97	1.00
678250	0.59	0.96	0.99
703000	0.40	0.95	0.99
727750	0.74	0.97	1.00
752500	0.74	0.97	1.00
777250	0.84	0.98	1.00
802000	0.11	0.87	0.94
826750	0.74	0.97	1.00
851500	0.76	0.97	1.00
876250	0.31	0.94	0.98
901000	0.74	0.97	1.00
925750	0.74	0.97	1.00
950500	0.87	0.99	1.00
975250	0.11	0.87	0.94
1000000	0.74	0.97	1.00

ATTACHMENT C

Test Plan/Report for TPA SCR #549

Test Plan Name: Test Time-Dependent, Climate-Correlated Fwet Parameter

Tested By: Carol S. Scherer **Date:** May18, 2005

Host Machine: SUN Ultra-4 server: Spock **Host OS:** Sun Solaris 5.8

Baseline Version: TPA 5.0.0o **Test Version: TPA** 5.0.0p

Testing Setup:

Directories/paths used for testing:
$HOME = spock/home/cscherer
Path for run directory: ***$HOME/scr549***

Environment variables:

TPA_TEST = $HOME /*scr549*
TPA_DATA = $HOME /*scr549*

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled " *TPA SCR # 549 - Test Directories*" (attached).

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***scr549***, ***scr549/tpa500o***

2. Copy **TPA** version 5.0.0p to ***$HOME/scr549***. Compile *tpa.e*. Create subdirectory ***standalone-releaset***, and copy releaset.e to subdirectory.

3. Copy **TPA** version 5.0.0o to ***$HOME/scr549/tpa500o***. Compile *tpa.e*.

Function Level Tests:

These tests are designed to demonstrate the functionality of the specified module.

1. Name: Compare Standalone Run of Releaset.e with TPA Run at 100,000 Years.

2. Paths for archives of results: ***$HOME /scr549/test-report/flt1***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: base case *tpa.inp* for version **TPA**5.0.0o and for version **TPA**5.0.0p. Change OutputMode to 1 and MaximumTime to 1.0e5 in both versions.

Utility scripts needed to perform the test: none

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to verify that the modified releaset.f can give the same results as **TPA**5.0.0o.

- assumptions: all setup instructions have been carried out.

- constraints: none.

- output files to compare or examine: *cumrelse.out, diagnose.out, ebsnef.dat, ebssf.dat, frac_rel.out, inv1000.out. maxrel.dat, rel_flow.out, relcum.out, releaset.out, relfrac.out,* and *trelease.out* from the standalone and **TPA**5.0.0o runs

- step by step test procedure to be used:

  1. —> change directory to <<run directory>>
  2. run *tpa.e* using command "***tpa.e > tpa_100K-AF-500p.out***"
  3. copy *wpflow.def* to ***tpa500o/data***
  4. copy *ebsrel.inp*, *ebstrh.dat*, *ebsflo.dat*, and *ebspac.nuc* to ***standalone-releaset***
  5. —> change directory to <<run directory>>***/tpa500o***
  6. run *tpa.e* using command "***tpa.e > tpa_100K-AF-500o.out***"
  7. —> change directory to <<run directory>>***/standalone-releaset***
  8. modify *ebsflo.dat* by changing all values in the last column to 1.0
  9. run *releaset.e*
  10. compare *cumrelse.out, diagnose.out, ebsnef.dat, ebssf.dat, frac_rel.out, inv1000.out. maxrel.dat, rel_flow.out, relcum.out, releaset.out, relfrac.out,* and *trelease.out* from the standalone and **TPA**5.0.0o runs.

- pass/fail criteria: the test passes if:

  1. All runs complete successfully.
  2. The only differences between the files from *releaset.e* standalone run and the **TPA**5.0.0o run are time/date stamps and header information, with one exception. The

ebsnef.dat file from the standalone run contains only the 22 aqueous nuclides; the *ebsnef.dat* file from the **TPA**5.0.0o run also contains the 11 colloidal nuclides.

Results of running test:

PASSED.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

1. Name: Compare Output from **TPA5.0.0o** and **TPA5.0.0p** at 1,000,000 Years.

   Paths for archives of results: ***$HOME /scr549/test-report/slt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use base case *tpa.inp* for each version and make the following changes:

   set OutputMode to 1
   set MaximumTime to 1,000,000
   set NumberOfTimeStepsAfterCompliancePeriod to 4800

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to show that the modified **TPA**5.0.0p code generates results that reflect the changes to *wpflow.def* and the time-dependent fwet/sawetfrac parameter at 1,000,000 years.

   - assumptions: all setup instructions have been carried out.

   - constraints: the files *tpa_1M-AF-500o.out* and *tpa_1M-AF-500p.out* do not exist in the run directory.

   - output files to compare or examine: *ebsnef.dat* from both runs

   - step by step test procedure to be used:

1. —> change directory to <<run directory>>/***tpa500o***
2. run *tpa.e* using command "***tpa.e > tpa_1M-AF-500o.out***"
3. —> change directory to <<run directory>>
4. run *tpa.e* using command "***tpa.e > tpa_1M-AF-500p.out***"
5. create *ebsnef-dat.xls* using the U234 release data (*ebsnef.dat*) from each run; add data from *climato2.dat*, and fmult, fow, drip/wp, and flow factor from *ebsflo.dat*. Flow factor, drip/wp, fmult, and fow are multiplied together to produce "flow multiplier".

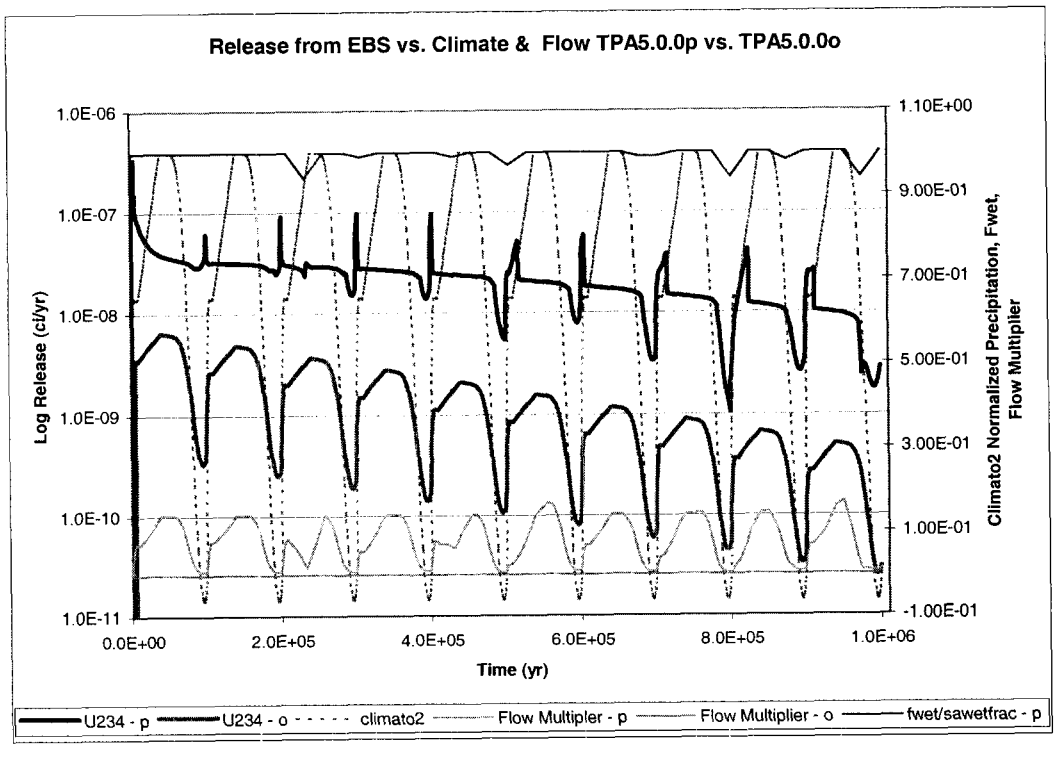
- pass/fail criteria: the test passes if:

  1. Both **TPA** runs complete successfully.

  2. See following graph "Release from EBS vs. Climate & Flow TPA5.0.0p vs TPA5.0.0o". The flow multiplier should change from a constant to a time-varying value that correlates directly and positively to the climate cycles and the fwet values. Release rates for U234 from **TPA**5.0.0p should be greater than release rates for U234 from **TPA**5.0.0o.

Results of running test:

PASSED.


Release from EBS vs. Climate & Flow TPA5.0.0p vs. TPA5.0.0o
1.0E-06
1.0E-07
1.0E-08
1.0E-09
1.0E-10
1.0E-11
Log Release (ci/yr)
1.10E+00
9.00E-01
7.00E-01
5.00E-01
3.00E-01
1.00E-01
-1.00E-01
Climato2 Normalized Precipitation, Fwet, Flow Multiplier
0.0E+00
2.0E+05
4.0E+05
6.0E+05
8.0E+05
1.0E+06
Time (yr)
U234 - p
U234 - o
climato2
Flow Multipler - p
Flow Multiplier - o
fwet/sawetfrac - p

NOTES:

05/18/5

Test Plan/Report for TPA SCR #549

Test Plan Name: Test Time-Dependent, Climate-Correlated Fwet Parameter

Tested By: Carol S. Scherer **Date:** May18, 2005

Host Machine: SUN Ultra-4 server: Spock **Host OS:** Sun Solaris 5.8

Baseline Version: TPA 5.0.0o **Test Version: TPA** 5.0.0p

Testing Setup:

Directories/paths used for testing:
$HOME = spock/home/cscherer
Path for run directory: ***$HOME/scr549***

Environment variables:

TPA_TEST = $HOME /*scr549*
TPA_DATA = $HOME /*scr549*

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 549 - Test Directories*" (attached).

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***scr549***, ***scr549/tpa500o***

2. Copy **TPA** version 5.0.0p to ***$HOME/scr549***. Compile *tpa.e*. Create subdirectory ***standalone-releaset***, and copy releaset.e to subdirectory.

3. Copy **TPA** version 5.0.0o to ***$HOME/scr549/tpa500o***. Compile *tpa.e*.

Function Level Tests:

These tests are designed to demonstrate the functionality of the specified module.

1. Name: Compare Standalone Run of Releaset.e with TPA Run at 100,000 Years.

2. Paths for archives of results: ***$HOME /scr549/test-report/flt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: base case *tpa.inp* for version **TPA**5.0.0o and for version **TPA**5.0.0p. Change OutputMode to 1 and MaximumTime to 1.0e5 in both versions.

   Utility scripts needed to perform the test: none

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that the modified releaset.f can give the same results as **TPA**5.0.0o.

   - assumptions: all setup instructions have been carried out.

   - constraints: none.

   - output files to compare or examine: *cumrelse.out, diagnose.out, ebsnef.dat, ebssf.dat, frac_rel.out, inv1000.out. maxrel.dat, rel_flow.out, relcum.out, releaset.out, relfrac.out,* and *trelease.out* from the standalone and **TPA**5.0.0o runs

   - step by step test procedure to be used:

     1. —> change directory to <<run directory>>
     2. run *tpa.e* using command "***tpa.e > tpa_100K-AF-500p.out***"
     3. copy *wpflow.def* to ***tpa500o/data***
     4. copy *ebsrel.inp*, *ebstrh.dat*, *ebsflo.dat*, and *ebspac.nuc* to ***standalone-releaset***
     5. —> change directory to <<run directory>>***/tpa500o***
     6. run *tpa.e* using command "***tpa.e > tpa_100K-AF-500o.out***"
     7. —> change directory to <<run directory>>***/standalone-releaset***
     8. modify *ebsflo.dat* by changing all values in the last column to 1.0
     9. run *releaset.e*
     10. compare *cumrelse.out, diagnose.out, ebsnef.dat, ebssf.dat, frac_rel.out, inv1000.out. maxrel.dat, rel_flow.out, relcum.out, releaset.out, relfrac.out,* and *trelease.out* from the standalone and **TPA**5.0.0o runs.

   - pass/fail criteria: the test passes if:

1. All runs complete successfully.
2. The only differences between the files from *releaset.e* standalone run and the **TPA**5.0.0o run are time/date stamps and header information, with one exception. The *ebsnef.dat* file from the standalone run contains only the 22 aqueous nuclides; the *ebsnef.dat* file from the **TPA**5.0.0o run also contains the 11 colloidal nuclides.

Results of running test:

PASSED.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

1. Name: Compare Output from **TPA5.0.0o** and **TPA5.0.0p** at 1,000,000 Years.

Paths for archives of results: ***$HOME /scr549/test-report/slt1***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: none.

Program modes to be used: use base case *tpa.inp* for each version and make the following changes:

set OutputMode to 1
set MaximumTime to 1,000,000
set NumberOfTimeStepsAfterCompliancePeriod to 4800

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA**5.0.0p code generates results that reflect the changes to *wpflow.def* and the time-dependent fwet/sawetfrac parameter at 1,000,000 years.

- assumptions: all setup instructions have been carried out.

- constraints: the files *tpa_1M-AF-500o.out* and *tpa_1M-AF-500p.out* do not exist in the run directory.

- output files to compare or examine: *ebsnef.dat* from both runs

- step by step test procedure to be used:

  1. —> change directory to <<run directory>>***/tpa500o***
  2. run *tpa.e* using command "***tpa.e > tpa_1M-AF-500o.out***"
  3. —> change directory to <<run directory>>
  4. run *tpa.e* using command "***tpa.e > tpa_1M-AF-500p.out***"
  5. create *ebsnef-dat.xls* using the U234 release data (*ebsnef.dat*) from each run; add data from *climato2.dat*, and fmult, fow, drip/wp, and flow factor from *ebsflo.dat*. Flow factor, drip/wp, fmult, and fow are multiplied together to produce "flow multiplier".

- pass/fail criteria: the test passes if:

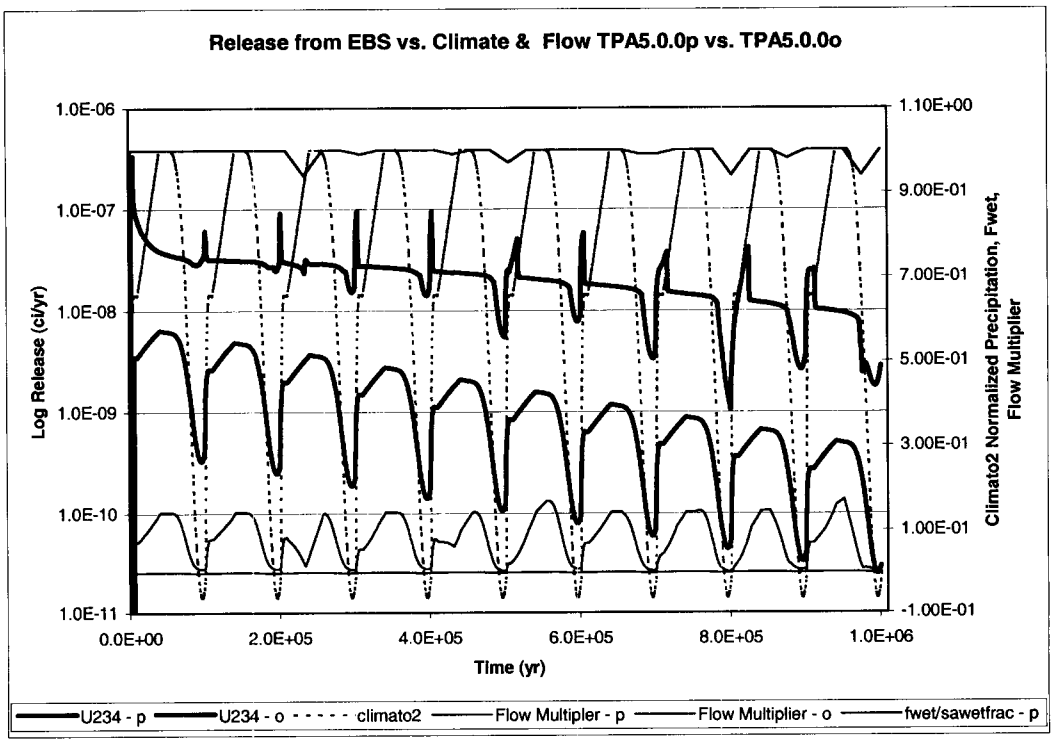
  1. Both **TPA** runs complete successfully.

  2. See following graph "Release from EBS vs. Climate & Flow TPA5.0.0p vs TPA5.0.0o". The flow multiplier should change from a constant to a time-varying value that correlates directly and positively to the climate cycles and the fwet values. Release rates for U234 from **TPA**5.0.0p should be greater than release rates for U234 from **TPA**5.0.0o.

Results of running test:

PASSED.

05/18/5


Release from EBS vs. Climate & Flow TPA5.0.0p vs. TPA5.0.0o
1.0E-06
1.0E-07
1.0E-08
1.0E-09
1.0E-10
1.0E-11
Log Release (ci/yr)
1.10E+00
9.00E-01
7.00E-01
5.00E-01
3.00E-01
1.00E-01
-1.00E-01
Climato2 Normalized Precipitation, Fwet, Flow Multiplier
0.0E+00
2.0E+05
4.0E+05
6.0E+05
8.0E+05
1.0E+06
Time (yr)
U234 - p
U234 - o
climato2
Flow Multipler - p
Flow Multiplier - o
fwet/sawetfrac - p

NOTES:

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-553	2. Software Title and Version: TPA 5.0.0	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): nfenv.f, seismo2.f, condxyzt.f, cond3dxyzt.h, exec.f, tpa.inp, mechfail.f, mechfail.def, nrutil.f

The thermal diffusivity (alpha) was calculated from:

`Condbf * 1e-3/(0.774*1.021)` where the `condbf = 0.27 W/m-K` which gives the 3.417e-4 value.

However, there is an error in this and we need to make a change. The conductivity of the backfill is not constant at 0.27 anymore and we should instead calculate the thermal diffusivity for tpa.inp input values of density, specific heat, and thermal conductivity of the backfill and then eliminate the ThermalDiffusivity[m2/s] input parameter from *tpa.inp*. Other parameters for air should be updated as well. This includes ThermalConductivityOfAir[W/(m-C)], VolumeOfThermalExpansion[1/K], and KinematicViscosity[m^2/s]. In addition, the Prandtl Number for air should be added.

The standard deviation of a particle size distribution needs to be modified to agree with equation 11-5 of the RARI report.

$$\sigma^2{}_{D_p} = \exp\left\{-\left[2\overline{\Phi}(ln\,2) + 4\sigma_\Phi^2\,(ln\,2)^2\right]\right\}$$

The TimeOfBackfillEmplaced[yr] parameter is used to both designate the time for emplacing backfill and the time at which repository closure occurs and ventilation ends.

5. Change Requested by: G. Adams Date: 1-20-2005	6. Change Authorized by (~~*Software Developer*~~): R. Janetzke Date: 1-20-2005

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See, "Description of Change(s) or Problem Resolution" attached.

8. Implemented by: G. Adams	Date: February 7, 2005

9. Description of Acceptance Tests:

See Attachment 1 (Test Plan for TPA SCR#553).

10. Tested by: O.Osidele	Date: March 18, 2005

CNWRA Form TOP-5 (05/2000)

Description of Change(s) or Problem Resolution

Used the following reference to establish thermal properties for air in tpa.inp: Incropera, Frank P. and David P. Dewitt. 1981. Fundamentals of Heat Transfer. New York, New York: John Wiley & Sons.

Parameters are based on a peak waste package temperature in a no-backfill condition of 165 °C or 438 K.
1) Changed parameter:
constant
KinematicViscosity[m^2/s]
32.39e-6

to

constant
KinematicViscosityOfAir[m^2/s]
30.95e-6

based on Table A.4 of the reference:
400K: 26.41e-6 m^2/s
450K: 32.39e-6 m^2/s
linear interpolation to 438K: 30.95e-6 m^2/s

2) Changed parameter:
constant
VolumeOfThermalExpansion[1/K]
2.85e-3

to

constant
VolumeOfThermalExpansionOfAir[1/K]
2.28e-3

based on:
Assumption of an ideal gas and using equation 9.10 from the above reference:
$\beta = 1 / T = 1/438K = 2.28e-3$

3) Added parameter:
constant
DensityOfAir[kg/m^3]
0.797

based on Table A.4 of the reference:
400K: 0.8711 kg/m^3
450K: 0.7740 kg/m^3
linear interpolation to 438K: 0.797 kg/m^3

4) Added parameter:
constant
SpecificHeatOfAir[kJ/kg-K]
1.019

based on Table A.4 of the reference:
400K: 1.014 kJ/kg-K

450K: 1.021 kJ/kg-K
linear interpolation to 438K: 1.019 kJ/kg-K

5) Added parameter:
constant
PrandtlNumberForAir[]
0.687

based on Table A.4 of the reference:
400K: 0.690
450K: 0.686
linear interpolation to 438K: 0.687

6) Removed parameter:
constant
ThermalDiffusivity[m^2/s]
3.417e-4

Replaced with the following calculation within nfenv.f:
Thermal Diffusivity of Backfill = conductivity of backfill / (density of air * specific heat of air)

7) Modified the calculation for standard deviation of a particle size distribution to agree with equation 11-5 of the RARI report.

8) Added parameter TimeOfRepositoryClosure[yr] and updated nfenv.f, exec.f, seismo2.f, cond3dxyzt.f, and mechfail.f to use this parameter in place of TimeOfBackfillEmplaced[yr].
constant
TimeOfRepositoryClosure[yr]
50.0

Removed parameter:
constant
TimeOfBackfillEmplaced[yr]
10000.0

9) Changed parameter
constant
ThermalConductivityOfAir[W/(m-C)]
37.3e-3

to

constant
ThermalConductivityOfAir[W/(m-C)]
36.5e-3

based on Table A.4 of the reference:
400K: 33.8e-3 W/(m-K)
450K: 37.3e-3 W/(m-K)
linear interpolation to 438K: 36.5e-3 W/(m-K)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
Modify from	NFENV	KinematicViscosity[m^2/s]		constant	32.39 e-6		GRA
Modify to	NFENV	KinematicViscosityOfAir[m^2/s]	Used for iterative thermal calculations	constant	30.95 e-6	Table A.4 (438K) of: Incropera, Frank P. And David P. Dewitt. 1981. Fundamentals of Heat Transfer. New York, New York: John Wiley & Sons.	GRA
Modify from	NFENV	VolumeOfThermalExpansion[1/K]		constant	2.85e-3		GRA

Modify to	NFENV	VolumeOfThermal ExpansionOfAir[1/K]	Used for iterative thermal calculations	constant	2.28e-3	Assumption of an ideal gas and using equation 9.10 from: Incropera, Frank P. And David P. Dewitt. 1981. Fundamentals of Heat Transfer. New York, New York: John Wiley & Sons.	GRA
Add	NFENV	DensityOfAir[kg/m^3]	Used for iterative thermal calculations	constant	0.797	Table A.4 (438K) of: Incropera, Frank P. And David P. Dewitt. 1981. Fundamentals of Heat Transfer. New York, New York: John Wiley & Sons.	GRA
Add	NFENV	SpecificHeatOfAir [kJ/kg-K]	Used for iterative thermal calculations	constant	1.019	Table A.4 (438K) of: Incropera, Frank P. And David P. Dewitt. 1981. Fundamentals of Heat Transfer. New York, New York: John Wiley & Sons.	GRA
Add	NFENV	PrandtlNumberFor Air[]	Used for iterative thermal calculations	constant	0.687	Table A.4 (438K) of: Incropera, Frank P. And David P. Dewitt. 1981. Fundamentals of Heat Transfer. New York, New York: John Wiley & Sons.	GRA
Delete	NFENV	ThermalDiffusivity [m^2/s]		constant	3.417 e-4		GRA

Add	Exec, Seismo 2, Nfenv	TimeOfRepository Closure[yr]	Used to determine when repository is closed and ventilation stops and potentially also when backfill may be emplaced.	Constant	50.0		GRA
Delete	Exec, Seismo 2, Nfenv	TimeOfBackfillEm placed[yr]		Constant	10000. 0		GRA
Modify from	Nfenv	ThermalConductivi tyOfAir[W/(m-C)]		Constant	37.3e-3		GRA
Modify to	Nfenv	ThermalConductivi tyOfAir[W/(m-C)]		Constant	36.5e-3		GRA

Attachment 1

Test Plan for TPA SCR#553

Tested by: Olufemi Osidele | Date: March 18, 2005

Host Machine: SUN Ultra-4 server: Spock | Host OS: Sun Solaris 5.9

Baseline Version: 5.0.0 | Test Version: 5.0.0m

General Remarks

Directory path for codes: base version: ~oosidele/tpa500
test version: ~oosidele/tpa500m

Environment variables: base version: setenv TPA_TEST ~/tpa500
setenv TPA_DATA ~/tpa500

test version: setenv TPA_TEST ~/tpa500m
setenv TPA_DATA ~/tpa500m

Special diagnostic code modifications required :

Source code files *nfenv.f* and *nrutil.f* were modified: (i) to force the execution of the function `zbrak()` and `zbrent()` with argument `fTargetDripShieldOuter`, and (ii) to write all variables to screen for the calculation of thermal diffusivity and standard deviation of particle size distribution (see files *nfenvSCR553test.f* and *nrutilSCR553test.f* on attached CD). Each code modification is tagged `SCR 553 test`.

Utility codes needed in the analysis of the test data: Microsoft Excel®

Test Description

1. <u>Parameter updates</u>

Objective: To update input parameters in *tpa.inp* as shown in the above table (Update Requirements for TPA.INP)

Affected module(s): EXEC, NFENV, SEISMO2

Assumptions: None

Output files to compare or examine: None

Test procedure:

(i) Search for the updated parameters in the *~oosidele/tpa500m* directory using the following command:

```
grep -in <search string> *.* tpa.inp ccdf/*.f codes/*.f
codes/gentpa/*.f codes/itym/src/*.f data/*.*
```

(ii) Examine *tpa.inp* for the updated parameter values

Pass/Fail criterion(ia):

(i) Search results should indicate that the updated parameters are in *tpa.inp* and the source code files of the affected modules
(ii) The updated parameter values should match those in the table (Update Requirements for TPA.INP).

Test results:

(i) See files *grepSearchPar.txt* and *grepSearch553.txt* on attached CD for screen dump of search results. Affected files are: *tpa.inp*, *exec.f*, *nfenv.f*, *seismo2.f*, *mechfail.f*, *condxyzt.f*, *mechfail.def*, and *cond3dxyzt.h*.

(ii) Files *tparun026ThDiff.inp* and *tparun026SD.inp* on the attached CD each contain the updated parameter values.

Test status: **PASS**

2. <u>Thermal diffusivity</u>

Objective: To replace the constant ThermalDiffusivity parameter with a calculation using parameters (`ThermalConductivityOfBackfill`, `DensityOfAir`, and `SpecificHeatOfAir`) in *tpa.inp*.

Affected module(s): NFENV

Assumptions: None

Output files to compare or examine: None.

Test procedure:

(i) Copy and paste screen output into Microsoft Excel spreadsheet;
(ii) Implement formula for calculating thermal conductivity independently in Excel;
(iii) Compare independent calculation with screen output.

Pass/Fail criterion(ia):

Independent calculation results should be identical to code calculation results.

Test results:

See files *nfenvSCR553test.f* for print statements and *tparun026_ThDiff.out* for screen outputs for 25 realizations.

compThDiff.xls shows the independent calculations in Excel. Results of independent calculation (Column 5) and code calculations (Column 1) are identical.

Test status: **PASS.**

3. Standard deviation of particle size distribution

Objective: To modify the calculation for standard deviation of a particle size distribution to agree with equation 11-5 of the RARI report.

Affected module(s): NFENV

Assumptions: None

Output files to compare or examine: None.

Test procedure:

(i) Copy and paste screen output into Microsoft Excel spreadsheet;
(ii) Implement formula for calculating standard deviation independently in Excel;
(iii) Compare independent calculation with screen output.

Pass/Fail criterion(ia):

Independent calculation results should be identical to code calculation results.

Test results:

See files *nrutilSCR553test.f* for print statements and *tparun026_SD_1.out* to *tparun026_SD_5.out* for screen outputs of five realizations.

compSD.xls shows the independent calculations in Excel. Results of independent calculation (Column 4) and code calculations (Column 1) are identical.

Test status: **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-554	2. Software Title and Version: TPA 5.0.0f	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *invent.f, nuclides.dat, burnup.dat, tpanames.dbs*

Thermal ouput in *burnup.dat* was divided by 475 kg. initial U mass (as for PWR assesmbly), but should have been divided by 200 kg. for BWR assembly.

O. Povetko also requested update to *nuclides.dat* file.

The **chains()** subroutine in the *invent.f* module produces negative results when t0 in *nuclides.dat* equals the emplacement time in *tpa.inp*. This effect is noticed in *ebspac.nuc*.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
O. Osidele, O. Povetko Date: 2-2-2005	R. Janetzke Date: 2-4-2005

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The revised *burnup.dat* was obtained from O.Povetko, based on calculations documented in Scientific Notebook #612 Section 17E. The revised data file *nuclides.dat* also provided by O.Povetko. Attachment 1 shows the contents of the current and revised files, and a plot of the current and revised thermal output for Boiling Water Reactor (BWR) SNF.

Inspection of the current and revised *burnup.dat* files shows that the thermal outputs listed for BWR SNF (in the `bwr` column) in the revised file is 2.375 times (i.e., 475/200) those in the current file.

Code changes for *invent.f* are at the end of Attachment 1.

8. Implemented by:	Date:
R. Janetzke, O. Osidele	2-24-2005

9. Description of Acceptance Tests:

See Attachment 2.

10. Tested by:	Date:
O. Osidele	3-2-2005

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)

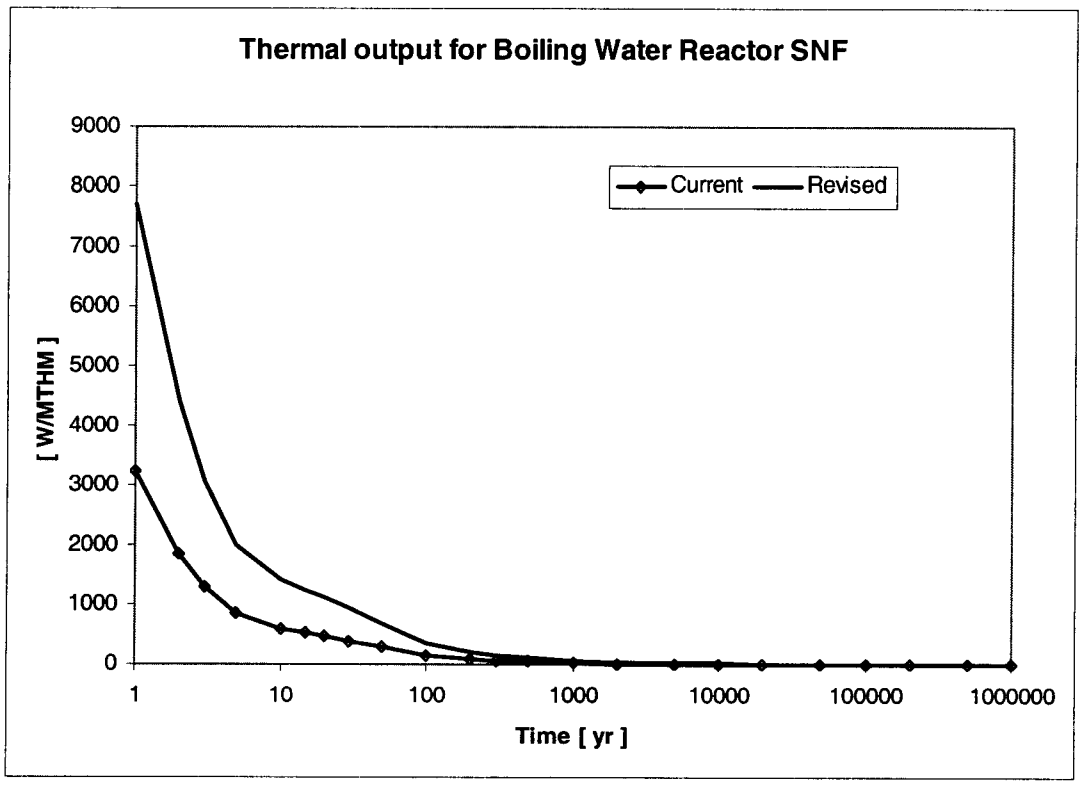
Attachment 1

Current *burnup.dat* file:

```
TITLE: Data for TPA 5.0.1 based on ORIGEN-ARP version 2.0 calculations, O.
Povetko 7-19-04
**
** time is years out of reactor.
** bwr is thermal output for boiling water reactor SNF.

** pwr is thermal output for pressurised water reactor SNF.

**
** Data from DOE AMR BBAC00000-01717-0210-0010REV 01 1999 ppX-3,X-4,X15-2,3,4

**
2008.                        ! Calendar year corresponding to time 0 in the
table.
0.35                         ! bwr blend

0.65                         ! pwr blend

Time (yr)    bwr (W/MTHM)       pwr (W/MTHM)
1            3240               13972.63158
2            1866.947368        7536.842105
3            1290.315789        4842.105263
5            844.8421053        2814.736842
10           595.7894737        1812
15           518.9473684        1557.052632
20           468                1398.315789
30           390.1052632        1159.368421
50           282.3157895        830.1052632
100          152.5894737        440.2105263
200          84.21052632        238.7368421
300          64.94736842        182.9052632
500          46.94736842        131.2
1000         26.88421053        73.74736842
2000         14.06736842        37.22105263
5000         8.915789474        23.11578947
10000        6.372631579        16.60631579
20000        3.667368421        9.650526316
50000        1.305684211        3.494736842
100000       0.516421053        1.408421053
200000       0.326526316        0.911157895
500000       0.269052632        0.753684211
1000000      0.192610526        0.537894737
```

Revised *burnup.dat* file:

```
TITLE: Data for TPA 5.0.1 based on SCALE5/ORIGEN-ARP calculations,O. Povetko 02-04-05
**
** time is years passed after discharge out of reactor.
** bwr is thermal output for boiling water reactor SNF.
** pwr is thermal output for pressurised reactor SNF.
**
** Input data for calculations from BWR  Source Term Generation and
** Evaluation, BBAC00000-01717-0210-0010REV 01 1999 Table 33 and p. XV-1;
** and from PWR Source Term Generation and Evaluation, BBAC00000-01717-0210-0010
** REV 01 1999 Table 11 and p. X-1
**
2008.                  ! Calendar year corresponding to time 0 in the table
0.35                   ! bwr blend
0.65                   ! pwr blend
Time (yr)     bwr (W/MTHM)  pwr (W/MTHM)
1             7695                14213
2             4434                7747
3             3065                5027
5             2007                2958
10            1415                1886
15            1233                1595
20            1112                1418
30            926.5               1164
50            670.5               830.1
100           362.4               440.2
200           200                 238.5
300           154.3               182.8
500           111.5               131.2
1000          63.85               73.7
2000          33.41               37.22
5000          21.18               23.12
10000         15.14               16.61
20000         8.71                9.655
50000         3.101               3.497
100000        1.227               1.409
200000        0.7755              0.9107
500000        0.639               0.7533
1000000       0.4575              0.5377
```


Thermal output for Boiling Water Reactor SNF
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
[W/MTHM]
Current
Revised
1
10
100
1000
10000
100000
1000000
Time [yr]

Current *nuclides.dat* file:

```
TITLE: TPA5.0.1 nuclide data used for the invent.f module.
** NOTE ON PARAMETERS CPMTU AND CPMGLASS:
**   For Colloids (e.g. Jc246, Jp242, ...) these parameters must be 0.00d+00.
**   If they are set to a value other than zero, they will be overwritten by
**   subroutine releasecolloids (called from module EBSREL).
**
**   Data from DOE SN0012T0810599.039 and ANL-WIS-MD-000006 REV 00 ICN 02, 2001
**
**   Decay flag information for groundwater protection calculations:
**   (1) beta/gamma, (2) alpha, (3) radon, and (4) uranium
**      idx = Nuclide index
**      NIS = namesisotopesave
**      NES = nameselemsave
**    CPMTU = cipermtuat10yr
**    DECAY = decay information
**      --- = unitless
** Year at which data is applicable follows:
2008.
** Number of nuclides to be read follows:
57
**idx,     NIS,    NIS2,    NIS3, NES,    wmole, halflife,   epalim,     CPMTU,  CPMGLASS,  DECAY
**---      ---,     ---,     ---, ---,  [g/mol],     [yr], [Ci/MTU],  [Ci/MTU],  [Ci/MTU],    ---
   01     U238    U238     U238     U  238.0d0   4.468d9      0.10  3.32d-01  6.75d-02      4
   02    Cm246   Cm246    CM246    Cm  246.0d0   4.731d3      0.10  2.05d-01  2.12d-05      2
   03    Pu242   Pu242    PU242    Pu  242.0d0   3.869d5      0.10  3.77d+00  2.35d-02      2
   04   Am242m  Am242m   AM242M    Am  242.0d0   1.520d2      0.10  1.51d+01  3.19d-02      1
   05    Pu238   Pu238    PU238    Pu  238.0d0   8.774d1      0.10  3.22d+03  1.23d+03      2
   06     U234    U234     U234     U  234.0d0   2.445d5      0.10  1.42d+00  2.27d-01      4
   07    Th230   Th230    TH230    Th  230.0d0   7.700d4      0.01  4.74d-04  1.24d-04      2
   08    Ra226   Ra226    RA226    Ra  226.0d0   1.600d3      0.10  0.00d+00  1.27d-05      3
   09    Pb210   Pb210    PB210    Pb  210.0d0   2.230d1      1.00  0.00d+00  8.46d-06      1
   10    Cm243   Cm243    CM243    Cm  243.0d0   2.850d1      0.10  2.23d+01  1.03d-03      2
   11    Am243   Am243    AM243    Am  243.0d0   7.380d3      0.10  3.21d+01  6.13d-02      2
   12    Pu239   Pu239    PU239    Pu  239.0d0   2.406d4      0.10  3.39d+02  1.85d+02      2
   13     U235    U235     U235     U  235.0d0   7.038d8      0.10  1.70d-02  2.82d-03      4
   14    Pa231   Pa231    PA231    Pa  231.0d0   3.277d4      0.10  5.81d-05  2.89d-02      2
   15    Ac227   Ac227    AC227    Ac  227.0d0   2.177d1      0.10  2.79d-05  2.60d-02      1
   16    Cm245   Cm245    CM245    Cm  245.0d0   8.499d3      0.10  6.00d-01  1.87d-04      2
   17    Pu241   Pu241    PU241    Pu  241.0d0   1.440d1   1000.00  1.72d+04  6.60d+00      1
   18    Am241   Am241    AM241    Am  241.0d0   4.322d2      0.10  3.76d+03  1.56d+02      2
   19    Np237   Np237    NP237    Np  237.0d0   2.140d6      0.10  4.17d-01  3.92d-01      2
   20     U233    U233     U233     U  233.0d0   1.585d5      0.10  8.43d-05  8.23d-02      4
   21    Th229   Th229    TH229    Th  229.0d0   7.339d3      0.10  0.00d+00  6.71d-04      2
   22    Cm244   Cm244    CM244    Cm  244.0d0   1.811d1   1000.00  2.81d+03  1.39d+00      2
   23    Pu240   Pu240    PU240    Pu  240.0d0   6.537d3      0.10  5.91d+02  6.66d+01      2
   24     U236    U236     U236     U  236.0d0   2.341d7      0.10  3.16d-01  1.98d-03      4
   25     U232    U232     U232     U  232.0d0   7.200d1      0.10  2.77d-02  1.39d-02      4
   26    Sm151   Sm151    SM151    Sm  151.0d0   8.999d1      1.00  4.63d+02  3.34d+02      1
   27    Cs137   Cs137    CS137    Cs  137.0d0   3.000d1      1.00  5.76d+04  3.01d+04      1
   28    Cs135   Cs135    CS135    Cs  135.0d0   2.300d6      1.00  8.63d-01  2.00d-01      1
   29     I129    I129     I129     I  129.0d0   1.570d7      0.10  3.88d-02  6.40d-03      1
   30    Sn126   Sn126    SN126    Sn  126.0d0   1.000d5      1.00  9.00d-01  6.02d-01      1
   31   Sn121m  Sn121m   SN121M    Sn  121.0d0   4.997d1      1.00  3.86d+00  6.34d-04      1
   32   Ag108m  Ag108m   AG108M    Ag  108.0d0   4.180d2      1.00  1.49d-02  0.00d+00      1
   33    Pd107   Pd107    PD107    Pd  107.0d0   6.496d6      1.00  1.94d-01  2.12d-02      1
   34     Tc99    Tc99     TC99    Tc   99.0d0   2.130d5     10.00  1.62d+01  9.54d+00      1
   35     Mo93    Mo93     MO93    Mo   93.0d0   3.498d3      1.00  7.09d-02  0.00d+00      1
   36     Nb94    Nb94     NB94    Nb   94.0d0   2.030d4      1.00  1.46d+00  5.83d-04      1
   37     Zr93    Zr93     ZR93    Zr   93.0d0   1.530d6      1.00  2.17d+00  2.27d+00      1
   38     Sr90    Sr90     SR90    Sr   90.0d0   2.912d1      1.00  3.82d+04  3.04d+04      1
   39     Se79    Se79     SE79    Se   79.0d0   1.100d6      1.00  1.08d-01  3.96d-01      1
   40     Ni63    Ni63     NI63    Ni   63.0d0   9.200d1      1.00  5.42d+02  1.00d+01      1
   41     Ni59    Ni59     NI59    Ni   59.0d0   8.000d4      1.00  4.52d+00  2.55d-01      1
   42     Cl36    Cl36     CL36    Cl   36.0d0   3.010d5      1.00  1.72d-02  0.00d+00      1
   43      C14     C14      C14     C   14.0d0   5.729d3      0.10  7.60d-01  2.21d-02      1
   44    Jc246   Jc246    JC246    Jc  246.0d0   4.731d3      0.00  0.00d+00  0.00d+00      2
   45    Jp242   Jp242    JP242    Jp  242.0d0   3.869d5      0.00  0.00d+00  0.00d+00      2
   46   Ja242m  Ja242m   JA242M    Ja  242.0d0   1.520d2      0.00  0.00d+00  0.00d+00      1
   47    Jp238   Jp238    JP238    Jp  238.0d0   8.774d1      0.00  0.00d+00  0.00d+00      2
   48    Jt230   Jt230    JT230    Jt  230.0d0   7.700d4      0.00  0.00d+00  0.00d+00      2
   49    Jc243   Jc243    JC243    Jc  243.0d0   2.850d1      0.00  0.00d+00  0.00d+00      2
   50    Jp239   Jp239    JP239    Jp  239.0d0   2.406d4      0.00  0.00d+00  0.00d+00      2
   51    Ja243   Ja243    JA243    Ja  243.0d0   7.380d3      0.00  0.00d+00  0.00d+00      2
   52    Jc245   Jc245    JC245    Jc  245.0d0   8.499d3      0.00  0.00d+00  0.00d+00      2
   53    Jp241   Jp241    JP241    Jp  241.0d0   1.440d1      0.00  0.00d+00  0.00d+00      1
   54    Ja241   Ja241    JA241    Ja  241.0d0   4.322d2      0.00  0.00d+00  0.00d+00      2
   55    Jc244   Jc244    JC244    Jc  244.0d0   1.811d1      0.00  0.00d+00  0.00d+00      2
   56    Jp240   Jp240    JP240    Jp  240.0d0   6.537d3      0.00  0.00d+00  0.00d+00      2
   57    Jt229   Jt229    JT229    Jt  229.0d0   7.339d3      0.00  0.00d+00  0.00d+00      2
```

Revised *nuclides.dat* file:

```
TITLE: TPA 5.0.1 nuclide data used for the invent.f module.
** NOTE ON PARAMETERS CPMTU AND CPMGLASS:
**   For Colloids (e.g. Jc246, Jc242, ...) these parameters must be 0.00d+00.
**   If they are set to a value other than zero, they will be overwritten by
**   subroutine releasecolloids (called from module EBSREL).
**
**   Data from  Inventory Abstraction ANL-WIS-MD-000006 REV 00 ICN 02, 2001; BWR  Source Term
Generation and
**   Evaluation, BBAC00000-01717-0210-0010REV 01 1999 pp.X15-2,3,4 and PWR  Source Term
Generation and
**   Evaluation, BBAC00000-01717-0210-0010REV 01 1999 ppX-3, X-4 and SN0012T0810599.039 DOE data
file
**   compiled by O.Povetko 02-04-05
**
**   Decay flag information for groundwater protection calculations:
**    (1) beta/gamma, (2) alpha, (3) radon, and (4) uranium
**       idx = Nuclide index
**       NIX = namesisotopesave
**       NES = nameslemsave
**     CPMTU = cipermtu
**  CMPGLASS = cipermtuglass
**     DECAY = decay information
**       --- = initless
**   Year at which data is applicable follows:
2033.
** Number of nuclides to be read follows:
57
**idx,     NIS,    NIS2,    NIS3, NES,    wmole, halflife,   epalim,     CPMTU,  CPMGLASS,  DECAY
**---      ---,     ---,     ---, ---,  [g/mol],     [yr], [Ci/MTU],  [Ci/MTU],  [Ci/MTU],    ---
   01     U238    U238     U238      U  238.0d0   4.468d9      0.10   3.32d-01   6.75d-02      4
   02    Cm246   Cm246    CM246     Cm  246.0d0   4.731d3      0.10   2.05d-01   2.12d-05      2
   03    Pu242   Pu242    PU242     Pu  242.0d0   3.869d5      0.10   3.77d+00   2.35d-02      2
   04   Am242m  Am242m   AM242M     Am  242.0d0   1.520d2      0.10   1.51d+01   3.19d-02      1
   05    Pu238   Pu238    PU238     Pu  238.0d0   8.774d1      0.10   3.22d+03   1.23d+03      2
   06    U234    U234     U234      U  234.0d0   2.445d5      0.10   1.42d+00   2.27d-01      4
   07    Th230   Th230    TH230     Th  230.0d0   7.700d4      0.01   4.74d-04   1.24d-04      2
   08    Ra226   Ra226    RA226     Ra  226.0d0   1.600d3      0.10   0.00d+00   1.27d-05      3
   09    Pb210   Pb210    PB210     Pb  210.0d0   2.230d1      1.00   0.00d+00   8.46d-06      1
   10    Cm243   Cm243    CM243     Cm  243.0d0   2.850d1      0.10   2.23d+01   1.03d-03      2
   11    Am243   Am243    AM243     Am  243.0d0   7.380d3      0.10   3.21d+01   6.13d-02      2
   12    Pu239   Pu239    PU239     Pu  239.0d0   2.406d4      0.10   3.39d+02   1.85d+02      2
   13     U235    U235     U235      U  235.0d0   7.038d8      0.10   1.70d-02   2.82d-03      4
   14    Pa231   Pa231    PA231     Pa  231.0d0   3.277d4      0.10   5.81d-05   2.89d-02      2
   15    Ac227   Ac227    AC227     Ac  227.0d0   2.177d1      0.10   2.79d-05   2.60d-02      1
   16    Cm245   Cm245    CM245     Cm  245.0d0   8.499d3      0.10   6.00d-01   1.87d-04      2
   17    Pu241   Pu241    PU241     Pu  241.0d0   1.440d1   1000.00   1.72d+04   6.60d+00      1
   18    Am241   Am241    AM241     Am  241.0d0   4.322d2      0.10   3.76d+03   1.56d+02      2
   19    Np237   Np237    NP237     Np  237.0d0   2.140d6      0.10   4.17d-01   3.92d-01      2
   20     U233    U233     U233      U  233.0d0   1.585d5      0.10   8.43d-05   8.23d-02      4
   21    Th229   Th229    TH229     Th  229.0d0   7.339d3      0.10   0.00d+00   6.71d-04      2
   22    Cm244   Cm244    CM244     Cm  244.0d0   1.811d1   1000.00   2.81d+03   1.39d+00      2
   23    Pu240   Pu240    PU240     Pu  240.0d0   6.537d3      0.10   5.91d+02   6.66d+01      2
   24     U236    U236     U236      U  236.0d0   2.341d7      0.10   3.16d-01   1.98d-03      4
   25     U232    U232     U232      U  232.0d0   7.200d1      0.10   2.77d-02   1.39d-02      4
   26    Sm151   Sm151    SM151     Sm  151.0d0   8.999d1      1.00   4.63d+02   3.34d+02      1
   27    Cs137   Cs137    CS137     Cs  137.0d0   3.000d1      1.00   5.76d+04   3.01d+04      1
   28    Cs135   Cs135    CS135     Cs  135.0d0   2.300d6      1.00   8.63d-01   2.00d-01      1
   29     I129    I129     I129      I  129.0d0   1.570d7      0.10   3.88d-02   6.40d-03      1
   30    Sn126   Sn126    SN126     Sn  126.0d0   1.000d5      1.00   9.00d-01   6.02d-01      1
   31   Sn121m  Sn121m   SN121M     Sn  121.0d0   4.997d1      1.00   3.86d+00   6.34d-04      1
   32   Ag108m  Ag108m   AG108M     Ag  108.0d0   4.180d2      1.00   1.49d-02   0.00d+00      1
   33    Pd107   Pd107    PD107     Pd  107.0d0   6.496d6      1.00   1.94d-01   2.12d-02      1
   34     Tc99    Tc99     TC99     Tc   99.0d0   2.130d5     10.00   1.62d+01   9.54d+00      1
   35     Mo93    Mo93     MO93     Mo   93.0d0   3.498d3      1.00   7.09d-02   0.00d+00      1
   36     Nb94    Nb94     NB94     Nb   94.0d0   2.030d4      1.00   1.46d+00   5.83d-04      1
   37     Zr93    Zr93     ZR93     Zr   93.0d0   1.530d6      1.00   2.17d+00   2.27d+00      1
   38     Sr90    Sr90     SR90     Sr   90.0d0   2.912d1      1.00   3.82d+04   3.04d+04      1
   39     Se79    Se79     SE79     Se   79.0d0   1.100d6      1.00   1.08d-01   3.96d-01      1
   40     Ni63    Ni63     NI63     Ni   63.0d0   9.200d1      1.00   5.42d+02   1.00d+01      1
   41     Ni59    Ni59     NI59     Ni   59.0d0   8.000d4      1.00   4.52d+00   2.55d-01      1
   42     Cl36    Cl36     CL36     Cl   36.0d0   3.010d5      1.00   1.72d-02   0.00d+00      1
   43      C14     C14      C14      C   14.0d0   5.729d3      0.10   7.60d-01   2.21d-02      1
   44    Jc246   Jc246    JC246     Jc  246.0d0   4.731d3      0.00   0.00d+00   0.00d+00      2
   45    Jp242   Jp242    JP242     Jp  242.0d0   3.869d5      0.00   0.00d+00   0.00d+00      2
   46   Ja242m  Ja242m   JA242M     Ja  242.0d0   1.520d2      0.00   0.00d+00   0.00d+00      1
   47    Jp238   Jp238    JP238     Jp  238.0d0   8.774d1      0.00   0.00d+00   0.00d+00      2
   48    Jt230   Jt230    JT230     Jt  230.0d0   7.700d4      0.00   0.00d+00   0.00d+00      2
   49    Jc243   Jc243    JC243     Jc  243.0d0   2.850d1      0.00   0.00d+00   0.00d+00      2
   50    Jp239   Jp239    JP239     Jp  239.0d0   2.406d4      0.00   0.00d+00   0.00d+00      2
```

51	Ja243	Ja243	JA243	Ja	243.0d0	7.380d3	0.00	0.00d+00	0.00d+00	2
52	Jc245	Jc245	JC245	Jc	245.0d0	8.499d3	0.00	0.00d+00	0.00d+00	2
53	Jp241	Jp241	JP241	Jp	241.0d0	1.440d1	0.00	0.00d+00	0.00d+00	1
54	Ja241	Ja241	JA241	Ja	241.0d0	4.322d2	0.00	0.00d+00	0.00d+00	2
55	Jc244	Jc244	JC244	Jc	244.0d0	1.811d1	0.00	0.00d+00	0.00d+00	2
56	Jp240	Jp240	JP240	Jp	240.0d0	6.537d3	0.00	0.00d+00	0.00d+00	2
57	Jt229	Jt229	JT229	Jt	229.0d0	7.339d3	0.00	0.00d+00	0.00d+00	2

invent.f

At line 454:

```
cc rwj 2-24-05; SCR 554
c     If any of the dn(2,*) are less then zero, that dt was too
c     small for this case.  Do not accept the values and reset to
c     input values.

      lnegflag = .false.

c     Test for negative values and set flag.
      do in = 1, 43
        if ( dn(2,in) .lt. 0.d0) lnegflag = .true.
      end do

c     If flag set copy input to output
      if (lnegflag) then
        do in = 1, 43
          dn(1,in) = dnt1(in)
          dn(2,in) = dnt1(in)
        end do
      end if
cc    End SCR 554
```

At line 1804:

```
cc rwj 2-22-05; SCR554; Copy all nuclides rather than just the first two.
c          call acopy( 1.d0, nt, amolepermtuat10yr, amolepermtu )
c          call acopy( 1.d0, nt, amolepermtuat10yrglass,
c    &                           amolepermtuglass )
          do i = 1,maxinvnuc
            amolepermtu(1,i) = amolepermtuat10yr(i)
            amolepermtu(2,i) = amolepermtuat10yr(i)
            amolepermtuglass(1,i) = amolepermtuat10yrglass(i)
            amolepermtuglass(2,i) = amolepermtuat10yrglass(i)
          end do
```

Attachment 2

Test Plan for TPA SCR#554

Tested by: Olufemi Osidele | Date: March 2, 2005

Host Machine: SUN Ultra-4 server: Spock | Host OS: Sun Solaris 5.9

Baseline Version: 5.0.0f | Test Version: 5.0.0k

General Remarks

Directory path for codes:	base version:	~oosidele/tpa500f
	test version:	~oosidele/tpa500k
Environment variables:	base version:	setenv TPA_TEST ~/tpa500f setenv TPA_DATA ~/tpa500f
	test version:	setenv TPA_TEST ~/tpa500k setenv TPA_DATA ~/tpa500k

Test Description

1. <u>Decay calculations</u>

Objective:

Correct the negative results produced in *ebspac.nuc* by the subroutine `chains()` when the initial time (`t0`) in *nuclides.dat* equals the emplacement time (`AverageCalendarYearAssumedForEmplacement[A.D.]`), currently `2033` in *tpa.inp*.

Affected module(s): INVENT

Assumptions: None

Output files to compare or examine: *ebspac.nuc*

Test procedure:

(i) Examine code modifications in *~oosidele/tpa500k/invent.f*;

(ii) Run the base version (*~oosidele/tpa500f/tpa.e*) for `t0 = 2008, 2020,` and `2033`;

(iii) Run the test version (*~oosidele/tpa500k/tpa.e*) for `t0 = 2008, 2020,` and `2033`; except for changes to the value of `t0`, this step is performed with the same nuclide inventory data (*nuclides.dat*) as step (ii);

(iv) Examine the contents of *ebspac.nuc* obtained for each trial run in (ii) and (iii).

Pass/Fail criterion(ia):

Trial run of base version should give negative results in *ebspac.nuc* for `t0 = 2033` only. All three trial runs of the test version should not produce negative results in *ebspac.nuc*.

Test results:

Test results are provided on attached CD ("Test Results for SCR# 554").

See files *ebspac500fY2008.nuc*, *ebspac500fY2020.nuc*, *ebspac500fY2033.nuc*, *ebspac500kY2008.nuc*, *ebspac500kY2020.nuc*, and *ebspac500kY2033.nuc* on attached CD for contents of *ebspac.nuc*. Negative values written to *ebspac500fY2033.nuc* do not appear in *ebspac500kY2033.nuc*.

Test status: **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-555	**2. Software Title and Version:** TPA 5.0.0x	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s):

nfenv.f, tpa.inp, tpanames.dbs, reflux2.i, reflux3.i

Remove subroutines **reflux1**()and **reflux2**() in the *nfenv.f* module.

5. Change Requested by: O. Pensado	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date:3-1-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Removed subroutines **reflux1()** and **reflux2()**.
Removed associated parameters and external subroutines from *nfenv.f* and *tpa.inp* files.
Renamed include file from *reflux2.i* to *reflux3.i.*
Add new *tpa.inp* parameter abbreviations to *tpanames.dbs.*

See Attachment 1.

8. Implemented by: Brandi L. Winfrey For	**Date:** 3 March 2005

9. Description of Acceptance Tests:

See Attachment 2.

10. Tested by: J. M. Menchaca J. M.	**Date:** 5-11-05

CNWRA Form TOP-5 (05/2000)

SCR555 UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
DELETE	Nfenv	SelectRefluxModel (1,2,3)	switch used to select between reflux1, reflux2, and reflux3 models:	iconstant	3	3. Deleted tpa.inp parameter when corresponding subroutine was deleted	BLW
DELETE	Nfenv	Reflux2Period	used by subroutine reflux2: number of years required for all dry-out zone-derived water to participate in a reflux cycle. user input, range = 1 - 1000. range is based on output of models (e.g. metra). units = years	constant	100	3. Deleted tpa.inp parameter when corresponding subroutine was deleted	BLW

DELETE	Nfenv	Reflux2LossI	used by subroutine reflux2: fraction of infiltration-derived water that escapes the reflux cycle each year. user input; range = 0.0 - 1.0	constant	0.1	3. Deleted tpa.inp parameter when corresponding subroutine was deleted	BLW
DELETE	Nfenv	Reflux2LossD	used by subroutine reflux2: fraction of dry-out zone-derived water that escapes the reflux cycle each year. user input, range = 0.0 - 1.0	constant	0.1	3. Deleted tpa.inp parameter when corresponding subroutine was deleted	BLW
DELETE	Nfenv	Reflux2Thickness	used by subroutine reflux2: thickness of dry-out zone around waste package. user input, range = 10m - 100m. range is based on output of models (e.g. metra). units = m	constant	100	3. Deleted tpa.inp parameter when corresponding subroutine was deleted	BLW
MODIFY FROM/TO	Nfenv	Reflux2Porosity Reflux3Porosity	used by subroutine reflux3: porosity of rock in dry-out zone (tsw)	constant	0.14	3. When subroutine reflux2 was deleted, renamed parameter for the subroutine it is currently used by: reflux3	BLW

MODIFY FROM/TO	Nfenv	Reflux2SatInit Reflux3SatInit	used by subroutine reflux3: initial saturation of dry-out zone rock (tsw)	constant	0.9	3. When subroutine reflux2 was deleted, renamed parameter for the subroutine it is currently used by: reflux3	BLW
MODIFY FROM/TO	Nfenv	Reflux2SatResid Reflux3SatResid	used by subroutine reflux3: residual saturation of dry-out zone rock (tsw)	constant	0.1	3. When subroutine reflux2 was deleted, renamed parameter for the subroutine it is currently used by: reflux3	BLW

Attachment 1

Include files:

reflux2.i - RENAME TO *reflux3.i*

Parameters:

In *tpa.inp*:
SelectRefluxModel(1,2,3) - DELETE
Reflux2Period - DELETE
Reflux2LossI - DELETE
Reflux2LossD - DELETE
Reflux2Porosity - CHANGE TO Reflux3Porosity
Reflux2SatInit - CHANGE TO Reflux3SatInit
Reflux2SatResid - CHANGE TO Reflux3SatResid

In *nvenv.f*:
iireflux - DELETE
ireflux - DELETE
irf2_thick - DELETE
irf2period - DELETE
irf2loss_i_val - DELETE
irf2loss_d_val - DELETE
irf2sat_init - CHANGE TO irf3sat_init
irf2sat_resid - CHANGE TO irf3sat_resid
irf2porosity - CHANGE TO irf3porosity
rf2sat_init - CHANGE TO rf3sat_init
rf2sat_resid - CHANGE TO rf3sat_resid
rf2porosity - CHANGE TO rf3porosity

External Subroutines:

Delete external subroutines used by reflux2 (located in module *nfenv.f* subroutine *reflux2*):
fill - DELETE
infil_calc - DELETE
rock - DELETE
dryout - DELETE

Code changes:

Delete if/else code to select between reflux models:

```
c       if (ireflux.eq.1) then
c
cc        GADAMS PA-SCR-553 2-4-2005: reflux1 uses the timeofbackfill to
cc        identify the time when ventilation ends.  Replaced the
cc        timeofbackfill parameter with timeofclosure
cc         call reflux1( isa, timeofbackfill, hloss_fact, ntim, tim(1),
cc      &   qm3peryrperwpinsa(1),
cc      &   temprep(1),
cc      &   qm3peryrperwpinsahitwp(1) )
c         call reflux1( isa, timeofclosure, hloss_fact, ntim, tim(1),
c      &   qm3peryrperwpinsa(1),
c      &   temprep(1),
c      &   qm3peryrperwpinsahitwp(1) )
cc        GADAMS PA-SCR-553 2-4-2005: End of change
c
```

```
c      else if (ireflux.eq.2) then
c       itpa = 1
c        call reflux2( itpa,isa, ntim, tim(1),
c     &   qm3peryrperwpinsa(1),
c     &   qm3peryrperwpinsahitwp(1) )
c      else if (ireflux.eq.3) then
c      else
c        print *, '            ***>>> Error in NFENV <<<***              '
c        print *,'"SelectRefluxModel(1,2,3)" in tpa.inp must be 1,2,or 3'
c        print *, ' '
c        print *, 'There are 3 reflux models '
c        print *, ' '
c        print *, 'The current value is ',ireflux
c        print *, ' '
c        STOP
c      endif
```

change call to reflux3:

from:

```
call reflux3( itpa, isa, ntim, tim(1),
     &                wpcellwidth, wpspacedrift,
     &                rf2porosity, rf2sat_init, rf2sat_resid,
     &                fracndrm, fracndto, fracndtorm,
     &                densboil, enthalphase, tempgradboil, cond,
     &                qm3peryrperwpinsa(1),
     &                qm3peryrperwpinsahitwp(1) )
```

to:

```
call reflux3( itpa, isa, ntim, tim(1),
     &                wpcellwidth, wpspacedrift,
     &                rf3porosity, rf3sat_init, rf3sat_resid,
     &                fracndrm, fracndto, fracndtorm,
     &                densboil, enthalphase, tempgradboil, cond,
     &                qm3peryrperwpinsa(1),
     &                qm3peryrperwpinsahitwp(1) )
```

Remove abbreviations for *tpa.inp* parameters from the *tpanames.dbs* file:

Reflux2Thickness	Ref2Thck
Reflux2Porosity	Ref2-Prs
Reflux2SatInit	Ref2StIt
Reflux2SatResid	Ref2StRs
Reflux2Period	Ref2-Prd
Reflux2LossI	Ref2LssI
Reflux2LossD	Ref2LssD

Add abbreviations for new *tpa.inp* parameters to the *tpanames.dbs file*:

Reflux3Porosity	RP1
Reflux3SatInit	RSI1
Reflux3SatResid	RSR1

Attachment 2

Test Plan for TPA SCR#555

Test Plan Name:

Tested By: Jose M. Menchaca

Date: May 06, 2005

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0.0l

Test Version: TPA 5.0.0l modified

Process Level (PL) Tests

PL-1. Name:
Path for run directory: ~jmench/tpa500l/SCR555/
Path for archive of results: ~jmench/tpa500l/SCR555/
Environment variables: setenv TPA_TEST ~/tpa500l
setenv TPA_DATA ~/tpa500l
Special input files or modifications to input files required :

Pertinent Lines in the tpa.inp file:

Special diagnostic code modifications required :

Program modes to be used (append flags, scenario/model switches, etc.): Default values

Utility scripts needed to perform the test:

Utility codes needed in the analysis of the test data: diff, grep

Test Description:

Item 1. Remove subroutines *reflux1* and *reflux2*.

A visual inspection aided by the grep routine verifies the deletion of the reflux1 and reflux2 subroutines.
Note that every occurrence of either reflux1 or reflux2 has been commented out.

```
/home/jmench/tpa500l{9}>grep -w "reflux[12]" *.f
nfenv.f:c     subroutine reflux1, original code: by S. Stothoff, March 10, 1997
nfenv.f:c                    3-2-2005 SCR555 BLW: remove reflux1 model
nfenv.f:c     subroutine reflux2, original code:
nfenv.f:c                    3-2-2005 SCR555 BLW: remove reflux2 model
nfenv.f:cc       GADAMS PA-SCR-553 2-4-2005: reflux1 uses the timeofbackfill to
nfenv.f:cc        call reflux1( isa, timeofbackfill, hloss_fact, ntim, tim(1),
nfenv.f:c        call reflux1( isa, timeofclosure, hloss_fact, ntim, tim(1),
nfenv.f:c        call reflux2( itpa,isa, ntim, tim(1),
nfenv.f:c        call reflux1( isa, timeofbackfill, hloss_fact, ntim, tim(1),
nfenv.f:c        call reflux2( itpa,isa, ntim, tim(1),
nfenv.f:cc        subroutine reflux1( iSA, tbackfill, hloss_fact, ntim, tim,
nfenv.f:c        subroutine reflux1( iSA, tclosure, hloss_fact, ntim, tim,
nfenv.f:cc     NAME:     reflux1
nfenv.f:cc              Module needed for reflux2 but not needed for stand-alone
nfenv.f:cc              reflux2.
nfenv.f:c       include 'reflux2.i'
nfenv.f:c               subroutine reflux2 (itpa,isa, ntim, tim, qm3peryrinsa,
nfenv.f:cc      for tpa vesion simply take reflux2 from stand-alone and insert
nfenv.f:cc       in reflux2.i.
nfenv.f:c       include 'reflux2.i'
nfenv.f:c       include 'reflux2.i'
nfenv.f:c       include 'reflux2.i'
nfenv.f:c      include 'reflux2.i'
nfenv.f:c      include 'reflux2.i' !n3
nfenv.f:c      include 'reflux2.i' !n3
nfenv.f:c      include 'reflux2.i'
/home/jmench/tpa500l{10}>
```

PASS

Item 2. Remove associated parameters and external subroutines from *nfenv.f* and *tpa.inp* files.

A visual inspection aided by the grep routine verifies the deletion of the appropriate values. Note that every occurrence of the values listed for deletion in "Update Requirements" table has been commented out. Additionally, note that the 3 values that listed as requiring modification in the "Update Requirements" table have been renamed to reflect the reflux 3 model.

```
/home/jmench/tpa5001{50}>grep SelectRefluxModel *.f codes/*.f
nfenv.f:c       name = 'SelectRefluxModel(1,2,3)'
nfenv.f:c        print *,'"SelectRefluxModel(1,2,3)" in tpa.inp must be 1,2,or 3'
nfenv.f:c        name = 'SelectRefluxModel(1,2,3)'
nfenv.f:c        print *,'"SelectRefluxModel(1,2,3)" in tpa.inp must be 1,2,or 3'
/home/jmench/tpa5001{51}>grep Reflux2Period *.f codes/*.f
nfenv.f:c       name = 'Reflux2Period'
nfenv.f:c        name = 'Reflux2Period'
/home/jmench/tpa5001{52}>grep RefluxLossI *.f codes/*.f
/home/jmench/tpa5001{53}>grep Reflux2LossI *.f codes/*.f
nfenv.f:c       name = 'Reflux2LossI'
nfenv.f:c        name = 'Reflux2LossI'
/home/jmench/tpa5001{54}>grep Reflux2LossD *.f codes/*.f
nfenv.f:c       name = 'Reflux2LossD'
nfenv.f:c        name = 'Reflux2LossD'
/home/jmench/tpa5001{55}>grep Reflux2Thickness *.f codes/*.f
nfenv.f:c       name = 'Reflux2Thickness'
nfenv.f:c        name = 'Reflux2Thickness'
/home/jmench/tpa5001{56}>grep Reflux *.f codes/*.f | grep Porosity
nfenv.f:c       name = 'Reflux2Porosity'
nfenv.f:        name = 'Reflux3Porosity'
nfenv.f:c        name = 'Reflux2Porosity'
/home/jmench/tpa5001{57}>grep Reflux *.f codes/*.f | grep SatInit
nfenv.f:c       name = 'Reflux2SatInit'
nfenv.f:        name = 'Reflux3SatInit'
nfenv.f:c        name = 'Reflux2SatInit'
/home/jmench/tpa5001{58}>grep Reflux *.f codes/*.f | grep Resid
nfenv.f:c       name = 'Reflux2SatResid'
nfenv.f:        name = 'Reflux3SatResid'
nfenv.f:c        name = 'Reflux2SatResid'

/home/jmench/tpa5001{11}>grep -i reflux tpa.inp
** BLW 3-2-2005 SCR555: remove reflux 1&2 models
**SelectRefluxModel(1,2,3)
LengthOfRefluxZone[m]
MaximumFluxInRefluxZone[m/s]
** BLW 3-2-2005 SCR555: remove reflux 1&2 models
**Reflux2Thickness
**Reflux2Porosity
Reflux3Porosity
**Reflux2SatInit
Reflux3SatInit
**Reflux2SatResid
Reflux3SatResid
** BLW 3-2-2005 SCR555: remove reflux 1&2 models
**Reflux2Period
** BLW 3-2-2005 SCR555: remove reflux 1&2 models
**Reflux2LossI
** BLW 3-2-2005 SCR555: remove reflux 1&2 models
**Reflux2LossD
```

PASS

Item 3. Rename include file.

A visual inspection aided by the diff routine verifies the name change of the reflux include file.

```
/home/jmench/tpa5001{9}>diff reflux3.i reflux2.i
/home/jmench/tpa5001{10}>echo No content change from reflux2.i to reflux3.i, just the name
changed.
No content change from reflux2.i to reflux3.i, just the name changed.
/home/jmench/tpa5001{11}>
```

PASS

Item 4. Add new *tpa.inp* parameter abbreviations to *tpanames.dbs*.

A visual inspection aided by the diff routine verifies the deletion of the appropriate values and the addition of new values to the tpanames.dbs file.

```
/home/jmench/tpa5001{15}>diff SCR555/tpanames.dbs.txt ./tpanames.dbs
22a23,29
> Reflux2Thickness                                          Ref2Thck
> Reflux2Porosity                                           Ref2-Prs
> Reflux2SatInit                                            Ref2StIt
> Reflux2SatResid                                           Ref2StRs
> Reflux2Period                                             Ref2-Prd
> Reflux2LossI                                              Ref2LssI
> Reflux2LossD                                              Ref2LssD
1702,1705d1708
< Reflux3Porosity                                           RP1
< Reflux3SatInit                                            RSI1
< Reflux3SatResid                                           RSR1
```

PASS

Run Test:

Final test is to run both versions and assure that the output is identical.

The diff output below demonstrates that the only differences in output is the time stamp for each file. Non-numerical differences occur in the files where it is to be expected after the changes to the tpa.inp:

cp.out
tpamax.out
tpameans.out
tpamin.out
tpanames.dbs

```
>  TPA 5.0.01, Job started: Tue May 10 17:21:44 2005
/home/jmench/tpa5001/SCR555{38}>diff AfterBLWChanges100kyr B4Changes100kyr
diff AfterBLWChanges100kyr/airpkdos.res B4Changes100kyr/airpkdos.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/arpkds_c.res B4Changes100kyr/arpkds_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/ashout.res B4Changes100kyr/ashout.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/cp.tpa B4Changes100kyr/cp.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
116a117
>                    3 = SelectRefluxModel(1,2,3)
120,122c121,127
<  1.400000000000000E-01 = Reflux3Porosity
<  9.000000000000000E-01 = Reflux3SatInit
<  1.000000000000000E-01 = Reflux3SatResid
---
>  1.000000000000000E+02 = Reflux2Thickness
>  1.400000000000000E-01 = Reflux2Porosity
>  9.000000000000000E-01 = Reflux2SatInit
>  1.000000000000000E-01 = Reflux2SatResid
>  1.000000000000000E+02 = Reflux2Period
>  1.000000000000000E-01 = Reflux2LossI
>  1.000000000000000E-01 = Reflux2LossD
diff AfterBLWChanges100kyr/cumrel.res B4Changes100kyr/cumrel.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/cumrel_c.res B4Changes100kyr/cumrel_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
```

```
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/dsfail.res B4Changes100kyr/dsfail.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/epa_ave.out B4Changes100kyr/epa_ave.out
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/epapktim.out B4Changes100kyr/epapktim.out
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/failt.out B4Changes100kyr/failt.out
4c4
<  Wed May 11 14:12:56 2005
---
>  Tue May 10 15:57:09 2005
diff AfterBLWChanges100kyr/ggenii.out B4Changes100kyr/ggenii.out
27c27
<  Executed on: 11-May-05 at 14:13:23                                    Page     0
---
>  Executed on: 10-May-05 at 15:57:38                                    Page     0
35c35
<  Executed on: 11-May-05 at 14:13:23                                    Page A.  1
---
>  Executed on: 10-May-05 at 15:57:38                                    Page A.  1
diff AfterBLWChanges100kyr/gmedia.out B4Changes100kyr/gmedia.out
7c7
<  Executed on: 11-May-05 at 14:13:23                                    Page     1
---
>  Executed on: 10-May-05 at 15:57:38                                    Page     1
diff AfterBLWChanges100kyr/gsccdf.res B4Changes100kyr/gsccdf.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/gsccdf_c.res B4Changes100kyr/gsccdf_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/gwccdf.res B4Changes100kyr/gwccdf.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/gwccdf_c.res B4Changes100kyr/gwccdf_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/gwpkdos.res B4Changes100kyr/gwpkdos.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/gwpkds_c.res B4Changes100kyr/gwpkds_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/gwttuzsz.res B4Changes100kyr/gwttuzsz.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/infilper.res B4Changes100kyr/infilper.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
```

```
diff AfterBLWChanges100kyr/mechfail.dat B4Changes100kyr/mechfail.dat
2c2
< DATE/Time: Wed May 11 14:12:56 2005
---
> DATE/Time: Tue May 10 15:57:08 2005
diff AfterBLWChanges100kyr/mechfail.inp B4Changes100kyr/mechfail.inp
2c2
< DATE/Time: Wed May 11 14:12:55 2005
---
> DATE/Time: Tue May 10 15:57:08 2005
diff AfterBLWChanges100kyr/mv.tpa B4Changes100kyr/mv.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/nearfld.res B4Changes100kyr/nearfld.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/nefii.dis B4Changes100kyr/nefii.dis
2c2
< EXECUTION DATE   May 11   AND TIME  14:13:2
---
> EXECUTION DATE   May 10   AND TIME  15:57:3
diff AfterBLWChanges100kyr/nefii.out B4Changes100kyr/nefii.out
8c8
<      *              EXECUTION DATE  May 11   AND TIME  14:13:2              *
---
>      *              EXECUTION DATE  May 10   AND TIME  15:57:3              *
diff AfterBLWChanges100kyr/nefiisz.dis B4Changes100kyr/nefiisz.dis
2c2
< EXECUTION DATE   May 11   AND TIME  14:13:2
---
> EXECUTION DATE   May 10   AND TIME  15:57:3
diff AfterBLWChanges100kyr/nefiisz.out B4Changes100kyr/nefiisz.out
8c8
<      *              EXECUTION DATE  May 11   AND TIME  14:13:2              *
---
>      *              EXECUTION DATE  May 10   AND TIME  15:57:3              *
diff AfterBLWChanges100kyr/nefiiuz.dis B4Changes100kyr/nefiiuz.dis
2c2
< EXECUTION DATE   May 11   AND TIME  14:12:5
---
> EXECUTION DATE   May 10   AND TIME  15:57:1
diff AfterBLWChanges100kyr/nefiiuz.out B4Changes100kyr/nefiiuz.out
8c8
<      *              EXECUTION DATE  May 11   AND TIME  14:12:5              *
---
>      *              EXECUTION DATE  May 10   AND TIME  15:57:1              *
diff AfterBLWChanges100kyr/npkdoset.res B4Changes100kyr/npkdoset.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/npkdst_c.res B4Changes100kyr/npkdst_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/pkmndose.res B4Changes100kyr/pkmndose.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/pkreltim.res B4Changes100kyr/pkreltim.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/pkrltm_c.res B4Changes100kyr/pkrltm_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
```

```
diff AfterBLWChanges100kyr/relccdf.res B4Changes100kyr/relccdf.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/releaset.out B4Changes100kyr/releaset.out
3c3
<  Wed May 11 14:12:56 2005
---
>  Tue May 10 15:57:09 2005
diff AfterBLWChanges100kyr/relgwgs.res B4Changes100kyr/relgwgs.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwna.tpa B4Changes100kyr/rgwna.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwnapani.tpa B4Changes100kyr/rgwnapani.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwnapdw.tpa B4Changes100kyr/rgwnapdw.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwnapext.tpa B4Changes100kyr/rgwnapext.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwnapinh.tpa B4Changes100kyr/rgwnapinh.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwnapmlk.tpa B4Changes100kyr/rgwnapmlk.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwnappla.tpa B4Changes100kyr/rgwnappla.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwnr.tpa B4Changes100kyr/rgwnr.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwsa.tpa B4Changes100kyr/rgwsa.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwsap.tpa B4Changes100kyr/rgwsap.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rgwsr.tpa B4Changes100kyr/rgwsr.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/rlccdf_c.res B4Changes100kyr/rlccdf_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
```

```
diff AfterBLWChanges100kyr/rlgwgs_c.res B4Changes100kyr/rlgwgs_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/samplpar.abb B4Changes100kyr/samplpar.abb
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:31 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/samplpar.hdr B4Changes100kyr/samplpar.hdr
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:31 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/samplpar.res B4Changes100kyr/samplpar.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/sp.tpa B4Changes100kyr/sp.tpa
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/totdos_c.res B4Changes100kyr/totdos_c.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/totdose.res B4Changes100kyr/totdose.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/tpa.out B4Changes100kyr/tpa.out
3c3
<         Job started: Wed May 11 14:06:31 2005
---
>         Job started: Tue May 10 15:50:30 2005
diff AfterBLWChanges100kyr/tpamax.out B4Changes100kyr/tpamax.out
7c7
< ** ** submitted for the run on Wed May 11 14:06:32 2005.
---
> ** ** submitted for the run on Tue May 10 15:50:30 2005.
833,836c833,835
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **iconstant
< **SelectRefluxModel(1,2,3)
< **3
---
> iconstant
> SelectRefluxModel(1,2,3)
> 3
850,853c849,851
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2Thickness
< **100.0
---
> constant
> Reflux2Thickness
> 100.0
855,856d852
< ** BLW 3-2-2005 SCR555: change parameter name
< **Reflux2Porosity
858c854
< Reflux3Porosity
---
> Reflux2Porosity
861,862d856
< ** BLW 3-2-2005 SCR555: change parameter name
< **Reflux2SatInit
864c858
< Reflux3SatInit
```

```
---
> Reflux2SatInit
867,868d860
< ** BLW 3-2-2005 SCR555: change parameter name
< **Reflux2SatResid
870c862
< Reflux3SatResid
---
> Reflux2SatResid
873,876c865,867
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2Period
< **100.0
---
> constant
> Reflux2Period
> 100.0
878,881c869,871
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2LossI
< **0.1
---
> constant
> Reflux2LossI
> 0.1
883,886c873,875
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2LossD
< **0.1
---
> constant
> Reflux2LossD
> 0.1
diff AfterBLWChanges100kyr/tpameans.out B4Changes100kyr/tpameans.out
7c7
< ** ** submitted for the run on Wed May 11 14:06:32 2005.
---
> ** ** submitted for the run on Tue May 10 15:50:30 2005.
833,836c833,835
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **iconstant
< **SelectRefluxModel(1,2,3)
< **3
---
> iconstant
> SelectRefluxModel(1,2,3)
> 3
850,853c849,851
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2Thickness
< **100.0
---
> constant
> Reflux2Thickness
> 100.0
855,856d852
< ** BLW 3-2-2005 SCR555: change parameter name
< **Reflux2Porosity
858c854
< Reflux3Porosity
---
> Reflux2Porosity
861,862d856
< ** BLW 3-2-2005 SCR555: change parameter name
< **Reflux2SatInit
864c858
< Reflux3SatInit
---
> Reflux2SatInit
867,868d860
< ** BLW 3-2-2005 SCR555: change parameter name
```

```
< **Reflux2SatResid
870c862
< Reflux3SatResid
---
> Reflux2SatResid
873,876c865,867
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2Period
< **100.0
---
> constant
> Reflux2Period
> 100.0
878,881c869,871
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2LossI
< **0.1
---
> constant
> Reflux2LossI
> 0.1
883,886c873,875
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2LossD
< **0.1
---
> constant
> Reflux2LossD
> 0.1
diff AfterBLWChanges100kyr/tpamin.out B4Changes100kyr/tpamin.out
7c7
< ** ** submitted for the run on Wed May 11 14:06:32 2005.
---
> ** ** submitted for the run on Tue May 10 15:50:30 2005.
833,836c833,835
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **iconstant
< **SelectRefluxModel(1,2,3)
< **3
---
> iconstant
> SelectRefluxModel(1,2,3)
> 3
850,853c849,851
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2Thickness
< **100.0
---
> constant
> Reflux2Thickness
> 100.0
855,856d852
< ** BLW 3-2-2005 SCR555: change parameter name
< **Reflux2Porosity
858c854
< Reflux3Porosity
---
> Reflux2Porosity
861,862d856
< ** BLW 3-2-2005 SCR555: change parameter name
< **Reflux2SatInit
864c858
< Reflux3SatInit
---
> Reflux2SatInit
867,868d860
< ** BLW 3-2-2005 SCR555: change parameter name
< **Reflux2SatResid
870c862
< Reflux3SatResid
---
```

```
> Reflux2SatResid
873,876c865,867
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2Period
< **100.0
---
> constant
> Reflux2Period
> 100.0
878,881c869,871
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2LossI
< **0.1
---
> constant
> Reflux2LossI
> 0.1
883,886c873,875
< ** BLW 3-2-2005 SCR555: remove reflux 1&2 models
< **constant
< **Reflux2LossD
< **0.1
---
> constant
> Reflux2LossD
> 0.1
diff AfterBLWChanges100kyr/tpanames.dbs B4Changes100kyr/tpanames.dbs
22a23,29
> Reflux2Thickness                                          Ref2Thck
> Reflux2Porosity                                           Ref2-Prs
> Reflux2SatInit                                            Ref2StIt
> Reflux2SatResid                                           Ref2StRs
> Reflux2Period                                             Ref2-Prd
> Reflux2LossI                                              Ref2LssI
> Reflux2LossD                                              Ref2LssD
1702,1705d1708
< Reflux3Porosity                                           RP1
< Reflux3SatInit                                            RSI1
< Reflux3SatResid                                           RSR1
<
diff AfterBLWChanges100kyr/wpsfail.res B4Changes100kyr/wpsfail.res
3c3
<  TPA 5.0.01, Job started: Wed May 11 14:06:32 2005
---
>  TPA 5.0.01, Job started: Tue May 10 15:50:30 2005
/home/jmench/tpa5001/SCR555{39}>
```

PASS

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-556	**2. Software Title and Version:** TPA 5.0.0q	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *tpa.inp, ebsrel.def, ebsrel.f,* and *releaset.f,*

1. Remove C-14 related parameters from *releaset.f* and *ebsrel.f*
2. Set Curium Kds to TPA version 4.1j Americium values.

5. Change Requested by: R. Codell, P. Bertetti Date: 2-2-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 2-2-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

1. The following C-14 related parameters are not used and are therefore being removed from the files listed in the affected modules section (see Attachment A for details):

RadiusOfSFGrain[m]
SubGrainFragmentRadiusAfterTransFrac[m]
ThicknessOfCladding[m]
SFC-14InventoryPerKgSF[ci]
CladC-14InventoryPerKgSF[ci]
ZyrOxideAndCrudC-14InvPerKgSF[ci]
GapAndGrainBoundaryInventoryPerKgSF[ci]

2. The Matrix Kd values for Curium are all currently 0. The Matrix Kd values for Curium are changed to the Americium values found in TPA Version 4.1j.

8. Implemented by: Jose M. Menchaca	**Date:** 03/11/05

9. Description of Acceptance Tests: See attachment for description of acceptance tests.

10. Tested by: R. Rice	**Date:** 05/17/05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)
Delete	EBSREL	RadiusOfSFGrain[m]		uniform	3.5e-6, 1.5e-5		
Delete	EBSREL	SubGrainFragmentRadiusAfterTransFrac[m]		normal	5.0e-7, 2.0e-6		
Delete	EBSREL	ThicknessOfCladding[m]		constant	6.1e-4		
Delete	EBSREL	SFC-14InventoryPerKgSF[ci]		constant	7.2e-4		
Delete	EBSREL	CladC-14InventoryPerKgSF[ci]		constant	4.89e-4		
Delete	EBSREL	ZyrOxideAndCrudC-14InvPerKgSF[ci]		constant	2.48e-5		

Delete	EBSREL	GapAndGrainBoundaryInventoryPerKgSF[ci]		constant	6.2e-6		
Modify From	UZFT	MatrixKD_TSw_Cm		constant	0.0		
Modify To	UZFT	MatrixKD_TSw_Cm		lognormal	1760., 73663.		
Modify From	UZFT	MatrixKD_CHnvCm		constant	0.0		
Modify To	UZFT	MatrixKD_TSwCm		lognormal	5340., 223529.		
Modify From	UZFT	MatrixKD_CHnzCm		constant	0.0		
Modify To	UZFT	MatrixKD_CHnzCm		lognormal	4855., 203209.		
Modify From	UZFT	MatrixKD_PPw_Cm		constant	0.0		
Modify To	UZFT	MatrixKD_PPw_Cm		lognormal	4005., 167647		
Modify From	UZFT	MatrixKD_UCF_Cm		constant	0.0		
Modify To	UZFT	MatrixKD_UCF_Cm		lognormal	4187., 175267.		
Modify From	UZFT	MatrixKD_BFw_Cm		constant	0.0		
Modify To	UZFT	MatrixKD_BFw_Cm		lognormal	1699., 71123.		
Modify From	UZFT	MatrixKD_UFZ_Cm		constant	0.0		
Modify To	UZFT	MatrixKD_UFZ_Cm		lognormal	1638., 68583.		

Attachment A

The following pages are the diff files for the subject files.

Differences in tpa.inp

```
diff -c tpa5001modifiedForSCR556/tpa.inp tpa5001
*** tpa5001modifiedForSCR556/tpa.inp    Tue Mar  8 11:40:58 2005
--- tpa5001/tpa.inp     Tue Mar  1 19:51:53 2005
***************
*** 2291,2327 ****
  InitialRadiusOfSFParticle[m]
  7.0e-4,  3.0e-3
  **
! *jmm uniform
! *jmm RadiusOfSFGrain[m]
! *jmm 3.5e-6, 1.5e-5
  **
  uniform
  CladdingCorrectionFactor
  0.0, 1.0
  **
! *jmm normal
! *jmm SubGrainFragmentRadiusAfterTransFrac[m]
! *jmm 5.0e-7,  2.0e-6
  **
! *jmm constant
! *jmm ThicknessOfCladding[m]
! *jmm 6.1e-4
  **
! *jmm constant
! *jmm SFC-14InventoryPerKgSF[ci]
! *jmm 7.2e-4
  **
! *jmm constant
! *jmm CladC-14InventoryPerKgSF[ci]
! *jmm 4.89e-4
  **
! *jmm constant
! *jmm ZyrOxideAndCrudC-14InvPerKgSF[ci]
! *jmm 2.48e-5
  **
! *jmm constant
! *jmm GapAndGrainBoundaryInventoryPerKgSF[ci]
! *jmm 6.2e-6
  **
  uniform
  SolubilityAm[kg/m3]
--- 2291,2327 ----
  InitialRadiusOfSFParticle[m]
  7.0e-4,  3.0e-3
  **
! uniform
! RadiusOfSFGrain[m]
! 3.5e-6, 1.5e-5
  **
  uniform
  CladdingCorrectionFactor
  0.0, 1.0
  **
! normal
! SubGrainFragmentRadiusAfterTransFrac[m]
! 5.0e-7,  2.0e-6
  **
! constant
! ThicknessOfCladding[m]
! 6.1e-4
  **
! constant
! SFC-14InventoryPerKgSF[ci]
```

```
! 7.2e-4
  **
! constant
! CladC-14InventoryPerKgSF[ci]
! 4.89e-4
  **
! constant
! ZyrOxideAndCrudC-14InvPerKgSF[ci]
! 2.48e-5
  **
! constant
! GapAndGrainBoundaryInventoryPerKgSF[ci]
! 6.2e-6
  **
  uniform
  SolubilityAm[kg/m3]
```

Differences in ebsrel.def

```
diff -c tpa5001modifiedForSCR556/data/ebsrel.def tpa5001/data
*** tpa5001modifiedForSCR556/data/ebsrel.def    Tue Mar  8 14:07:45 2005
--- tpa5001/data/ebsrel.def     Fri Oct 17 17:34:05 2003
***************
*** 46,55 ****
--- 46,62 ----
  |
  \C-14 generation
   2.17412E-03            ! r0z: initial radius of SF particle [m]
+  1.25000E-05            ! radu: radius of the SF grain [m]
+  1.77073E-06            ! radsg: subgrain fragment radius after trans. frac. [m]
   1.0                    ! claddingcorfact: cladding correction factor
   100.0                  ! cladve, velocity enhancement factor (1 to 240)
   2.0                  ! ltube0, half length of fuel rod, meters  ebsrel: eltube0
   0.005                  ! rrod, radius of fuel in rod, meters
+  6.10000E-04            ! thclad: thickness of cladding [m]
+  7.20000E-04            ! cfuel: C-14 [ci] /kg SF
+  4.89000E-04            ! czmetal: C-14 [ci] /kg SF in Zyr. clad & other metals
+  2.48000E-05            ! czoxide: C-14/kg SF in initial Zry oxide & crud
+  6.20000E-06            ! cgap: C-14/kg SF in grain and gap
  |
  \glass model
   5.63e-2                ! simglass m^2/kg
```

Differences in ebsrel.f

```
diff -c tpa5001modifiedForSCR556/ebsrel.f tpa5001
*** tpa5001modifiedForSCR556/ebsrel.f   Fri Mar 11 11:57:14 2005
--- tpa5001/ebsrel.f    Tue Mar  1 19:51:51 2005
***************
*** 256,268 ****
        common / ebsrel26 / i_oxgnovpr
        common / ebsrel27 / i_cc03
        common / ebsrel29 / i_r0z
! cjmm      common / ebsrel30 / i_radu scheduled for deletion because of SCR 556
! cjmm      common / ebsrel31 / i_radsg
! cjmm      common / ebsrel32 / i_thclad
! cjmm      common / ebsrel33 / i_cfuel
! cjmm      common / ebsrel34 / i_czmetal
! cjmm      common / ebsrel35 / i_czoxide
! cjmm      common / ebsrel36 / i_cgap
        common / ebsrel37 / i_driftdia
        common / ebsrel38 / i_sawetfrac, i_wp_payload
        common / ebsrel39 / imvindex(maxnnucl,2,maxnsubarea)
--- 256,268 ----
        common / ebsrel26 / i_oxgnovpr
        common / ebsrel27 / i_cc03
        common / ebsrel29 / i_r0z
!       common / ebsrel30 / i_radu
!       common / ebsrel31 / i_radsg
!       common / ebsrel32 / i_thclad
!       common / ebsrel33 / i_cfuel
!       common / ebsrel34 / i_czmetal
!       common / ebsrel35 / i_czoxide
!       common / ebsrel36 / i_cgap
        common / ebsrel37 / i_driftdia
        common / ebsrel38 / i_sawetfrac, i_wp_payload
        common / ebsrel39 / imvindex(maxnnucl,2,maxnsubarea)
***************
*** 623,664 ****
          name = 'InitialRadiusOfSFParticle[m]'
          i_r0z =  ispquery( name )

! cjmm        call clearchar( 60, name )
! cjmm        name = 'RadiusOfSFGrain[m]'
! cjmm        i_radu =  ispquery( name )

! cjmm        call clearchar( 60, name )
! cjmm        name = 'SubGrainFragmentRadiusAfterTransFrac[m]'
! cjmm        i_radsg =  ispquery( name )

          call clearchar( 60, name )
          name = 'CladdingCorrectionFactor'
          i_claddingcorfact =  ispquery( name )

! cjmm        call clearchar( 60, name )
! cjmm        name = 'ThicknessOfCladding[m]'
! cjmm        i_thclad =  ispquery( name )
  c
  c css 2-14-2005; SCR519:  these 4 parameters are written out
  c     to ebsrel.inp and then read in by releaset; however, releaset
  c     does not actually use them
  c
! cjmm c     CFUEL
! cjmm         call clearchar( 60, name )
! cjmm         name = 'SFC-14InventoryPerKgSF[ci]'
! cjmm         i_cfuel =  ispquery( name )
! cjmm c     CZMETAL
! cjmm         call clearchar( 60, name )
! cjmm         name = 'CladC-14InventoryPerKgSF[ci]'
! cjmm         i_czmetal =  ispquery( name )
! cjmm c     CZOXIDE
! cjmm         call clearchar( 60, name )
! cjmm         name = 'ZyrOxideAndCrudC-14InvPerKgSF[ci]'
! cjmm         i_czoxide =  ispquery( name )
! cjmm c     CGAP
! cjmm         call clearchar( 60, name )
! cjmm         name = 'GapAndGrainBoundaryInventoryPerKgSF[ci]'
! cjmm         i_cgap =  ispquery( name )
```

```
  c
  c end change:  SCR519
  c
--- 623,664 ----
          name = 'InitialRadiusOfSFParticle[m]'
          i_r0z =  ispquery( name )

!         call clearchar( 60, name )
!         name = 'RadiusOfSFGrain[m]'
!         i_radu =  ispquery( name )

!         call clearchar( 60, name )
!         name = 'SubGrainFragmentRadiusAfterTransFrac[m]'
!         i_radsg =  ispquery( name )

          call clearchar( 60, name )
          name = 'CladdingCorrectionFactor'
          i_claddingcorfact =  ispquery( name )

!         call clearchar( 60, name )
!         name = 'ThicknessOfCladding[m]'
!         i_thclad =  ispquery( name )
  c
  c css 2-14-2005; SCR519:  these 4 parameters are written out
  c     to ebsrel.inp and then read in by releaset; however, releaset
  c     does not actually use them
  c
! c     CFUEL
!         call clearchar( 60, name )
!         name = 'SFC-14InventoryPerKgSF[ci]'
!         i_cfuel =  ispquery( name )
! c     CZMETAL
!         call clearchar( 60, name )
!         name = 'CladC-14InventoryPerKgSF[ci]'
!         i_czmetal =  ispquery( name )
! c     CZOXIDE
!         call clearchar( 60, name )
!         name = 'ZyrOxideAndCrudC-14InvPerKgSF[ci]'
!         i_czoxide =  ispquery( name )
! c     CGAP
!         call clearchar( 60, name )
!         name = 'GapAndGrainBoundaryInventoryPerKgSF[ci]'
!         i_cgap =  ispquery( name )
  c
  c end change:  SCR519
  c
***************
*** 1152,1173 ****
  C   LINE 48
        write(iebsrelinp, 100 ) aline

! cjmm      RADU = valuesp(i_radu)
! cjmm      read(iebsreltmp, 100 ) aline
! cjmm      write( aline(1:14), fmt='(1pe14.5)' ) RADU
  C   LINE 49
! cjmm      write(iebsrelinp, 100 ) aline

! cjmm      RADSG = valuesp(i_radsg)
! cjmm      read(iebsreltmp, 100 ) aline
! cjmm      write( aline(1:14), fmt='(1pe14.5)' ) RADSG
  C   LINE 50
! cjmm      write(iebsrelinp, 100 ) aline

        claddingcorfact = valuesp(i_claddingcorfact)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) claddingcorfact
! C   LINE 49
        write(iebsrelinp, 100 ) aline

  c   cladding velocity enhancement factor
--- 1152,1173 ----
  C   LINE 48
        write(iebsrelinp, 100 ) aline

!       RADU = valuesp(i_radu)
```

```
!       read(iebsreltmp, 100 ) aline
!       write( aline(1:14), fmt='(1pe14.5)' ) RADU
  C   LINE 49
!       write(iebsrelinp, 100 ) aline

!       RADSG = valuesp(i_radsg)
!       read(iebsreltmp, 100 ) aline
!       write( aline(1:14), fmt='(1pe14.5)' ) RADSG
  C   LINE 50
!       write(iebsrelinp, 100 ) aline

        claddingcorfact = valuesp(i_claddingcorfact)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) claddingcorfact
! C   LINE 51
        write(iebsrelinp, 100 ) aline

  c   cladding velocity enhancement factor
***************
*** 1174,1180 ****
        CLADVE = valuesp(i_claddingvefact)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) CLADVE
! C   glass & cladding LINE 50
        write(iebsrelinp, 100 ) aline

  c   half length of fuel rod
--- 1174,1180 ----
        CLADVE = valuesp(i_claddingvefact)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) CLADVE
! C   glass & cladding LINE 52
        write(iebsrelinp, 100 ) aline

  c   half length of fuel rod
***************
*** 1181,1187 ****
        ELTUBE = valuesp(i_rodhalflength)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) ELTUBE
! C   glass & cladding LINE 51
        write(iebsrelinp, 100 ) aline

  c   fuel radius in rod
--- 1181,1187 ----
        ELTUBE = valuesp(i_rodhalflength)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) ELTUBE
! C   glass & cladding LINE 53
        write(iebsrelinp, 100 ) aline

  c   fuel radius in rod
***************
*** 1188,1227 ****
        RROD = valuesp(i_fuelradius)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) RROD
! C   glass & cladding LINE 52
        write(iebsrelinp, 100 ) aline

! cjmm      THCLAD = valuesp(i_thclad)
! cjmm      read(iebsreltmp, 100 ) aline
! cjmm      write( aline(1:14), fmt='(1pe14.5)' ) THCLAD
  C   glass & cladding LINE 55
! cjmm      write(iebsrelinp, 100 ) aline

! cjmm      CFUEL = valuesp(i_cfuel)
! cjmm      read(iebsreltmp, 100 ) aline
! cjmm      write( aline(1:14), fmt='(1pe14.5)' ) CFUEL
! cjmmC   glass & cladding LINE 56
! cjmm      write(iebsrelinp, 100 ) aline
! cjmm
! cjmm      CZMETAL = valuesp(i_czmetal)
! cjmm      read(iebsreltmp, 100 ) aline
! cjmm      write( aline(1:14), fmt='(1pe14.5)' ) CZMETAL
```

```
! cjmmC   glass & cladding LINE 57
! cjmm      write(iebsrelinp, 100 ) aline
! cjmm
! cjmm      CZOXIDE = valuesp(i_czoxide)
! cjmm      read(iebsreltmp, 100 ) aline
! cjmm      write( aline(1:14), fmt='(1pe14.5)' ) CZOXIDE
! cjmmC   glass & cladding LINE 58
! cjmm      write(iebsrelinp, 100 ) aline
! cjmm
! cjmm      CGAP = valuesp(i_cgap)
! cjmm      read(iebsreltmp, 100 ) aline
! cjmm      write( aline(1:14), fmt='(1pe14.5)' ) CGAP
! cjmmC   glass & cladding LINE 59
! cjmm      write(iebsrelinp, 100 ) aline
! cjmm
! C   Copy LINE 53 - LINE 54
        do i = 1, 2
          read(iebsreltmp, 100 ) aline
          write(iebsrelinp, 100 ) aline
--- 1188,1227 ----
        RROD = valuesp(i_fuelradius)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) RROD
! C   glass & cladding LINE 54
        write(iebsrelinp, 100 ) aline

!       THCLAD = valuesp(i_thclad)
!       read(iebsreltmp, 100 ) aline
!       write( aline(1:14), fmt='(1pe14.5)' ) THCLAD
  C   glass & cladding LINE 55
!       write(iebsrelinp, 100 ) aline

!       CFUEL = valuesp(i_cfuel)
!       read(iebsreltmp, 100 ) aline
!       write( aline(1:14), fmt='(1pe14.5)' ) CFUEL
! C   glass & cladding LINE 56
!       write(iebsrelinp, 100 ) aline
!
!       CZMETAL = valuesp(i_czmetal)
!       read(iebsreltmp, 100 ) aline
!       write( aline(1:14), fmt='(1pe14.5)' ) CZMETAL
! C   glass & cladding LINE 57
!       write(iebsrelinp, 100 ) aline
!
!       CZOXIDE = valuesp(i_czoxide)
!       read(iebsreltmp, 100 ) aline
!       write( aline(1:14), fmt='(1pe14.5)' ) CZOXIDE
! C   glass & cladding LINE 58
!       write(iebsrelinp, 100 ) aline
!
!       CGAP = valuesp(i_cgap)
!       read(iebsreltmp, 100 ) aline
!       write( aline(1:14), fmt='(1pe14.5)' ) CGAP
! C   glass & cladding LINE 59
!       write(iebsrelinp, 100 ) aline
!
! C   Copy LINE 60 - LINE 61
        do i = 1, 2
          read(iebsreltmp, 100 ) aline
          write(iebsrelinp, 100 ) aline
***************
*** 1232,1283 ****
        SIMGLASS = valuesp(i_simglass)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) SIMGLASS
! C   glass & cladding LINE 55
        write(iebsrelinp, 100 ) aline

        PHGLASS = valuesp(i_phglass)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) PHGLASS
! C   glass & cladding LINE 56
        write(iebsrelinp, 100 ) aline

        RLOGKEFFHI = valuesp(i_logkeffhi)
```

```
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) RLOGKEFFHI
! C   glass & cladding LINE 57
        write(iebsrelinp, 100 ) aline

        ETAHI = valuesp(i_etahi)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) ETAHI
! C   glass & cladding LINE 58
        write(iebsrelinp, 100 ) aline

        EAHI = valuesp(i_eahi)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) EAHI
! C   glass & cladding LINE 59
        write(iebsrelinp, 100 ) aline

        RLOGKEFFLOW = valuesp(i_logkefflow)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) RLOGKEFFLOW
! C   glass & cladding LINE 60
        write(iebsrelinp, 100 ) aline

        ETALOW = valuesp(i_etalow)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) ETALOW
! C   glass & cladding LINE 61
        write(iebsrelinp, 100 ) aline

        EALOW = valuesp(i_ealow)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) EALOW
! C   glass & cladding LINE 62
        write(iebsrelinp, 100 ) aline

! C   Copy LINE 63 - LINE 64
        do i = 1, 2
          read(iebsreltmp, 100 ) aline
          write(iebsrelinp, 100 ) aline
--- 1232,1283 ----
        SIMGLASS = valuesp(i_simglass)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) SIMGLASS
! C   glass & cladding LINE 62
        write(iebsrelinp, 100 ) aline

        PHGLASS = valuesp(i_phglass)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) PHGLASS
! C   glass & cladding LINE 63
        write(iebsrelinp, 100 ) aline

        RLOGKEFFHI = valuesp(i_logkeffhi)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) RLOGKEFFHI
! C   glass & cladding LINE 64
        write(iebsrelinp, 100 ) aline

        ETAHI = valuesp(i_etahi)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) ETAHI
! C   glass & cladding LINE 65
        write(iebsrelinp, 100 ) aline

        EAHI = valuesp(i_eahi)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) EAHI
! C   glass & cladding LINE 66
        write(iebsrelinp, 100 ) aline

        RLOGKEFFLOW = valuesp(i_logkefflow)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) RLOGKEFFLOW
! C   glass & cladding LINE 67
        write(iebsrelinp, 100 ) aline
```

```
        ETALOW = valuesp(i_etalow)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) ETALOW
! C   glass & cladding LINE 68
        write(iebsrelinp, 100 ) aline

        EALOW = valuesp(i_ealow)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) EALOW
! C   glass & cladding LINE 69
        write(iebsrelinp, 100 ) aline

! C   Copy LINE 70 - LINE 71
        do i = 1, 2
          read(iebsreltmp, 100 ) aline
          write(iebsrelinp, 100 ) aline
***************
*** 1289,1334 ****
        CR_LENGTH = valuesp(i_cracklength)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) CR_LENGTH
! C   glass & cladding LINE 65
        write(iebsrelinp, 100 ) aline

        CR_AREA_A = valuesp(i_crackarea)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) CR_AREA_A
! C   glass & cladding LINE 66
        write(iebsrelinp, 100 ) aline

        CR_AREA_B = valuesp(i_crackgrowthslope)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) CR_AREA_B
! C   glass & cladding LINE 67
        write(iebsrelinp, 100 ) aline

        EL_INTERNAL = valuesp(i_filmpathlength)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) EL_INTERNAL
! C   glass & cladding LINE 68
        write(iebsrelinp, 100 ) aline

        A_INTERNAL = valuesp(i_filmcrosssection)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) A_INTERNAL
! C   glass & cladding LINE 69
        write(iebsrelinp, 100 ) aline

        D_WATER = valuesp(i_waterdiffusivity)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) D_WATER
! C   glass & cladding LINE 70
        write(iebsrelinp, 100 ) aline

        FTILT = valuesp(i_diffusiontiltfraction)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) FTILT
! C   glass & cladding LINE 71
        write(iebsrelinp, 100 ) aline

! C   Copy 22 lines  LINE 72 to LINE 93
        do i = 1, 22
          read(iebsreltmp, 100 ) aline
          write(iebsrelinp, 100 ) aline
--- 1289,1334 ----
        CR_LENGTH = valuesp(i_cracklength)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) CR_LENGTH
! C   glass & cladding LINE 72
        write(iebsrelinp, 100 ) aline

        CR_AREA_A = valuesp(i_crackarea)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) CR_AREA_A
```

```
! C   glass & cladding LINE 73
        write(iebsrelinp, 100 ) aline

        CR_AREA_B = valuesp(i_crackgrowthslope)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) CR_AREA_B
! C   glass & cladding LINE 74
        write(iebsrelinp, 100 ) aline

        EL_INTERNAL = valuesp(i_filmpathlength)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) EL_INTERNAL
! C   glass & cladding LINE 75
        write(iebsrelinp, 100 ) aline

        A_INTERNAL = valuesp(i_filmcrosssection)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) A_INTERNAL
! C   glass & cladding LINE 76
        write(iebsrelinp, 100 ) aline

        D_WATER = valuesp(i_waterdiffusivity)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) D_WATER
! C   glass & cladding LINE 77
        write(iebsrelinp, 100 ) aline

        FTILT = valuesp(i_diffusiontiltfraction)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) FTILT
! C   glass & cladding LINE 78
        write(iebsrelinp, 100 ) aline

! C   Copy 22 lines  LINE 79 to LINE 100
        do i = 1, 22
          read(iebsreltmp, 100 ) aline
          write(iebsrelinp, 100 ) aline
***************
*** 1337,1346 ****
        DRIFTDIA = valuesp(i_driftdia)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) DRIFTDIA
! c   LINE 94
        write(iebsrelinp, 100 ) aline

! c   LINE 95 - 103  (until "\END" is read)
        do i = 1, 1000
          read( iebsreltmp, 100, end=993 ) aline
          write(iebsrelinp, 100 ) aline
--- 1337,1346 ----
        DRIFTDIA = valuesp(i_driftdia)
        read(iebsreltmp, 100 ) aline
        write( aline(1:14), fmt='(1pe14.5)' ) DRIFTDIA
! c   LINE 101
        write(iebsrelinp, 100 ) aline

! c   LINE 102 - 110  (until "\END" is read)
        do i = 1, 1000
          read( iebsreltmp, 100, end=993 ) aline
          write(iebsrelinp, 100 ) aline
```

Differences in releaset.f

```
diff -c tpa5001modifiedForSCR556/codes/releaset.f tpa5001/codes
*** tpa5001modifiedForSCR556/codes/releaset.f   Tue Mar  8 11:54:50 2005
--- tpa5001/codes/releaset.f    Sat Feb 12 19:19:04 2005
***************
*** 484,496 ****
  c                     of time [ci]
  C    oxz:           number of moles of uo2 oxidized/mole o (not o2)
  C    r0z:           radius of SF particle [m]
! cjmm    radu:          initial radius of uo2 grain [m], scheduled for deletion
! cjmm    radsg:         subgrain radius after transgranular fracture [m], scheduled for deletion
! cjmm    thclad:        thickness of cladding, m, scheduled for deletion
! cjmm    cfuel:         ci c14 / kg of fuel in fuel, scheduled for deletion
! cjmm    czmetal:       ci c14 / kg of fuel in zirconium cladding, scheduled for deletion
! cjmm     czoxide:        ci c14/kg of fuel in initial zirconium oxide and crud, scheduled for
deletion
! cjmm    cgap:          ci of c14 / kg of fuel in grain boundary and gap, scheduled for deletion
  C    gscmrl:        gaseous cumulative release
  C    isconf & v:    scenario container numbers by subarea
  c    nremain:       remaining waste packages after initially defective ones
--- 484,496 ----
  c                     of time [ci]
  C    oxz:           number of moles of uo2 oxidized/mole o (not o2)
  C    r0z:           radius of SF particle [m]
! c    radu:          initial radius of uo2 grain [m]
! C    radsg:         subgrain radius after transgranular fracture [m]
! C    thclad:        thickness of cladding, m
! C    cfuel:         ci c14 / kg of fuel in fuel
! C    czmetal:       ci c14 / kg of fuel in zirconium cladding
! C    czoxide:       ci c14/kg of fuel in initial zirconium oxide and crud
! C    cgap:          ci of c14 / kg of fuel in grain boundary and gap
  C    gscmrl:        gaseous cumulative release
  C    isconf & v:    scenario container numbers by subarea
  c    nremain:       remaining waste packages after initially defective ones
***************
*** 1288,1295 ****
          integer ntemp, nvar
          integer ncon, kcon, icon, nchns, ni
          real*8 sol, rd, rde, amall, halflife, curall, fggap
! cjmm        real*8 r0z, radu, radsg
!         real*8 r0z
          real*8 alam, atoms, atall, am
          real*8 fueden, amassc
          integer kmax, kount
--- 1288,1294 ----
          integer ntemp, nvar
          integer ncon, kcon, icon, nchns, ni
          real*8 sol, rd, rde, amall, halflife, curall, fggap
!         real*8 r0z, radu, radsg
          real*8 alam, atoms, atall, am
          real*8 fueden, amassc
          integer kmax, kount
***************
*** 1313,1319 ****
          common /cther1/ ttemp(maxtim), tcan(maxtim)
          common /cwast1/ fueden, amassc
          common /cther0/ ntemp
! cjmm        common /rcarbon1/      radu, radsg
          common /path  / kmax, kount, dxsav, xp(200), yp(100, 200)
          common /rkutta/ eps, tiny, dtinit, dtmin, dtmax
          common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
--- 1312,1318 ----
          common /cther1/ ttemp(maxtim), tcan(maxtim)
          common /cwast1/ fueden, amassc
          common /cther0/ ntemp
!         common /rcarbon1/      radu, radsg
          common /path  / kmax, kount, dxsav, xp(200), yp(100, 200)
          common /rkutta/ eps, tiny, dtinit, dtmin, dtmax
          common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
***************
*** 1376,1385 ****
          real*8 phvalue,oxgnovpr,pco3,usrlrate,preexpo
          common /rcarbon4/ cladfactor,cladve,velfuel,velcladunzip,ltube,
       &         rrod,ltube0
```

```
- cjmm        common /rcarbon4/ cladfactor,cladve,velfuel,velcladunzip,ltube,
- cjmm     &         rrod,ltube0
          real*8 cladfactor,cladve,velfuel,velcladunzip,ltube,rrod,ltube0
- cjmm        real*8 cladfactor,cladve,velfuel,velcladunzip,ltube,rrod,ltube0

  C-----------------------------------------------------------------------
  c
--- 1375,1381 ----
***************
*** 1787,1795 ****
          real*8 rdp2, dissip2
          real*8 oxwidth
          real*8 pi
! cjmm        real*8 r0z, radu, radsg, cladfactor
!         real*8 r0z, cladfactor
! cjmm        real*8 cladve,velfuel,velcladunzip,ltube,rrod,ltube0
          real*8 cladve,velfuel,velcladunzip,ltube,rrod,ltube0
          real*8 saream
          real*8 alam, atoms, atall, am
--- 1783,1789 ----
          real*8 rdp2, dissip2
          real*8 oxwidth
          real*8 pi
!         real*8 r0z, radu, radsg, cladfactor
          real*8 cladve,velfuel,velcladunzip,ltube,rrod,ltube0
          real*8 saream
          real*8 alam, atoms, atall, am
***************
*** 1820,1830 ****

          common /cwast1/ fueden, amassc
          common /damvalues/ rdpxx, dissipxx, adflux
! cjmm        common /rcarbon1/      radu, radsg
          common /rcarbon4/ cladfactor,cladve,velfuel,velcladunzip,ltube,
       1         rrod,ltube0
- cjmm        common /rcarbon4/ cladfactor,cladve,velfuel,velcladunzip,ltube,
- cjmm     1         rrod,ltube0
          common /oxidized/ oxwidth
          common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
       &                  dele(maxele),cd(maxnuc,maxmem),
--- 1814,1822 ----

          common /cwast1/ fueden, amassc
          common /damvalues/ rdpxx, dissipxx, adflux
!         common /rcarbon1/      radu, radsg
          common /rcarbon4/ cladfactor,cladve,velfuel,velcladunzip,ltube,
       1         rrod,ltube0
          common /oxidized/ oxwidth
          common /cnucl2/ ncon(maxele), sol(maxele), rde(maxele),
       &                  dele(maxele),cd(maxnuc,maxmem),
***************
*** 3014,3033 ****
          implicit none


!         real*8  amassc, pco3, cftime,
!      &          ctemp, cvol, defectt
! cjmm        real*8  amassc, pco3, cftime, cfuel, cgap,
! cjmm     &          ctemp, cvol, czmetal, czoxide, defectt
          real*8  usrlrate,preexpo
          real*8  diff
          real*8  xfrac
          real*8  floref, flowfactr, fueden,
!      &          oxgnovpr, phvalue, r0z, rpor
! cjmm &          oxgnovpr, phvalue, r0z, radu, radsg, rpor
          real*8  ctfmult,ctfow
          real*8  cladfactor
!         real*8  wetfrac, simtimex, tcan, tcaqu, tflo, ttemp
! cjmm        real*8  wetfrac, simtimex, tcan, tcaqu, tflo, thclad, ttemp
          real*8  xco, xcon, yco
          real*8  qin
          integer nbt
--- 3006,3021 ----
          implicit none
```

```
!         real*8  amassc, pco3, cftime, cfuel, cgap,
!      &          ctemp, cvol, czmetal, czoxide, defectt
          real*8  usrlrate,preexpo
          real*8  diff
          real*8  xfrac
          real*8  floref, flowfactr, fueden,
!      &          oxgnovpr, phvalue, r0z, radu, radsg, rpor
          real*8  ctfmult,ctfow
          real*8  cladfactor
!         real*8  wetfrac, simtimex, tcan, tcaqu, tflo, thclad, ttemp
          real*8  xco, xcon, yco
          real*8  qin
          integer nbt
***************
*** 3090,3098 ****
        common /cther1/ ttemp(maxtim), tcan(maxtim)
        common /cther2/ ctemp
        common /cwast1/ fueden, amassc
! cjmm      common /rcarbon1/      radu, radsg
! cjmm      common /rcarbon2/ cfuel, czmetal, czoxide, cgap
! cjmm      common /rcarbon3/ thclad
        real*8 cladve,velfuel,velcladunzip,ltube,rrod,ltube0
        common /rcarbon4/ cladfactor,cladve,velfuel,velcladunzip,ltube,
       1                  rrod,ltube0
--- 3078,3086 ----
        common /cther1/ ttemp(maxtim), tcan(maxtim)
        common /cther2/ ctemp
        common /cwast1/ fueden, amassc
!       common /rcarbon1/      radu, radsg
!       common /rcarbon2/ cfuel, czmetal, czoxide, cgap
!       common /rcarbon3/ thclad
        real*8 cladve,velfuel,velcladunzip,ltube,rrod,ltube0
        common /rcarbon4/ cladfactor,cladve,velfuel,velcladunzip,ltube,
       1                  rrod,ltube0
***************
*** 3148,3155 ****
  c   phvalue:            pH
  C   ppor:               porosity of packing
  C   r0z:                initial radius of uo2 grain, m
! cjmm   radu:               radius of uo2 fragment, m, destined for deletion
! cjmm   radsg:              subgrain radius after transgranular fracture [m]
  c   cladfactor:         cladding protection factor - 1.0=no protection
  C   rpor:               porosity:: three layers damaged, disturbed, host rock
  C   wetfrac(i):         the fractional liuid level in the wp below which
--- 3136,3143 ----
  c   phvalue:            pH
  C   ppor:               porosity of packing
  C   r0z:                initial radius of uo2 grain, m
! C   radu:               radius of uo2 fragment, m
! C   radsg:              subgrain radius after transgranular fracture [m]
  c   cladfactor:         cladding protection factor - 1.0=no protection
  C   rpor:               porosity:: three layers damaged, disturbed, host rock
  C   wetfrac(i):         the fractional liuid level in the wp below which
***************
*** 3165,3171 ****
  C   tcan(time,subarea): wp surface temp at above times
  C   tcaqu:              time at which aqueous condition begins in  the subarea
  C   tflo:               time of table entry i for floref
! cjmm   thclad:             thickness of cladding, m, scheduled for deletion
  C   time1,2,3:          times corresponding to releases for each type of
  C                       container failure
  C   ttemp(time):        times in table at which temperatures are given
--- 3153,3159 ----
  C   tcan(time,subarea): wp surface temp at above times
  C   tcaqu:              time at which aqueous condition begins in  the subarea
  C   tflo:               time of table entry i for floref
! C   thclad:             thickness of cladding, m
  C   time1,2,3:          times corresponding to releases for each type of
  C                       container failure
  C   ttemp(time):        times in table at which temperatures are given
***************
*** 3400,3416 ****
         read (4, *)
         read (4, *)
```

```
         read (4, *) r0z
! cjmm       read (4, *) radu
! cjmm       read (4, *) radsg
         read (4, *) cladfactor
         read (4, *) cladve
         read (4, *) ltube0
         read (4, *) rrod
! cjmm       read (4, *) thclad
! cjmm       read (4, *) cfuel
! cjmm       read (4, *) czmetal
! cjmm       read (4, *) czoxide
! cjmm       read (4, *) cgap
         read(4,*)
         read(4,*)
         read (4, *) simglass
--- 3388,3404 ----
         read (4, *)
         read (4, *)
         read (4, *) r0z
!        read (4, *) radu
!        read (4, *) radsg
         read (4, *) cladfactor
         read (4, *) cladve
         read (4, *) ltube0
         read (4, *) rrod
!        read (4, *) thclad
!        read (4, *) cfuel
!        read (4, *) czmetal
!        read (4, *) czoxide
!        read (4, *) cgap
         read(4,*)
         read(4,*)
         read (4, *) simglass
/home/jmench{25}>
```

Differences in tpanames.dbs

```
diff -c tpa5001modifiedForSCR556/data/tpanames.dbs tpa5001/data
*** tpa5001modifiedForSCR556/data/tpanames.dbs  Fri Mar 11 14:27:57 2005
--- tpa5001/data/tpanames.dbs   Fri Feb 25 20:26:30 2005
***************
*** 360,366 ****
--- 360,373 ----
  GapFractionForSE79                                    G%-Se79
  GapFractionForNB94                                    G%-Nb94
  InitialRadiusOfSFParticle[m]                          InitRSFP
+ RadiusOfSFGrain[m]                                    Rad-SFG
  CladdingCorrectionFactor                              CladCorF
+ SubGrainFragmentRadiusAfterTransFrac[m]               SbGFRATF
+ ThicknessOfCladding[m]                               ThckCldg
+ SFC-14InventoryPerKgSF[ci]                           SFC-14I
+ CladC-14InventoryPerKgSF[ci]                         CC-14I
+ ZyrOxideAndCrudC-14InvPerKgSF[ci]                    ZO&CC-14
+ GapAndGrainBoundaryInventoryPerKgSF[ci]              GAGBI
  FractionOfFlowHittingWP                               WP-%FHit
  SolubilityAm[kg/m3]                                   Solbl-Am
  SolubilityNp[kg/m3]                                   Solbl-Np
```

Test Plan for TPA SCR#556

Test Plan Name: Removal of C-14 parameters and modified Cm matrix Kds

Tested By: R. Rice

Date: May 16, 2005

Host Machine: Toshiba Laptop

Host OS: XP Professional

Baseline Version: 5.0.0q

Test Version: 5.0.0r

System Level (SL) Tests

SL-1. Name: Removal of C-14 parameters

Path for run directory: c:\SCR556_working\tpa500q\basecase\meanvalue and c:\SCR556_working\tpa500r\basecase\meanvalue

Path for archive of results: \SCR556_working\tpa500q\basecase\meanvalue and \SCR556_working\tpa500r\basecase\meanvalue (archived on CD)

Environment variables: TPA_DATA=c:\SCR556_working\tpa500q\
TPA_TEST=c:\SCR556_working\tpa500q\

and

TPA_DATA=c:\SCR556_working\tpa500r\
TPA_TEST=c:\SCR556_working\tpa500r\

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Using the meanvalues from the *tpa.inp* file generated using the basecase TPA code for Versions 5.0.0q and 5.0.0r, compare the RELEASET input file, *ebsrel.inp*, to verify removal of the C-14 parameters; also, check the RELEASET output file, *ebsnef.dat*, to verify the values in these files are not changed (note that to use the same TPA code input parameters, meanvalues need to be used because two of the removed C-14 parameters were non-constant sampled parameters)

- Objective: Verify these modifications have removed C-14 parameters and RELEASET output is not changed

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** *ebsrel.inp* and *ebsnef.dat*

- **Step by step test procedure to be used:**

  Execute the TPA Versions 5.0.0q and 5.0.0r code using the basecase *tpa.inp* file, and then using the meanvalue *tpa.inp* file, through execution of the RELEASET code (UZFT and subsequent calculations are not relevant for this test). Then, perform the following:

  1. Perform a file comparison between the RELEASET input files *ebsrel.inp* from the Versions 5.0.0q and 5.0.0r runs
  2. Perform a file comparison between the RELEASET output files *ebsnef.dat* from the Versions 5.0.0q and 5.0.0r runs

- **Pass/Fail criteria:**

  Criteria 1: Differences between RELEASET input files *ebsrel.inp* from the Versions 5.0.0q and 5.0.0r meanvalue runs should only be the removal of C-14 parameters

  Criteria 2: No differences between RELEASET output files *ebsnef.dat* from the Versions 5.0.0q and 5.0.0r meanvalue runs

Test Results: The following text displays the differences between the RELEASET input files *ebsrel.inp* from the Versions 5.0.0q and 5.0.0r runs. Note that 7 parameters (in bold below) related to C-14 were removed. The file that was contains the comparison information is in the c:\SCR556_working\tpa500r\basecase\meanvalue subdirectory and is called "file_comparison_ebsrel.inp".

```
Comparing files ebsrel.inp and
C:\SCR556_WORKING\TPA500Q\BASECASE\MEANVALUE\EBSREL.INP
***** ebsrel.inp
  1.85000E-03      ! r0z: initial radius of SF particle [m]
  5.00000E-01      ! claddingcorfact: cladding correction factor
***** C:\SCR556_WORKING\TPA500Q\BASECASE\MEANVALUE\EBSREL.INP
  1.85000E-03      ! r0z: initial radius of SF particle [m]
  9.25000E-06      ! radu: radius of the SF grain [m]
  1.25000E-06      ! radsg: subgrain fragment radius after trans. frac. [m]
  5.00000E-01      ! claddingcorfact: cladding correction factor
*****

***** ebsrel.inp
  5.00000E-03      ! rrod, radius of fuel in rod, meters
|
***** C:\SCR556_WORKING\TPA500Q\BASECASE\MEANVALUE\EBSREL.INP
  5.00000E-03      ! rrod, radius of fuel in rod, meters
  6.10000E-04      ! thclad: thickness of cladding [m]
  7.20000E-04      ! cfuel: C-14 [ci] /kg SF
  4.89000E-04      ! czmetal: C-14 [ci] /kg SF in Zyr. clad & other metals
```

```
 2.48000E-05        ! czoxide: C-14/kg SF in initial Zry oxide & crud
 6.20000E-06        ! cgap: C-14/kg SF in grain and gap
|
*****
```

The following text displays that there are no differences between the RELEASET input files *ebsrel.inp* from the Versions 5.0.0q and 5.0.0r runs. The file that was contains the comparison information is in the c:\SCR556_working\tpa500r\basecase\meanvalue subdirectory and is called "file_comparison_ebsnef.dat".

```
Comparing files ebsnef.dat and
C:\SCR556_WORKING\TPA500Q\BASECASE\MEANVALUE\EBSNEF.DAT
FC: no differences encountered
```

Results from all tests are contained on the CD attached to this test plan.

- Overall test status: <u>PASS</u>

SL-2. Name: Addition of TPA Version 4.1j values for Cm matrix Kds to *tpa.inp* and removal of C-14 parameters

Path for run directory: c:\SCR556_working\tpa500q and c:\SCR556_working\tpa500r (note: there is no run)

Path for archive of results: \SCR556_working\tpa500r (archived on CD)

Environment variables: TPA_DATA=c:\SCR556_working\tpa500q\
TPA_TEST=c:\SCR556_working\tpa500q\

and

TPA_DATA=c:\SCR556_working\tpa500r\
TPA_TEST=c:\SCR556_working\tpa500r\
(note: there is no run)

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Compare the TPA code input files *tpa.inp* from Versions 5.0.0q and 5.0.0r to verify TPA Version 4.1j values for Cm matrix Kds were added and C-14 related parameters were removed

- **Objective:** Verify TPA Version 4.1j values for Cm matrix Kds were added to the *tpa.inp* file and that C-14 related parameters (the 7 identified in the previous test, SL-1) have been removed

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** none (only a file comparison between *tpa.inp* files from Versions 5.0.0q and 5.0.0r)

- **Step by step test procedure to be used:**
  1. Use the XP DOS command "fc" to compare *tpa.inp* files from the TPA Versions 5.0.0q and 5.0.0r code

- **Pass/Fail criteria:**

Criteria 1:	Cm matrix Kds values should be changed from 0 to TPA Version 4.1j values
Criteria 2:	C-14 related parameters (identified previously in test SL-1) should be removed/commented out in the TPA Version 5.0.0r code *tpa.inp* file

Test Results: The following text displays the differences between the *tpa.inp* input files *ebsrel.inp* from the Versions 5.0.0q and 5.0.0r runs. Note that C-14 related parameters were commented out; however, Cm matrix Kds were not changed. The file that was contains the comparison information is in the c:\SCR556_working\tpa500r subdirectory and is called "file_comparison_tpa.inp".

```
Comparing files tpa.inp and C:\SCR556_WORKING\TPA500Q\TPA.INP
***** tpa.inp
title
 Input file tpa.inp as supplied with TPA Version 5.0.0r Code.
 Base case.
***** C:\SCR556_WORKING\TPA500Q\TPA.INP
title
 Input file tpa.inp as supplied with TPA Version 5.0.0q Code.
 Base case.
*****

***** tpa.inp
**
*jmm SCR556
*jmm uniform
*jmm RadiusOfSFGrain[m]
*jmm 3.5e-6, 1.5e-5
**
***** C:\SCR556_WORKING\TPA500Q\TPA.INP
**
uniform
RadiusOfSFGrain[m]
3.5e-6, 1.5e-5
**
*****

***** tpa.inp
**
*jmm SCR556
*jmm normal
*jmm SubGrainFragmentRadiusAfterTransFrac[m]
*jmm 5.0e-7,  2.0e-6
**
*jmm SCR556
*jmm constant
*jmm ThicknessOfCladding[m]
*jmm 6.1e-4
**
*jmm SCR556
*jmm constant
*jmm SFC-14InventoryPerKgSF[ci]
*jmm 7.2e-4
```

```
**
*jmm SCR556
*jmm constant
*jmm CladC-14InventoryPerKgSF[ci]
*jmm 4.89e-4
**
*jmm SCR556
*jmm constant
*jmm ZyrOxideAndCrudC-14InvPerKgSF[ci]
*jmm 2.48e-5
**
*jmm SCR556
*jmm constant
*jmm GapAndGrainBoundaryInventoryPerKgSF[ci]
*jmm 6.2e-6
**
***** C:\SCR556_WORKING\TPA500Q\TPA.INP
**
normal
SubGrainFragmentRadiusAfterTransFrac[m]
5.0e-7, 2.0e-6
**
constant
ThicknessOfCladding[m]
6.1e-4
**
constant
SFC-14InventoryPerKgSF[ci]
7.2e-4
**
constant
CladC-14InventoryPerKgSF[ci]
4.89e-4
**
constant
ZyrOxideAndCrudC-14InvPerKgSF[ci]
2.48e-5
**
constant
GapAndGrainBoundaryInventoryPerKgSF[ci]
6.2e-6
**
*****
```

Results from all tests are contained on the CD attached to this test plan.

- Overall test status: FAIL

Note that Cm Matrix Kds will be added to the *tpa.inp* file through SCR552

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-560	2. Software Title and Version: TPA 5.0.01	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *reader.f, dcags.f, tpa.inp, repdes.dat, volcano.f*

The current repository design does not reflect the latest design from DOE.
There is a spelling error in *dcags.f* for the AshBulkDensity parameter.
The number of packages failed in volcano.f at line 514 can exceed the number in the subarea due to round off error.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
S. Mohanty Date: 2-23-05	R. Janetzke R. Janetzke Date: 2-23-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): The **drifts** subroutine in *reader.f* was changed to accept multiple panels for a repository design rather than just multiple emplacement blocks. Each panel is allowed multiple emplacement blocks. The specification of emplacement direction is the same as before. The *repdes.dat* file contains a new angle as well as new outlines for the panels and emplacement blocks. The *tpa.inp* file was changed to specify the new subareas (7 with an 8th for contingency). Also, the maximum subarea for volcanic event was changed from 10 to 7.

The spelling for the ash bulk density parameter was corrected to **AshBulkDensity[g/cm3]** in the *dcags.f* module.

The **dnint()** function was used in *volcano.f* to prevent round off inconsistencies.

8. Implemented by:	Date:
R. Janetzke R. Janetzke	3-8-05

9. Description of Acceptance Tests: The file named "Test_Plan_SCR560_v004.wpd" on the CD attached to this SCR contains a description of the Acceptance Tests for the 3 items listed in Box #4 above.

10. Tested by: R. Rice	Date: 4-18-05 4/18/05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)

Modify From	reader	subarea	subarea coordinates	10 edaii 1-cw 547514.88,4079310.61 548069.2,4079136.5 547847.3,4077816.2 547370.95,4077922.04 547514.88,4079310.61 edaii 2-cw 548069.2,4079136.5 548569.32,4078981. 548504.06,4077664.24 547847.3,4077816.2 548069.2,4079136.5 edaii 3-cw 547370.95,4077922.04 547847.3,4077816.2 548322.7,4077192.2 547474.7,4077281.6 547370.95,4077922.04 edaii 4-cw 547847.3,4077816.2 548504.06,4077664.24 548479.71,4077173.06 548322.7,4077192.2 547847.3,4077816.2 edaii 5-cw 547474.7,4077281.6 547887.3,4077238.1 547897.79,4076045.46 547655.97,4076123.07 547474.7,4077281.6	N/A		

				edaii 6-cw 547887.3,4077238.1 548322.7,4077192.2 548155.7,4075962.63 547897.79,4076045.46 547887.3,4077238.1 edaii 7-cw 548322.7,4077192.2 548479.71,4077173.06 548455,4076674.51 548155.7,4075962.63 548322.7,4077192.2 edaii 8-cw 547645.27,4079656.06 548588.98,4079377.55 548569.32,4078981 547514.88,4079310.61 547645.27,4079656.06 edaii 9-cw 547732.82,4080960.00 548251.91,4080817.50 548116.89,4079516.81 547645.27,4079656.06 547732.82,4080960.00 edaii 10-cw 548251.91,4080817.50 548664.55,4080675.00 548588.98,4079377.55 548116.89,4079516.81 548251.91,4080817.50			

Modify To	reader	subarea	subarea coordinates	7 Subarea 1 (Top Left) 547390., 4080177. 547535., 4080512. 547582., 4079221. 547346., 4079145. 547390., 4080177. Subarea 2 547535., 4080512. 547729., 4080943. 547955., 4079338. 547582., 4079221. 547535., 4080512. Subarea 3 547729., 4080943. 549744., 4081576. 549068., 4079690. 547955., 4079338. 547729., 4080943. Subarea 4 547346., 4079145. 547582., 4079221. 547606., 4078451. 547456., 4078400. 547346., 4079145. Subarea 5 547582., 4079221. 547955., 4079338. 548056., 4078603. 547606., 4078451. 547582., 4079221.	N/A		

				Subarea 6 547955., 4079338. 548606., 4079545. 548553., 4078770. 548056., 4078603. 547955., 4079338. Subarea 7 547803., 4078308. 548542., 4078549. 548523., 4078132. 547802., 4077893. 547803., 4078308. **Subarea 8 (contingency) **547802., 4077893. **548523., 4078132. **548430., 4076303. **547799., 4076093. **547802., 4077893.			
Modify From	Volcano	Subarea OfVolcanicEvent[ ]	Subarea in which the conduit is considered.	Iuniform	1, 10		
Modify To	Volcano	Subarea OfVolcanicEvent[ ]	Subarea in which the conduit is considered.	Iuniform	1, 7		

Test Plan for TPA SCR#560

Test Plan Name: Repository Layout/Ash Bulk Density/Volcano WPs Failed

Tested By: R. Rice **Date:** March 23, 2005

Host Machine: Toshiba Laptop **Host OS:** XP Professional

Baseline Version: 5.0.0l **Test Version:** 5.0.0m

System Level (SL) Tests

SL-1. Name: Repository Layout #1

Path for run directory: c:\SCR560\tpa500m\SL-1\basecase

Path for archive of results: \SCR560\tpa500m\SL-1\basecase (archived on CD)

Environment variables: TPA_DATA=c:\SCR560\tpa500m
TPA_DATA=c:\SCR560\tpa500m

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Using the repository area, the WP and drift spacing in the *tpa.inp* file, and the coordinates in *repdes.dat*, hand calculations (EXCEL spreadsheet) will verify the correct determination of the drift location, the number of WPs in each drift, drift spacing, and the drift angle. Also, the correct assignment of WPs to each subarea, which is available in the screen print and *drifts.dat*, will be verified. A plot will show the location of the drifts relative to the repository outline as specified in *repdes.dat* and the subarea coordinates specified in the *tpa.inp* file.

- **Objective:** Verify correct drift location, number of WPs in each drift, drift spacing, number of WPs in each subarea, and drift angle.
- **Assumptions:** None, other than the assumptions made in the TPA code
- **Constraints:** None

- Output files to compare or examine: *drifts.dat* and screenprint

- Step by step test procedure to be used:

Execute the TPA Version 5.0.0m code using the basecase *tpa.inp* file and capture the screenprint. Then, perform the following:

1. Plot drift endpoints in *drifts.dat*, repository design endpoints in *repdes.dat*, and the subarea coordinates in the *tpa.inp* file
2. Use EXCEL spreadsheet to compute distance between drift endpoints and subarea boundary
3. Use EXCEL spreadsheet to compute number of WPs in each drift
4. Use EXCEL spreadsheet to compute the drift spacing from drift endpoints in *drifts.dat*
5. Use EXCEL spreadsheet to compute number of WPs in each subarea
6. Use EXCEL spreadsheet to compute drift angle

- Pass/Fail criteria: (For steps 2-6 above)

Criteria 1: Drift endpoints and subarea boundaries should coincide (visual inspection of the plot)

Criteria 2: EXCEL spreadsheet calculated distance between a drift endpoint in *drifts.dat* and the subarea boundary should be zero*

Criteria 3: EXCEL spreadsheet calculated number of WPs and the number of WPs in each drift from *drifts.dat* should be equal*

Criteria 4: EXCEL spreadsheet calculated drifts spacing from drift endpoints in *drifts.dat* should be equal* to the value set in the *tpa.inp* file

Criteria 5: EXCEL spreadsheet calculated number of WPs in a subarea should be equal* to the number of WPs in a subarea shown in the screenprint

Criteria 6: EXCEL spreadsheet calculated drift angle from drift endpoints in *drifts.dat* should be equal* to the value set in the *tpa.inp* file

* within an acceptable tolerance (less than 5%)

Test Results: The EXCEL spreadsheet file (SCR560_repository_and_drift_coordinates_v003.xls) in the /SCR560/ subdirectory on the attached CD contains results for this test. The WORKSHEETS in this EXCEL file show that the Pass/Fail Criteria listed above were met.

- Overall test status: **PASS**

SL-1b. Name: Repository Layout #1b

Path for run directory: c:\SCR560\tpa500m\SL-1\basecase\test\test2

Path for archive of results: \SCR560\tpa500m\SL-1\basecase\test\test2 (archived on CD)

Environment variables: TPA_DATA=c:\SCR560\tpa500m
TPA_DATA=c:\SCR560\tpa500m

Special input files or modifications to input files required: *repdes.dat* and *tpa.inp*

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: The panel, emplacement block, and subarea coordinates with be modified to rectangles, which will facilitate the ability to easily check results in the *drifts.dat* file and screenprint. Note that the *tpa.inp* file subarea coordinates were modified and 1 subarea specified. Also, parameters for drift spacing and WP spacing were changed to 100 and 5 m and the MTUs in the repository changed to 100,000. Therefore, the emplacement block will contain 10,000 WPs.

- Objective: Verify correct drift location, number of WPs in each drift, drift spacing, number of WPs in each subarea, and drift angle.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *drifts.dat* and screenprint

- Step by step test procedure to be used:

Execute the TPA Version 5.0.0m code using the basecase *tpa.inp* file and capture the screenprint.

1. Inspect drift endpoints in *drifts.dat*, repository design endpoints in *repdes.dat*, and the subarea coordinates in the *tpa.inp* file.
2. Modify subarea coordinates to make a smaller and larger subarea than the panel and emplacement block rectangles (these latter two are the same dimensions) and repeat Steps #1-3)

- Pass/Fail criteria:

Criteria 1: For panel and emplacement block coordinates that do not change, information in the *drifts.dat* file should not change.

Criteria 2: The number of WPs in each subarea should be consistent with the area that the subarea overlaps in the emplacement block (i.e., the drifts in the *drifts.dat* file).

Test Results: The screenprint below shows results from "test5". (Note that in the run directory listed above, there are *tpa.inp* and *tpa.out* [screenprint] files for tests 1 - 10). In the following test, the subarea was made larger than the emplacement block; however, more WPs were assigned to the subarea than expected (15,000 instead of 10,000) and there are more MTUs in the repository (15,000) than 10,000 MTUs specified in the *tpa.inp* file (this is test5).

```
==========================================================================
      exec: Welcome to TPA Version 5.0.0m
    Job started: Thu Apr 07 09:12:04 2005
==========================================================================

 ***>>> Error in Reader <<<***
 (amtu .lt. 60000.0d0) .or. amtu .gt. 80000.0d0)
 amtu =  150000.0000000000
 Repository area & AML not consistent
 trying to bury either too much or too little waste
 need to try to bury 70,000 MTU

REPOSITORY DESIGN INFORMATION
Subarea  Area      Waste   Number of WP
  #     [m^2]     [MTU]
  1  15000000.0  150000.0      15000

Total Area [acre]        = 3706.449221645664
Total Buried Waste [MTU]  = 150000.0000000000
Repository AML [MTU/acre] = 40.47000000000000

Specified Global Parameters:

          Compliance Period =  10000.0 (yr)
      Maximum Simulation Time =  10000.0 (yr)
       Number Of Realizations =      1
          Number Of Subareas =      1
          Volcanism scenario =      1 (yes=1, no=0)
           Faulting scenario =      0 (yes=1, no=0)
   Mechanical failure scenarios:
                 Seismicity =      1 (yes=1, no=0)
           Drift Degradation =      1 (yes=1, no=0)
    Distance to Receptor Group =     18.0 (km)

**>>> CAUTION: CHECKING OF NUCLIDES AND CHAINS IS DISABLED <<<**
**>>> You may not be using the standard chains specified   <<<**
**>>> in the invent module.                                <<<**
**>>> (see "CheckNuclidesAndChains(yes=1,no=0)" in tpa.inp)<<<**
```

```
The specified path for data  = $TPA_DATA/
The specified path for codes = $TPA_TEST/

**To modify global parameters or the path, stop code execution using control-C**

 ***>>> WARNING: THE APPEND OPTION IS SELECTED <<<***
(see "OutputMode(0=None,1=All,2=UserDefined)" in tpa.inp)
For "SelectAppendFiles", a value of 0 (all append files) was set in tpa.inp.
By selecting this option, files are written which may require   6 megs of disk space.
(more disk space could be needed)

-----------------------------------------------------------------------
   subarea  1 of  1          realization   1 of   1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:   0.0000E+00
      Mean Annual Infiltration at Start(AAI0):   5.8542E+00
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Weld Failure
    ebsfail: time of WP failure  =     162.1  yr
exec: calling volcano
exec: failed WPs from Volcanic  event =  10000 at time =     0.0 yr
exec: failed WPs from CORROSION event =   5000 at time =    162.1 yr
 *** failed WPs: all WPs failed ( 15000 ) ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 1
          Tc99    1.2058E+02 [Ci/yr/SA] at  7.205E+03 yr
          Cs135   6.5441E+00 [Ci/yr/SA] at  7.205E+03 yr
          C14     2.4235E+00 [Ci/yr/SA] at  7.205E+03 yr
          Ni59    2.0743E+00 [Ci/yr/SA] at  7.205E+03 yr
          Se79    8.1763E-01 [Ci/yr/SA] at  7.205E+03 yr
          Pb210   7.0989E-01 [Ci/yr/SA] at  1.000E+04 yr
exec: calling uzft
               Highest release rates from UZ
          Tc99    1.1641E+02 [Ci/yr/SA] at  7.551E+03 yr
          Se79    6.8527E-01 [Ci/yr/SA] at  1.000E+04 yr
          I129    2.8180E-01 [Ci/yr/SA] at  7.551E+03 yr
          Np237   1.3771E-01 [Ci/yr/SA] at  1.000E+04 yr
          Cm245   1.2890E-01 [Ci/yr/SA] at  1.000E+04 yr
          Cl36    1.2184E-01 [Ci/yr/SA] at  7.551E+03 yr
exec: calling szft
               Highest release rates from SZ
          Tc99    1.1077E+02 [Ci/yr/SA] at  8.101E+03 yr
          I129    2.6818E-01 [Ci/yr/SA] at  8.101E+03 yr
          Cl36    1.1570E-01 [Ci/yr/SA] at  8.101E+03 yr
          Se79    4.2588E-03 [Ci/yr/SA] at  1.000E+04 yr
          Pu239   9.0314E-04 [Ci/yr/SA] at  1.000E+04 yr
          Pu240   6.3409E-04 [Ci/yr/SA] at  1.000E+04 yr
```

```
exec: calling dcagw
            Highest annual dose GW pathway
        Tc99   7.8812E+01 [mrem/yr]  at  8.101E+03 yr
        I129   2.1121E+01 [mrem/yr]  at  8.101E+03 yr
        Pu239  8.7623E-01 [mrem/yr]  at  1.000E+04 yr
        Pu240  6.1523E-01 [mrem/yr]  at  1.000E+04 yr
        Am243  4.9701E-01 [mrem/yr]  at  1.000E+04 yr
        Cl36   4.5385E-01 [mrem/yr]  at  8.101E+03 yr
       At end of TPI, annual dose GW pathway
        Tc99   5.3562E+01 [mrem/yr]
        I129   1.4265E+01 [mrem/yr]
        Pu239  8.7623E-01 [mrem/yr]
        Pu240  6.1523E-01 [mrem/yr]
        Am243  4.9701E-01 [mrem/yr]
        Cl36   3.0293E-01 [mrem/yr]
          sum  7.0130E+01 [mrem/yr]
               There is no GS release
exec: end realizations

exec: Peak Mean Dose is 1.00390E-01 rem/yr at   8101.3 yr, based on     1 realizations.

exec:  Run Successfully Completed
```

Because there are more WPs assigned to the subarea than the number of WPs in an emplacement block, the test criteria were not satisfied. It is recommended that the algorithm (which uses drift and subarea coordinates) to determine of number of WPs in a subarea be examined and modified as needed. It appears as though this algorithm extends the drift endpoints to intersect a subarea and then uses this increased drift length to determine the number of WPs in a subarea. That is, the drift endpoints should not be extended.

- Overall test status: <u>FAIL</u> (SCR #570 addresses this test failure)

SL-2. Name: AshBulkDensity[g/cm3] Parameter Name Correction

Path for run directory: c:\SCR560\tpa500l\SL-2\basecase
c:\SCR560\tpa500m\SL-2\basecase

Path for archive of results: \SCR560\tpa500l\SL-2\basecase (archived on CD)
\SCR560\tpa500m\SL-2\basecase (archived on CD)

Environment variables: TPA_DATA=c:\SCR560\tpa500l
TPA_DATA=c:\SCR560\tpa500l

TPA_DATA=c:\SCR560\tpa500m
TPA_DATA=c:\SCR560\tpa500m

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Activate Volcano with AshEvolutionMode equal to 0 (no_remob) in the *tpa.inp* file

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Execute the TPA Version 5.0.0l and 5.0.0m codes using the basecase *tpa.inp* file with Volcano activated and the AshEvolutionMode set equal to 0 for no_remob. Since the AshBulkDensity[g/cm3] parameter name is incorrect in Version 5.0.0l, the TPA Version 5.0.0l code execution should stop when there is a query for a parameter with the incorrect name. The error message in the screenprint should describe the reasons for stopping code execution. Then, under the same conditions in the *tpa.inp* file for Version 5.0.0m (i.e., Volcano activated and the AshEvolutionMode set equal to 0 for no_remob), the TPA code execution should be successful.

- Objective: Verify the parameter name "AshBulkDensity[g/cm3]" has been corrected.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: screenprint (saved as the file *tpa.out*)

- Step by step test procedure to be used:

Execute the TPA Version 5.0.0l and 5.0.0m codes using the basecase *tpa.inp* file with Volcano activated and the AshEvolutionMode set equal to 0 for no_remob. Capture the screenprint.

1. Examine the screenprint (*tpa.out*) to verify the problem in the AshBulkDensity[g/cm3] name in Version 5.0.0l
2. Examine the screenprint (*tpa.out*) to verify the parameter name AshBulkDensity[g/cm3] has been correct in Version 5.0.0m

- Pass/Fail criteria:

Criteria 1: Version 5.0.0l screenprint (*tpa.out*) should indicate an incorrect name for the parameter "AshBulkDensity[g/cm3]".

Criteria 2: Version 5.0.0m screenprint (*tpa.out*) should indicate successful completion of the TPA code

Test Results: The screenprints (*tpa.out*) from the TPA Version 5.0.0l code and from the TPA Version 5.0.0m code are provided below.

<u>Screenprint TPA Version 5.0.0l code</u>

```
=====================================================================
      exec: Welcome to TPA Version 5.0.0l
    Job started: Fri Apr 01 08:42:53 2005
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea  Area      Waste   Number of WP
  #    [m^2]     [MTU]
  1   723591.3   11535.2      1462
  2   784763.0   12363.6      1567
  3   390372.0    6083.2       771
  4   207581.3    3384.8       429
  5   378857.2    5980.6       758
  6   424872.5    6698.6       849
  7   163938.3    2556.4       324
  8   393468.9    6667.1       845
  9   660785.5    7708.5       977
 10   589497.1    7061.5       895

Total Area [acre]        = 1165.734397566135
Total Buried Waste [MTU] = 70039.53000000000
Repository AML [MTU/acre] = 60.08189356531916

Specified Global Parameters:

        Compliance Period = 10000.0 (yr)
     Maximum Simulation Time = 10000.0 (yr)
      Number Of Realizations =     1
        Number Of Subareas =    10
```

```
          Volcanism scenario =      1 (yes=1, no=0)
           Faulting scenario =      0 (yes=1, no=0)
    Mechanical failure scenarios:
                 Seismicity =      1 (yes=1, no=0)
           Drift Degradation =      1 (yes=1, no=0)
     Distance to Receptor Group =     18.0 (km)

**>>> CAUTION: CHECKING OF NUCLIDES AND CHAINS IS DISABLED <<<**
**>>> You may not be using the standard chains specified   <<<**
**>>> in the invent module.                                <<<**
**>>> (see "CheckNuclidesAndChains(yes=1,no=0)" in tpa.inp)<<<**

The specified path for data  = $TPA_DATA/
The specified path for codes = $TPA_TEST/

**To modify global parameters or the path, stop code execution using control-C**
-----------------------------------------------------------------------
   subarea   1 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
      Mean Annual Infiltration at Start(AAI0):    5.8542E+00
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
exec: calling volcano
exec: failed WPs from INITIAL   event =     15 at time =      0.0 yr
exec: failed WPs from Volcanic  event =   1197 at time =   7038.2 yr
 *** failed WPs:  1212   out of  1462  ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 1
          C14     1.1022E-03 [Ci/yr/SA] at  3.635E+03 yr
          Tc99    6.7921E-04 [Ci/yr/SA] at  3.635E+03 yr
          Cs135   5.0809E-04 [Ci/yr/SA] at  3.635E+03 yr
          Pu239   1.6750E-04 [Ci/yr/SA] at  1.000E+04 yr
          Jp239   1.4238E-04 [Ci/yr/SA] at  1.000E+04 yr
          Pu240   1.3373E-04 [Ci/yr/SA] at  1.000E+04 yr
exec: calling uzft
               Highest release rates from UZ
          Tc99    6.4788E-04 [Ci/yr/SA] at  3.812E+03 yr
          I129    7.4521E-05 [Ci/yr/SA] at  3.812E+03 yr
          Jp239   6.8307E-05 [Ci/yr/SA] at  1.000E+04 yr
          Jp240   5.4706E-05 [Ci/yr/SA] at  1.000E+04 yr
          Se79    4.2421E-05 [Ci/yr/SA] at  4.945E+03 yr
          Cl36    3.1878E-05 [Ci/yr/SA] at  3.812E+03 yr
exec: calling szft
               Highest release rates from SZ
          Tc99    5.1580E-04 [Ci/yr/SA] at  5.184E+03 yr
          I129    5.9431E-05 [Ci/yr/SA] at  5.184E+03 yr
```

```
        Cl36    2.5345E-05 [Ci/yr/SA] at  5.184E+03 yr
        Se79    7.3039E-14 [Ci/yr/SA] at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   2 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow

. . .

. . .

. . .

exec: calling szft
                Highest release rates from SZ
        Tc99    1.7208E-04 [Ci/yr/SA] at  4.607E+03 yr
        I129    1.9854E-05 [Ci/yr/SA] at  4.607E+03 yr
        Cl36    8.4779E-06 [Ci/yr/SA] at  4.607E+03 yr
        Se79    5.2787E-15 [Ci/yr/SA] at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea  10 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling eqvdia
exec: calling nfenvFI
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
   ebsfail: No Weld Failure
   *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =      9 at time =      0.0 yr
exec: failed WPs from Volcanic  event =    834 at time =   7038.2 yr
 *** failed WPs:  843   out of  895  ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 10
        C14     3.4260E-04 [Ci/yr/SA] at  2.729E+03 yr
        Tc99    1.8881E-04 [Ci/yr/SA] at  2.729E+03 yr
        Cs135   1.4150E-04 [Ci/yr/SA] at  2.729E+03 yr
        Pu240   4.0438E-05 [Ci/yr/SA] at  4.093E+03 yr
        Jp240   3.4372E-05 [Ci/yr/SA] at  4.093E+03 yr
        Pu239   3.4255E-05 [Ci/yr/SA] at  5.564E+03 yr
exec: calling uzft
                Highest release rates from UZ
        Tc99    1.8146E-04 [Ci/yr/SA] at  2.796E+03 yr
        Cs135   1.3596E-04 [Ci/yr/SA] at  2.796E+03 yr
        Pu240   4.0191E-05 [Ci/yr/SA] at  4.191E+03 yr
        Pu239   3.4214E-05 [Ci/yr/SA] at  5.564E+03 yr
        Jp240   3.0159E-05 [Ci/yr/SA] at  5.434E+03 yr
        Jp239   2.7478E-05 [Ci/yr/SA] at  5.971E+03 yr
exec: calling szft
                Highest release rates from SZ
```

```
        Tc99    1.4652E-04 [Ci/yr/SA] at  9.323E+03 yr
        I129    1.7423E-05 [Ci/yr/SA] at  9.323E+03 yr
        Cl36    7.3616E-06 [Ci/yr/SA] at  9.323E+03 yr
        Se79    4.1338E-14 [Ci/yr/SA] at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
exec: calling dcagw
              Highest annual dose GW pathway
        I129    2.4266E-02 [mrem/yr]  at  8.897E+03 yr
        Tc99    1.2434E-03 [mrem/yr]  at  8.691E+03 yr
        Cl36    2.3940E-04 [mrem/yr]  at  8.691E+03 yr
        Se79    7.2576E-12 [mrem/yr]  at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
      At end of TPI, annual dose GW pathway
        I129    2.1891E-02 [mrem/yr]
        Tc99    1.1185E-03 [mrem/yr]
        Cl36    2.1534E-04 [mrem/yr]
        Se79    7.2576E-12 [mrem/yr]
          sum  2.3225E-02 [mrem/yr]
   The remaining  16   nuclide(s) have zero release
exec: calling ashplumo
exec: calling ashrmovo
exec: calling dcags

 ***>>> Error in ispquery <<<***
 can not find name of parameter
 dump of first 15 PDFs defined
 ipdf, description
1  GenerateRestartFiles(yes=1,no=0)
2  ImportanceAnalysisFlag(yes=1,no=0)
3  SubsystemNaturalStudy
4  BarrierBiosphereStudy
5  ComponentPrecipitationStudy
6  BarrierUpperUnsaturatedZoneStudy
7  ComponentTivaCanyonStudy
8  BarrierLowerUnsaturatedZoneStudy
9  ComponentTSwStudy
10  ComponentCHnvStudy
11  ComponentCHnzStudy
12  ComponentPPwStudy
13  ComponentUCFStudy
14  ComponentBFwStudy
15  BarrierSaturatedZoneStudy

 ***>>> Error in ispquery <<<***
 can not find name of parameter
 in above list of all PDF names
 name =AshBulkDensity[g/m3]
```

Screenprint TPA Version 5.0.0m code

```
==================================================================
     exec: Welcome to TPA Version 5.0.0m
    Job started: Fri Apr 01 08:53:53 2005
```

```
==================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
  #     [m^2]     [MTU]
  1   221574.0    3566.3       452
  2   447909.0    7203.6       913
  3  2619149.5   41951.1      5317
  4   150452.0    2319.7       294
  5   318060.0    4994.4       633
  6   437858.0    6888.0       873
  7   301280.0    3116.5       395

Total Area [acre]        = 1111.016184828268
Total Buried Waste [MTU] = 70039.53000000000
Repository AML [MTU/acre] = 63.04096281984062

Specified Global Parameters:

          Compliance Period =  10000.0 (yr)
      Maximum Simulation Time =  10000.0 (yr)
       Number Of Realizations =     1
          Number Of Subareas =     7
          Volcanism scenario =     1 (yes=1, no=0)
           Faulting scenario =     0 (yes=1, no=0)
   Mechanical failure scenarios:
                 Seismicity =     1 (yes=1, no=0)
           Drift Degradation =     1 (yes=1, no=0)
    Distance to Receptor Group =    18.0 (km)

**>>> CAUTION: CHECKING OF NUCLIDES AND CHAINS IS DISABLED <<<**
**>>> You may not be using the standard chains specified   <<<**
**>>> in the invent module.                                <<<**
**>>> (see "CheckNuclidesAndChains(yes=1,no=0)" in tpa.inp)<<<**

The specified path for data  = $TPA_DATA/
The specified path for codes = $TPA_TEST/

**To modify global parameters or the path, stop code execution using control-C**
-------------------------------------------------------------------
   subarea   1 of   7          realization    1 of    1
-------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
      Mean Annual Infiltration at Start(AAI0):    5.8542E+00
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
exec: calling volcano
exec: failed WPs from INITIAL   event =      5 at time =      0.0 yr
exec: failed WPs from Volcanic  event =    384 at time =   7038.2 yr
```

```
 *** failed WPs:  389   out of  452  ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 1
        C14     2.2931E-04 [Ci/yr/SA] at  4.093E+03 yr
        Tc99    1.5035E-04 [Ci/yr/SA] at  4.093E+03 yr
        Cs135   1.1117E-04 [Ci/yr/SA] at  4.093E+03 yr
        Pu239   3.2243E-05 [Ci/yr/SA] at  1.000E+04 yr
        Jp239   2.7407E-05 [Ci/yr/SA] at  1.000E+04 yr
        Pu240   2.6110E-05 [Ci/yr/SA] at  4.093E+03 yr
exec: calling uzft
            Highest release rates from UZ
        Tc99    1.4118E-04 [Ci/yr/SA] at  4.394E+03 yr
        I129    1.6053E-05 [Ci/yr/SA] at  4.394E+03 yr
        Jp239   1.3061E-05 [Ci/yr/SA] at  1.000E+04 yr
        Jp240   1.0555E-05 [Ci/yr/SA] at  4.945E+03 yr
        Se79    9.7952E-06 [Ci/yr/SA] at  6.113E+03 yr
        Cl36    6.8585E-06 [Ci/yr/SA] at  4.394E+03 yr
exec: calling szft
            Highest release rates from SZ
        Tc99    1.2122E-04 [Ci/yr/SA] at  5.696E+03 yr
        I129    1.3825E-05 [Ci/yr/SA] at  5.696E+03 yr
        Cl36    5.8890E-06 [Ci/yr/SA] at  5.696E+03 yr
        Se79    7.3191E-14 [Ci/yr/SA] at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   2 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow

. . .

. . .

. . .

exec: calling szft
            Highest release rates from SZ
        Tc99    2.5162E-04 [Ci/yr/SA] at  8.897E+03 yr
        I129    2.9324E-05 [Ci/yr/SA] at  8.897E+03 yr
        Cl36    1.2403E-05 [Ci/yr/SA] at  8.897E+03 yr
        Se79    1.0765E-15 [Ci/yr/SA] at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   7 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
```

```
exec: failed WPs from INITIAL   event =     4 at time =     0.0 yr
exec: failed WPs from Volcanic  event =   391 at time =  7038.2 yr
 *** failed WPs: all WPs failed ( 395 ) ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 7
        C14     1.4520E-04 [Ci/yr/SA] at  7.038E+03 yr
        Tc99    1.3279E-04 [Ci/yr/SA] at  7.038E+03 yr
        Cs135   1.0027E-04 [Ci/yr/SA] at  7.038E+03 yr
        Pu239   1.9105E-05 [Ci/yr/SA] at  1.000E+04 yr
        Jp239   1.6239E-05 [Ci/yr/SA] at  1.000E+04 yr
        I129    1.5436E-05 [Ci/yr/SA] at  7.038E+03 yr
exec: calling uzft
            Highest release rates from UZ
        Tc99    1.2598E-04 [Ci/yr/SA] at  7.914E+03 yr
        I129    1.4681E-05 [Ci/yr/SA] at  7.914E+03 yr
        Jp239   6.8750E-06 [Ci/yr/SA] at  1.000E+04 yr
        Cl36    6.2232E-06 [Ci/yr/SA] at  7.914E+03 yr
        Jp240   5.4828E-06 [Ci/yr/SA] at  1.000E+04 yr
        Se79    1.9343E-06 [Ci/yr/SA] at  1.000E+04 yr
exec: calling szft
            Highest release rates from SZ
        Tc99    1.2205E-04 [Ci/yr/SA] at  9.107E+03 yr
        I129    1.4274E-05 [Ci/yr/SA] at  9.107E+03 yr
        Cl36    6.0344E-06 [Ci/yr/SA] at  9.107E+03 yr
        Se79    1.5819E-15 [Ci/yr/SA] at  1.000E+04 yr
    The remaining  16   nuclide(s) have zero release
exec: calling dcagw
            Highest annual dose GW pathway
        I129    2.7902E-02 [mrem/yr]  at  8.897E+03 yr
        Tc99    1.4344E-03 [mrem/yr]  at  8.897E+03 yr
        Cl36    2.7515E-04 [mrem/yr]  at  8.897E+03 yr
        Se79    2.3407E-12 [mrem/yr]  at  1.000E+04 yr
    The remaining  16   nuclide(s) have zero release
        At end of TPI, annual dose GW pathway
        I129    2.4939E-02 [mrem/yr]
        Tc99    1.2800E-03 [mrem/yr]
        Cl36    2.4533E-04 [mrem/yr]
        Se79    2.3407E-12 [mrem/yr]
          sum  2.6464E-02 [mrem/yr]
    The remaining  16   nuclide(s) have zero release
exec: calling ashplumo
exec: calling ashrmovo
exec: calling dcags
            Highest annual dose from GS
        Pu240  8.5007E+03 [mrem/yr] at  7.038E+03 yr
        Pu239  8.4155E+03 [mrem/yr] at  7.038E+03 yr
        Am243  5.1496E+02 [mrem/yr] at  7.038E+03 yr
        Pu242  1.0665E+02 [mrem/yr] at  7.038E+03 yr
        Np237  4.8624E+01 [mrem/yr] at  7.038E+03 yr
         U234  2.3482E+01 [mrem/yr] at  7.038E+03 yr
exec: end realizations

exec: Peak Mean Dose is 1.76550E+01 rem/yr at   7038.2 yr, based on     1 realizations.
```

exec: Run Successfully Completed

- Overall test status: <u>PASS</u>

SL-3. Name: Maximum Number of Volcanic Failures in a Subarea

Path for run directory: c:\SCR560\tpa500l\SL-3\basecase
c:\SCR560\tpa500m\SL-3\basecase

Path for archive of results: \SCR560\tpa500l\SL-3\basecase (archived on CD)
\SCR560\tpa500m\SL-3\basecase (archived on CD)

Environment variables: TPA_DATA=c:\SCR560\tpa500l
TPA_DATA=c:\SCR560\tpa500l

TPA_DATA=c:\SCR560\tpa500m
TPA_DATA=c:\SCR560\tpa500m

Special input files or modifications to input files required: Increase the dike width and length to very large values that encompass the entire repository; set the dike angle at zero and volcano diameter at zero; set subarea for volcanic event at 3 in the *tpa.inp* file; and set the time for the volcanic event and initially defective WPs equal to 0.

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Activate Volcano in the *tpa.inp* file

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: To evaluate whether the number of WPs failed in a subarea exceeds the number of WPs in the subarea, execute the TPA Version 5.0.0l code to demonstrate this situation; then, execute the TPA Version 5.0.0m code (using the same input conditions) to show that the number of failed WPs from an intrusive volcanic event equals the actual number of WPs in the subarea. All WPs will be failed by setting dike lengths and widths are large values to encompass the entire repository and at an angle and location to intersect all drifts. Initial defective WPs and the time of the volcanic event will be set equal to 0.

- Objective: Verify the TPA code cannot have more VOLCANO intrusive WP failures in a subarea than the number of

WPs in that subarea.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: screenprint (saved as the file *tpa.out*)

- Step by step test procedure to be used:

1. Execute the TPA Version 5.0.0l and 5.0.0m codes using the basecase *tpa.inp* file with Volcano activated and other *tpa.inp* file parameters set equal as described above. That is, the dike lengths and widths set equal to large values (i.e., 1,000,000), the dike angle at 0 degrees, the volcano diameter set equal to 0 (i.e., so there are no ejected WPs), the subarea of volcanic event set equal to 3, time 0 for the volcanic event, and zero initial defective WPs in the *tpa.inp* file.
2. Capture the screenprint.
3. Examine the screenprint (*tpa.out*) to verify that more WPs are failed than are present in a subarea for Version 5.0.0l.
4. Examine the screenprint (*tpa.out*) to verify that there are not more WPs are failed than are present in a subarea for Version 5.0.0m (i.e., all subarea WPs have failed).

- Pass/Fail criteria:

Criterion 1: Version 5.0.0l screenprint (*tpa.out*) should indicate more WPs are failed than are present in a subarea.

Criterion 2: Version 5.0.0m screenprint (*tpa.out*) should indicate all WPs in the subarea have failed.

Test Results: The screenprint (*tpa.out*) from the TPA Version 5.0.0m code is provided below. This output appears to show a problem with the VOLCANO module in failing all of the WPs in a particular subarea. (Note that TPA Version 5.0.0l screenprint shows the same behavior, and therefore is not presented here.)

```
=====================================================================
      exec: Welcome to TPA Version 5.0.0m
    Job started: Wed Apr 06 09:10:14 2005
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea  Area      Waste   Number of WP
  #    [m^2]     [MTU]
  1   221574.0   3566.3      452
  2   447909.0   7203.6      913
  3  2619149.5  41951.1     5317
  4   150452.0   2319.7      294
  5   318060.0   4994.4      633
  6   437858.0   6888.0      873
```

```
  7   301280.0    3116.5       395

Total Area [acre]        =  1111.016184828268
Total Buried Waste [MTU]  =  70039.53000000000
Repository AML [MTU/acre] =  63.04096281984062

Specified Global Parameters:

          Compliance Period =  10000.0 (yr)
      Maximum Simulation Time =  10000.0 (yr)
       Number Of Realizations =     1
          Number Of Subareas =     7
          Volcanism scenario =     1 (yes=1, no=0)
           Faulting scenario =     0 (yes=1, no=0)
   Mechanical failure scenarios:
                 Seismicity =     1 (yes=1, no=0)
           Drift Degradation =     1 (yes=1, no=0)
    Distance to Receptor Group =     18.0 (km)

**>>> CAUTION: CHECKING OF NUCLIDES AND CHAINS IS DISABLED <<<**
**>>> You may not be using the standard chains specified   <<<**
**>>> in the invent module.                                <<<**
**>>> (see "CheckNuclidesAndChains(yes=1,no=0)" in tpa.inp)<<<**

The specified path for data  = $TPA_DATA/
The specified path for codes = $TPA_TEST/

**To modify global parameters or the path, stop code execution using control-C**

  ***>>> WARNING: THE APPEND OPTION IS SELECTED <<<***
(see "OutputMode(0=None,1=All,2=UserDefined)" in tpa.inp)
For "SelectAppendFiles", a value of 0 (all append files) was set in tpa.inp.
By selecting this option, files are written which may require    6 megs of disk space.
(more disk space could be needed)

-----------------------------------------------------------------------
   subarea   1 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
      Mean Annual Infiltration at Start(AAI0):    5.8542E+00
exec: calling eqvdia
exec: calling nfenvFI
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
exec: calling volcano
exec: failed WPs from Volcanic  event =    388 at time =      0.0 yr
 *** failed WPs:  388   out of  452  ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
             Highest release rates from Sub Area 1
```

```
        C14     1.2375E-04 [Ci/yr/SA] at  3.076E+03 yr
        Tc99    8.0512E-05 [Ci/yr/SA] at  5.184E+03 yr
        Pu239   6.5634E-05 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   5.9912E-05 [Ci/yr/SA] at  5.184E+03 yr
        Pu240   5.9782E-05 [Ci/yr/SA] at  5.832E+03 yr
        Jp239   5.5789E-05 [Ci/yr/SA] at  1.000E+04 yr
exec: calling uzft
            Highest release rates from UZ
        Tc99    8.0413E-05 [Ci/yr/SA] at  5.308E+03 yr
        Jp239   2.7278E-05 [Ci/yr/SA] at  1.000E+04 yr
        Jp240   2.4385E-05 [Ci/yr/SA] at  6.113E+03 yr
        I129    9.1985E-06 [Ci/yr/SA] at  5.308E+03 yr
        Se79    7.0766E-06 [Ci/yr/SA] at  6.875E+03 yr
        Cl36    3.9218E-06 [Ci/yr/SA] at  5.308E+03 yr
exec: calling szft
            Highest release rates from SZ
        Tc99    7.9937E-05 [Ci/yr/SA] at  6.560E+03 yr
        I129    9.1757E-06 [Ci/yr/SA] at  6.560E+03 yr
        Cl36    3.9011E-06 [Ci/yr/SA] at  6.560E+03 yr
        Se79    1.2460E-12 [Ci/yr/SA] at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   2 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
   ebsfail: No Weld Failure
   *** No Corrosion WP Failure ***
exec: failed WPs from Volcanic  event =    876 at time =      0.0 yr
 *** failed WPs:  876   out of  913  ***
 *** ejected WPs:  0
exec: calling ebsrel
    ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 2
        C14     5.0337E-04 [Ci/yr/SA] at  3.076E+03 yr
        Tc99    3.1889E-04 [Ci/yr/SA] at  5.184E+03 yr
        Pu239   2.7506E-04 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   2.3799E-04 [Ci/yr/SA] at  5.184E+03 yr
        Jp239   2.3380E-04 [Ci/yr/SA] at  1.000E+04 yr
        Pu240   2.3230E-04 [Ci/yr/SA] at  7.376E+03 yr
exec: calling uzft
    *** NEFTRAN is skipped for this UZ path since no layers have significant ground water travel
time. ***
            Highest release rates from UZ
        Tc99    3.1889E-04 [Ci/yr/SA] at  5.184E+03 yr
        Pu239   2.7506E-04 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   2.3799E-04 [Ci/yr/SA] at  5.184E+03 yr
        Jp239   2.3380E-04 [Ci/yr/SA] at  1.000E+04 yr
        Pu240   2.3230E-04 [Ci/yr/SA] at  7.376E+03 yr
        Jp240   1.9745E-04 [Ci/yr/SA] at  7.376E+03 yr
```

```
exec: calling szft
                Highest release rates from SZ
          Tc99    3.1681E-04 [Ci/yr/SA] at  6.258E+03 yr
          I129    3.6470E-05 [Ci/yr/SA] at  6.258E+03 yr
          Cl36    1.5516E-05 [Ci/yr/SA] at  6.258E+03 yr
          Se79    2.1612E-11 [Ci/yr/SA] at  1.000E+04 yr
          Np237   4.5601E-25 [Ci/yr/SA] at  1.000E+04 yr
    The remaining  15   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   3 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
exec: failed WPs from Volcanic  event =   4316 at time =      0.0 yr
 *** failed WPs:  4316   out of  5317  ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
             Highest release rates from Sub Area 3
          C14     1.1499E-03 [Ci/yr/SA] at  3.076E+03 yr
          Tc99    7.4732E-04 [Ci/yr/SA] at  5.184E+03 yr
          Pu239   7.0053E-04 [Ci/yr/SA] at  1.000E+04 yr
          Jp239   5.9545E-04 [Ci/yr/SA] at  1.000E+04 yr
          Pu240   5.7227E-04 [Ci/yr/SA] at  8.293E+03 yr
          Cs135   5.5845E-04 [Ci/yr/SA] at  5.184E+03 yr
exec: calling uzft
                Highest release rates from UZ
          Tc99    7.4631E-04 [Ci/yr/SA] at  5.564E+03 yr
          Jp239   2.8070E-04 [Ci/yr/SA] at  1.000E+04 yr
          Jp240   2.2857E-04 [Ci/yr/SA] at  8.897E+03 yr
          I129    8.5753E-05 [Ci/yr/SA] at  5.434E+03 yr
          Se79    6.5789E-05 [Ci/yr/SA] at  7.376E+03 yr
          Cl36    3.6551E-05 [Ci/yr/SA] at  5.434E+03 yr
exec: calling szft
                Highest release rates from SZ
          Tc99    7.4191E-04 [Ci/yr/SA] at  7.038E+03 yr
          I129    8.5496E-05 [Ci/yr/SA] at  6.715E+03 yr
          Cl36    3.6336E-05 [Ci/yr/SA] at  6.715E+03 yr
    The remaining  17   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   4 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
```

```
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
exec: failed WPs from Volcanic  event =    201 at time =      0.0 yr
 *** failed WPs:  201   out of  294  ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 4
        C14     4.0242E-05 [Ci/yr/SA] at  3.076E+03 yr
        Tc99    2.6506E-05 [Ci/yr/SA] at  5.184E+03 yr
        Pu239   1.9943E-05 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   1.9788E-05 [Ci/yr/SA] at  5.184E+03 yr
        Pu240   1.7957E-05 [Ci/yr/SA] at  5.971E+03 yr
        Jp239   1.6952E-05 [Ci/yr/SA] at  1.000E+04 yr
exec: calling uzft
            Highest release rates from UZ
        Tc99    2.6482E-05 [Ci/yr/SA] at  5.434E+03 yr
        Jp239   7.5927E-06 [Ci/yr/SA] at  1.000E+04 yr
        Jp240   6.4337E-06 [Ci/yr/SA] at  7.551E+03 yr
        I129    3.0401E-06 [Ci/yr/SA] at  5.434E+03 yr
        Se79    2.3483E-06 [Ci/yr/SA] at  6.875E+03 yr
        Cl36    1.2958E-06 [Ci/yr/SA] at  5.434E+03 yr
exec: calling szft
            Highest release rates from SZ
        Tc99    2.6338E-05 [Ci/yr/SA] at  6.715E+03 yr
        I129    3.0335E-06 [Ci/yr/SA] at  6.715E+03 yr
        Cl36    1.2893E-06 [Ci/yr/SA] at  6.560E+03 yr
        Se79    2.1877E-13 [Ci/yr/SA] at  1.000E+04 yr
    The remaining  16   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   5 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
exec: failed WPs from Volcanic  event =    633 at time =      0.0 yr
 *** failed WPs: all WPs failed ( 633 ) ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 5
        C14     4.6321E-04 [Ci/yr/SA] at  3.076E+03 yr
        Tc99    2.8930E-04 [Ci/yr/SA] at  5.184E+03 yr
        Pu239   2.3292E-04 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   2.1632E-04 [Ci/yr/SA] at  4.607E+03 yr
        Pu240   2.0015E-04 [Ci/yr/SA] at  7.038E+03 yr
        Jp239   1.9798E-04 [Ci/yr/SA] at  1.000E+04 yr
exec: calling uzft
            Highest release rates from UZ
        Tc99    2.8903E-04 [Ci/yr/SA] at  5.308E+03 yr
        Jp239   9.6814E-05 [Ci/yr/SA] at  1.000E+04 yr
```

```
        Jp240   8.2536E-05 [Ci/yr/SA] at  7.376E+03 yr
        I129    3.3198E-05 [Ci/yr/SA] at  5.184E+03 yr
        Se79    2.5616E-05 [Ci/yr/SA] at  5.971E+03 yr
        Cl36    1.4172E-05 [Ci/yr/SA] at  4.717E+03 yr
exec: calling szft
              Highest release rates from SZ
        Tc99    2.8746E-04 [Ci/yr/SA] at  6.258E+03 yr
        I129    3.3136E-05 [Ci/yr/SA] at  6.258E+03 yr
        Cl36    1.4101E-05 [Ci/yr/SA] at  6.113E+03 yr
        Se79    3.7224E-12 [Ci/yr/SA] at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   6 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
   ebsfail: No Weld Failure
   *** No Corrosion WP Failure ***
exec: failed WPs from Volcanic  event =    782 at time =      0.0 yr
 *** failed WPs:  782   out of  873  ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
             Highest release rates from Sub Area 6
        C14     2.0149E-04 [Ci/yr/SA] at  3.076E+03 yr
        Tc99    1.3132E-04 [Ci/yr/SA] at  5.184E+03 yr
        Pu239   1.0972E-04 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   9.8098E-05 [Ci/yr/SA] at  5.184E+03 yr
        Jp239   9.3262E-05 [Ci/yr/SA] at  1.000E+04 yr
        Pu240   9.2518E-05 [Ci/yr/SA] at  7.376E+03 yr
exec: calling uzft
              Highest release rates from UZ
        Tc99    1.3103E-04 [Ci/yr/SA] at  5.696E+03 yr
        Jp239   4.3288E-05 [Ci/yr/SA] at  1.000E+04 yr
        Jp240   3.5642E-05 [Ci/yr/SA] at  8.293E+03 yr
        I129    1.5052E-05 [Ci/yr/SA] at  5.696E+03 yr
        Se79    1.1497E-05 [Ci/yr/SA] at  1.000E+04 yr
        Cl36    6.4124E-06 [Ci/yr/SA] at  5.564E+03 yr
exec: calling szft
              Highest release rates from SZ
        Tc99    1.3043E-04 [Ci/yr/SA] at  6.875E+03 yr
        I129    1.5033E-05 [Ci/yr/SA] at  6.715E+03 yr
        Cl36    6.3891E-06 [Ci/yr/SA] at  6.715E+03 yr
        Se79    2.3158E-14 [Ci/yr/SA] at  1.000E+04 yr
   The remaining  16   nuclide(s) have zero release
-----------------------------------------------------------------------
   subarea   7 of   7          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling eqvdia
exec: calling nfenvFl
```

```
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Weld Failure
    *** No Corrosion WP Failure ***
exec: failed WPs from Volcanic  event =    395 at time =      0.0 yr
 *** failed WPs: all WPs failed ( 395 ) ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
            Highest release rates from Sub Area 7
         C14     9.3199E-05 [Ci/yr/SA] at  3.076E+03 yr
         Tc99    6.0836E-05 [Ci/yr/SA] at  5.184E+03 yr
         Cs135   4.5545E-05 [Ci/yr/SA] at  5.184E+03 yr
         Pu239   3.9594E-05 [Ci/yr/SA] at  1.000E+04 yr
         Pu240   3.6825E-05 [Ci/yr/SA] at  5.434E+03 yr
         Jp239   3.3655E-05 [Ci/yr/SA] at  1.000E+04 yr
exec: calling uzft
               Highest release rates from UZ
         Tc99    6.0618E-05 [Ci/yr/SA] at  5.832E+03 yr
         Jp239   1.5599E-05 [Ci/yr/SA] at  1.000E+04 yr
         Jp240   1.3540E-05 [Ci/yr/SA] at  6.875E+03 yr
         I129    6.9861E-06 [Ci/yr/SA] at  5.832E+03 yr
         Se79    5.2117E-06 [Ci/yr/SA] at  1.000E+04 yr
         Cl36    2.9751E-06 [Ci/yr/SA] at  5.832E+03 yr
exec: calling szft
               Highest release rates from SZ
         Tc99    6.0342E-05 [Ci/yr/SA] at  6.875E+03 yr
         I129    6.9776E-06 [Ci/yr/SA] at  6.875E+03 yr
         Cl36    2.9645E-06 [Ci/yr/SA] at  6.875E+03 yr
         Se79    2.1578E-14 [Ci/yr/SA] at  1.000E+04 yr
    The remaining  16   nuclide(s) have zero release
exec: calling dcagw
               Highest annual dose GW pathway
         I129    1.6131E-02 [mrem/yr]  at  6.560E+03 yr
         Tc99    8.3917E-04 [mrem/yr]  at  6.715E+03 yr
         Cl36    1.5991E-04 [mrem/yr]  at  6.560E+03 yr
         Se79    7.0079E-11 [mrem/yr]  at  1.000E+04 yr
         Np237   5.7735E-22 [mrem/yr]  at  1.000E+04 yr
    The remaining  15   nuclide(s) have zero release
        At end of TPI, annual dose GW pathway
         I129    1.5493E-02 [mrem/yr]
         Tc99    8.1226E-04 [mrem/yr]
         Cl36    1.5240E-04 [mrem/yr]
         Se79    7.0079E-11 [mrem/yr]
         Np237   5.7735E-22 [mrem/yr]
           sum  1.6457E-02 [mrem/yr]
    The remaining  15   nuclide(s) have zero release
                 There is no GS release
exec: end realizations

exec: Peak Mean Dose is 1.71300E-05 rem/yr at   6559.6 yr, based on     1 realizations.

exec:  Run Successfully Completed
```

Because it was not possible to fail all WPs in a subarea, the test criteria were not be satisfied. It is recommended that the algorithm, which uses drift and subarea coordinates to determine of number of WPs disrupted by a volcanic event, be examined and modified as needed.

- Overall test status: FAIL (SCR #570 addresses this test failure)

```
**
**          ***>>> VOLCANO <<<***
**
iconstant
VolcanoModel(1=Geometric,2=Distribution)
1
**
finiteexponential
TimeOfNextVolcanicEventinRegionOfInterest[yr]
100.0, 10000.0, 1.0e-7
**
** for Geometric Model
constant
XLocationInRegionOfInterest[m]
548000.0
**
constant
YLocationInRegionOfInterest[m]
4078000.0
**
uniform
RNtoDetermineIfExtrusiveOrIntrusiveVolcanicEvent
0.0, 1.0
**
constant
FractionOfTimeVolcanicEventIsExtrusive
0.999
**
uniform
AngleOfVolcanicDikeMeasuredFromNorthClockwise[degrees]
0.0, 15.0
**
uniform
LengthOfVolcanicDike[m]
2000.0, 11000.0
**
uniform
WidthOfVolcanicDike[m]
1.0, 10.0
**
uniform
DiameterOfVolcanicConduit[m]
28.0, 280.0
**
** For Geometric Model, set SubareaOfVolcanicEvent[] to
**    constant, 3
iuniform
SubareaOfVolcanicEvent[]
1, 7
**1, 10
** SCR560
**
** For Distribution model only.
**
beta
NumberOfWPsEntrainedByEjecta[]
1.0, 150.0, 1.0, 2.0
```

```
**
usersuppliedpwisecdf
NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[]
19
0.      0.000
8.941e-6 0.084
.01788 0.094
.05364 0.117
.08941 0.141
.1252  0.175
.1609  0.213
.1886  0.257
.1887  0.475
.2527  0.562
.2813  0.588
.2814  0.712
.4470  0.781
.5633  0.813
.6974  0.843
.8156  0.881
.8157  0.967
.8444  0.969
.8445  1.000
**
```

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-561	2. Software Title and Version: TPA 5.0.0p	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *strmtube.dat*

The stream tube information in *strmtube.dat* needs to be updated for the new repository footprint.

5. Change Requested by: J. Winterle Date: 3-10-05	6. Change Authorized by (*Software Developer*): R. Janetzke Date: 3-10-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The *strmtube.dat* file was modified (See Attachment A) to be consistent with the new subarea definitions. The most significant change is that the northernmost streamtube (no. 3) was made wider by a factor of 1.77 along its entire length. This was done because the new repository footprint extends farther north. To keep travel times approximately the same, the specified flux for streamtube no. 3 also had to be increased by a factor of 1.77.

The only other changes were to adjust the specified streamtube centerlines for all three streamtubes so that it actually goes down the center of the streamtube (whereas, before these centerlines were purposely made crooked so that they would pick up specific subareas).

8. Implemented by: J. Winterle	Date: 3-11-05

9. Description of Acceptance Tests:

Attachment B shows the difference between the p version and the q version of *strmtube.dat* file. The numbers for the flow rate and the streamtube no. 3 width were increased by 1.77 for the q version. The center line values between the p and q version were changed and Attachment A agrees with the q version by visual inspection.

10. Tested by: A. Lozano	Date: 4-15-05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)

ATTACHMENT A

```
TITLE: TPA5 Stream Tube data for the saturated zone.
TITLE: Created by J.R. Winterle (jrw) 3/11/05
TITLE: Based on 3D saturated zone flow path simulation results
TITLE: Three streamtubes to 18-km distance based on most recent repository design
**      Change from previous version is increase in nothernmost streamtube (No. 3)
**      to accomodate more recent footprint design and subarea layout that extends
**      farther to the north.  Streamtube no. 3 width and flux were increased
**      by a factor or 1.77.
**
  3      Number of stream tubes.
**
** Flow Rates (m^3/yr/m)
**
  3
263.
252.
274.
**
** Distance to Receptor Well
**  set 2 values: should match "DistanceToReceptorGroup..." in tpa.inp and the
**  well pumping and mixing zone data for DCAGW in tpa.inp )
**
10.0, 18.0
**
**
** Following inputs define center line coordinates for flow paths from beneath the
** repository area to the entrance of the stream tubes, which begin on the eastern edge of the
** repository footprint.  These points are used to determine which subareas contribute to which
** streamtubes -- the line closest to the centroid of a particular subarea will receive the mass
** for that subarea in its associated streamtube. (updated 3/11/05 to be consistent with updated
** subarea pattern)
**
**  Streamtube 1 is southernmost
**
1
  3       Number of stream tube points for tube 1.
UTM-x[m]   UTM-y[m]
547400.,  4077400.
548000.,  4077000.
548450.,  4076700.
**
**  Streamtube 2 is central
2
  3       Number of stream tube points for tube 2.
UTM-x[m]   UTM-y[m]
547250.,  4079200.
548100.,  4078620.
548550.,  4078320.
**
**  Streamtube 3 is northernmost
3
  3       Number of stream tube points for tube 3.
UTM-x[m]   UTM-y[m]
547550.,  4081060.
548450.,  4080465.
549230.,  4079950.
**
**
**  DEFINITION OF STREAMTUBE SEGMENT GEOMETRIES
**
** I/F_Dist is linear distance from Repository boundary
** width[m] is the average width of the streamtube since the last I/F_Dist
** tube_length[m] is the cumulative flow distance for all segments
**
** Southernmost streamtube
  10      Number of points for tube 1.
I/F_Dist   width[m]  tube_length[m]
0.0     1400.,  0.
1.5     1500.,  1500.
2.5     450.,   2500.
4.0     300.,   4000.
```

```
6.5     225.,   6500.
9.0     350.,   9000.
12.5    550.,   12500.
13      450.,   13000.
15      375.,   15000.
18.0    220.,   18000.
**
** Central streamtube
  8       Number of points for tube 2.
I/F_Dist   width[m]  tube_length[m]
0.0     1500.,  0.
1.0     1500.,  1350.
3.0     450.,   4350.
9.5     250.,   10850.
13.0    400.,   14350.
13.5    375.,   14850.
15.0    325.,   16350.
18.0    225.,   19350.
**
** Northernmost streamtube
  10      Number of points for tube 3.
I/F_Dist   width[m]  tube_length[m]
0.0     2300.,  0.
1.5     2100.,  2200.
2.0     880.,   4600.
3.0     530.,   6100.
7.0     400.,   10600.
10.0    310.,   13900.
13.0    440.,   16900.
13.5    400.,   17400.
15.0    310.,   18900.
18.0    265.,   21900.
**
endoffile
```

ATTACHMENT B

Changes to strmtube.dat

Differences between p version on left (Pre) and q version on right (Post changes).

```
**                                          **
** Flow Rates (m^3/yr/m)                    ** Flow Rates (m^3/yr/m)
**                                          **
 3                                           3
263.                                        263.
252.                                        252.
155.              X 1.77                    274.

** for that subarea in its associated streamtube. (updated 3/11/05 to be
consistent with updated
** subarea pattern)
**
**  Streamtube 1 is southernmost ( Alligned center lines )
**
1
 3       Number of stream tube points for tube 1.
UTM-x[m]   UTM-y[m]                         UTM-x[m]   UTM-y[m]
547400.,  4077550.                          547400.,  4077400.
548000.,  4076750.                          548000.,  4077000.
548400.,  4076600.                          548450.,  4076700.
**
**  Streamtube 2 is central
2
 3       Number of stream tube points for tube 2.
UTM-x[m]   UTM-y[m]                         UTM-x[m]   UTM-y[m]
547550.,  4079400.                          547250.,  4079200.
548000.,  4078800.                          548100.,  4078620.
548475.,  4077500.                          548550.,  4078320.
**
**  Streamtube 3 is northernmost
3
 3       Number of stream tube points for tube 3.
UTM-x[m]   UTM-y[m]                         UTM-x[m]   UTM-y[m]
547700.,  4081000.                          547550.,  4081060.
548200.,  4080400.                          548450.,  4080465.
548600.,  4080200.                          549230.,  4079950.
**
**
**  DEFINITION OF STREAMTUBE SEGMENT GEOMETRIES
**
** I/F_Dist is linear distance from EDAII boundary
** width[m] is the average width of the streamtube since the last I/F_Dist
** tube_length[m] is the cumulative flow distance for all segments
**
** Southernmost streamtube
  10      Number of points for tube 1.
I/F_Dist   width[m]  tube_length[m]
0.0   1400.,      0.                        No changes
1.5   1500.,      1500.
2.5   450.,       2500.
```

```
4.0   300., 4000.
6.5   225., 6500.
9.0   350., 9000.
12.5  550., 12500.
13    450., 13000.
15    375., 15000.
18.0  220., 18000.
**
** Central streamtube
  8      Number of points for tube 2.
I/F_Dist   width[m]  tube_length[m]
0.0   1500.,0.                            No changes
1.0   1500.,1350.
3.0   450., 4350.
9.5   250., 10850.
13.0  400., 14350.
13.5  375., 14850.
15.0  325., 16350.
18.0  225., 19350.
**
** Northernmost streamtube
  10      Number of points for tube 3.
I/F_Dist   width[m]  tube_length[m]
0.0   1300.,0.    1300 X 1.77 = 2300      0.0   2300.,0.
1.5   1200.,2200. (Aprox)width x 1.77     1.5   2100.,2200.
2.0   500., 4600.                         2.0   880., 4600.
3.0   300., 6100.                         3.0   530., 6100.
7.0   225., 10600.                        7.0   400., 10600.
10.0  175., 13900.                        10.0  310., 13900.
13.0  250., 16900.                        13.0  440., 16900.
13.5  225., 17400.                        13.5  400., 17400.
15.0  175., 18900.                        15.0  310., 18900.
18.0  150., 21900.                        18.0  265., 21900.
**
endoffile
```

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*):	**2. Software Title and Version:**	**3. Project No:**
PA-SCR-562	TPA 5.0.0m	20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *setupCommons.h, buildInputFiles.h, dsfail.f, exec.f, nfenv.f, dsfailt.def, tpa.inp*

1) The following parameters need to be removed from *tpa.inp*:
   A) TiCorrosionRateVsFluorideSlope[]
   B) MinimumFluoride[mol/L]
   C) MaximumFluoride[mol/L]
   D) UseFluorideEnhancingFactor(0=no,1=yes)
   These parameters need to be retained in *dsfailt.def*. The user can change the parameters in *dsfailt.def*, if necessary.
2) Observed that the name for the fluoride data file, fluoride.dat is both present in dsfailt.def and hardcoded in *dsfail.f*. If the user changes the fluoride data file in dsfailt.def, it has no effect (the changed name does not appear in *dsfailt.inp*).
3) There is a spelling error that appears in *dsfail.rlt*: "No failure of the drip *shiled* in:."
4) The thermal conductivity of the backfill in *tpa.inp* applies to both thermal model 1 and thermal model 2. This value incorporates the conduction through the backfill as well as other mechanisms such as convection. However, for thermal model 2, the convection through the backfill is calculated directly. Therefore, separate parameters need to be used for thermal models 1 and 2.
5) It is not clear how natural backfill degradation is turned off from *tpa.inp*.

5. Change Requested by:	**6. Change Authorized by** (*Software Developer*):
O. Pensaldo Date: 3-24-2005	R. Janetzke Date: 3-24-2005

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

1)Removed the parameters TiCorrosionRateVsFluorideSlope[], MinimumFluoride[mol/L], MaximumFluoride[mol/L], and UseFluorideEnhancingFactor(0=no,1=yes) from *tpa.inp* and *dsfail.f*.
2) Modified *dsfail.f* to allow the user to change the name for the fluoride data file.
3) Changed ThermalConductivityOfBackfill[W/(m-C)] to ThermalConductivityOfBackfillModelOne[W/(m-C)] and added parameter ThermalConductivityOfBackfillModelTwo[W/(m-C)]. Also, placed these parameters near the parameter, SelectThermalModel(1,2) within *tpa.inp*.
4) Corrected the spelling error in *exec.f* (changed shiled to shield).
5) Added a note in *tpa.inp* section Disruptive Scenario Flags to indicate that both SeismicDisruptiveScenarioFlag(yes=1,no=0) and DriftDegradationScenarioFlag(yes=1,no=0) must be set to no(0) in order to turn off natural backfill accumulation.

8. Implemented by:	**Date:**
G. Adams	April 18, 2005

9. Description of Acceptance Tests (used tpa500s for Pre and tpa500t for post

1)Checked the tpa.inp file in the t version for removal of TiCorrosionRateVsFluorideSlope[], MinimumFluoride[mol/L], MaximumFluoride[mol/L], and UseFluorideEnhancingFactor(0=no,1=yes) from *tpa.inp* and *dsfail.f*.
Passed - All 4 parameters were removed from tpa.inp. **Passed** - All 4 parameters were removed from dsfail.f.

2) Modified *dsfail.f* to allow the user to change the name for the fluoride data file.
Passed - The modified version of *dsfail.f* obtains the name of the fluoride data file from *dsfailt.def*.

3) Confirmed that the change from ThermalConductivityOfBackfill[W/(m-C)] to ThermalConductivityOfBackfillModelOne[W/(m-C)] was made and that the parameter ThermalConductivityOfBackfillModelTwo[W/(m-C)] was added. Also, placed these parameters near the parameter, SelectThermalModel(1,2) within *tpa.inp*.
Passed - Modification was made in tpa.inp and nfenv.f .

4) Corrected the spelling error in *exec.f* (changed shiled to shield). **Passed** - the spelling error was corrected.

5) Added a note in *tpa.inp* section Disruptive Scenario Flags to indicate that both SeismicDisruptiveScenarioFlag(yes=1,no=0) and DriftDegradationScenarioFlag(yes=1,no=0) must be set to no(0) in order to turn off natural backfill accumulation
Passed - The note was added to tpa.inp .

10. Tested by:	**Date:**
A. Lozano	April 26, 2005

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
DELETE	DSFAIL	TiCorrosionRateVsFluorideSlope[]					GRA
DELETE	DSFAIL	MinimumFluoride[mol/L]					GRA
DELETE	DSFAIL	MaximumFluoride[mol/L]					GRA
DELETE	DSFAIL	UseFluorideEnhancingFactor(0=no, 1=yes)					GRA

MODIFY	NFENV	ThermalConductivityOfBackfill[W/(m-C)] to ThermalConductivityOfBackfillModelOne[W/(m-C)]		triangular	0.12, 0.27, 1.0	Note: No change to the distribution or range from what Rfedors provided	GRA
ADD	NFENV	ThermalConductivityOfBackfillModelTwo[W/(m-C)]	Used to calculate the heat transfer through the backfill material in Thermal Model 2 calculations.	constant	0.27	Quartz sand thermal conductivity Civilian Radioactive Waste Management System Management & Operating Contractor (1999). From an LSN search (DEN001435856 - ALC.20040610.8358), a document titled Repository Thermal Design Review 1999 by Meieran, Osnes, Roberds, and Smyder (pages 6-7), identifies a thermal conductivity less than 0.33 W/m-K for dry sand. The document also refers to a conductivity range between 0.12 and 0.28 W/m-K.	GRA

ADD	Disruptive Scenario Flags	NOTE: Both SeismicDisruptiveScenarioFlag(yes=1,no=0) and DriftDegradationScenarioFlag(yes=1,no=0) must be set to no(0) in order to turn off natural backfill accumulation.	Clarifying text in tpa.inp			Users would not be aware that both flags need to be set to no(0) in order to eliminate the effects of drift degradation.	GRA

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-564	2. Software Title and Version: TPA 5.0.0t	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *exec.f, tpa.inp, volcano.f*

1. Should arrange the code so that each realization always has an intrusive event, and a simple flag (0,1) for extrusive event with default = 1 (include extrusive event). The current sampling of the 2 current parameters is confusing and not useful; no basis for probabilistic sampling of intrusive:extrusive. So, for `VolcanismDisruptiveScenarioFlag` = 1:
   a) Always have an intrusive event, with groundwater release pathway
   b) If `ExtrusiveEventFlag` = 1 [default], then do airborne release pathway, else only do intrusive event. There are no conditions where there is only an extrusive event without an intrusive event. All igneous events (i.e., `VolcanismDisruptiveScenarioFlag` = 1) have an intrusive event.

2. There is no longer any need for calculating area of the volcanic dike or any need for the volcanic dike width parameter. No need to calculate overlap of conduit and dike area.

3. In *exec.f*, number of WPs ejected is always reported for subarea 2. This should vary according to the subarea for the volcanic event.

4. The dike center should be sampled uniformly over the repository footprint.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
B. Hill	R. Janetzke Date: 4-3-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See Attachment A.

8. Implemented by:	Date:
C. Scherer / Carol S. Scherer	4-22-05
R. Janetzke R. Janetzke	4-23-05

9. Description of Acceptance Tests:

See Attachment B for inspection tests that apply to both the UNIX and PC versions.

See Attachment C for PC platform tests.

See Attachment D for UNIX platform tests.

10. Tested by:	Date:
Albert Lozano / D. Stead Dave Stead	4-4-06

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 564

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its function in TPA code (calculated from . . ., used for calculating . . ., used to relate . . . etc.)	Distribution	Range	Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source
add	VOLCANO	ExtrusiveEventFlag	Flag set to 1 if there should be an extrusive event in addition to intrusive event or 0 if there should only be an intrusive event	iflag	1	User option.	B. Hill
delete	VOLCANO	RntoDetermineIfExtrusiveOrIntrusiveEvent		uniform	0.0, 1.0		B. Hill
delete	VOLCANO	FractionOfTimeVolcanicEventIsExtrusive		constant	0.999		B. Hill

delete	VOLCANO	WidthOfVolcanic Dike[m]		uniform	1.0, 10.0		R. Janetzke
delete	VOLCANO	XLocationInRegi onOfInterest		constant	548000		R. Janetzke
delete	VOLCANO	YLocationInRegi onOfInterest		constant	4079000		R. Janetzke
add	VOLCANO	RNToDetermine CenterOfVolcani cDike[]	The dike center will be located randomly along the drift center lines found in *drifts.dat*.	Uniform	0.0, 1.0		R. Janetzke

ATTACHMENT A

Description of Change(s) or Problem Resolution

1. Delete `RntoDetermineIfExtrusiveOrIntrusiveVolcanicEvent`, `FractionOfTimeVolcanicEventIsExtrusive`, and `WidthofVolcanicDike[m]` from *tpa.inp*. Add parameter `ExtrusiveEventFlag (iflag,1)` to *tpa.inp*. Modify *volcano.f* so that `ExtrusiveEventFlag` is used in conditional statement checks instead of `RntoDetermineIfExtrusiveOrIntrusiveVolcanicEvent`.

2. Remove obsolete code from *volcano.f* that used the dike width to calculate dike area, and remove code that calculates where the conduit falls with respect to the dike. Remove the parameter `FractionOfTimeVolcanicEventIsExtrusive` from *tpa.inp*.

3. In *exec.f*, (approx. line 4235), the number of WPs ejected by the volcanic event was hardcoded to always be reported from subarea 2 for the geometric volcano model. The code was changed to use eventsubarea (variable for input parameter `SubareaOfVolcanicEvent[]`; iuniform; 1,7) to report the ejected WPs, as was already done for the distribution volcano model.

4. The center of the dike is now calculated using a single random number and the drift end points as found in *drifts.dat*. The AMTU ejected and number of packages entrained are now treated the same for both geometric and distribution models. The methods for determining these values retain their original distinction.

ATTACHMENT B

Pre Change is tpa500t. Post Change is tpa500u

Acceptance of Change(s) or Problem Resolution

1. **Passed** - `RntoDetermineIfExtrusiveOrIntrusiveVolcanicEvent, FractionOfTimeVolcanicEventIsExtrusive, and WidthofVolcanicDike[m]` were deleted from *tpa.inp*.

```
**
** 4-5-05  css SCR564: remove current Extrusive parameters and replace
**         with ExtrusiveEventFlag(0=no,1=yes)
**uniform
**RNtoDetermineIfExtrusiveOrIntrusiveVolcanicEvent
**0.0, 1.0
****
**constant
**FractionOfTimeVolcanicEventIsExtrusive
**0.999
**
**
** 4-20-05  css SCR564: WidthOfVolcanicDike no longer used - remove
**uniform
**WidthOfVolcanicDike[m]
**1.0, 10.0
**
```

Passed - `ExtrusiveEventFlag (iflag,1)` was added to *tpa.inp*.

```
**
** 4-5-05  css SCR564: remove current Extrusive parameters and replace
**         with ExtrusiveEventFlag(0=no,1=yes)
iflag
ExtrusiveEventFlag(0=no,1=yes)
1
**
```

Modify *volcano.f* so that ExtrusiveEventFlag is used in conditional statement checks instead of RntoDetermineIfExtrusiveOrIntrusiveVolcanicEvent.

```
c css 04/05/05; SCR564:  remove Extrusive parameters and add extrusive
c     event flag
c
cc        call clearchar( 60, name )
cc        name = 'RNtoDetermineIfExtrusiveOrIntrusiveVolcanicEvent'
cc        iextint = ispquery( name )
cc
cc        call clearchar( 60, name )
cc        name = 'FractionOfTimeVolcanicEventIsExtrusive'
cc        ifractext = ispquery( name )

       call clearchar( 60, name )
       name = 'ExtrusiveEventFlag(0=no,1=yes)'
       iextrusive = ispquery( name )
c end change:  SCR564
c
```

```
c css 04/05/05; SCR564:  remove Extrusive parameters and replace
c     with extrusive event flag
cc        if( pext .le. fext ) then
       if (extrusive .eq. 1) then
c end change:  SCR564
           lExtrusive = .TRUE.
       else
           lExtrusive = .FALSE.
       end if

       if ( lExtrusive ) then
         wpentrained  = valuesp( iwpentrained )
       else
         wpentrained  = 0.0d0
       end if
```

2. Remove obsolete code from *volcano.f* that used the dike width to calculate dike area, and remove code that calculates where the conduit falls with respect to the dike. Remove the parameter `FractionOfTimeVolcanicEventIsExtrusive` from *tpa.inp*.

```
c css 04/05/05; SCR564:  remove obsolete parameters & variables
ccc     dikeonlyarea
ccc     fext
ccc     iextint
ccc     ifractext
ccc     iwidth
ccc     pext
ccc     width
c end change:  SCR564

cc rwj 4-22-05 scr564
     integer iwpspace
     integer irnloc

c css 04/05/05; SCR 564:  remove Extrusive parameters and add
c     extrusive event flag; remove variables no longer used
cc      integer iextint
cc      integer ifractext

     integer extrusive
     integer iextrusive
c end change:  SCR 564

cc rwj 4-22-05 scr564
cc      call clearchar( 60, name )
cc      name = 'XLocationInRegionOfInterest[m]'
cc      ixloc = ispquery( name )
cc
cc      call clearchar( 60, name )
cc      name = 'YLocationInRegionOfInterest[m]'
cc      iyloc = ispquery( name )
c
c css 04/20/05; SCR564:  remove width of dike; area of dike no
```

```
c     longer used
cc        call clearchar( 60, name )
cc        name = 'WidthOfVolcanicDike[m]'
cc        iwidth = ispquery( name )
c end change:  SCR564

cc rwj 4-23-05; scr564;
       call clearchar( 60, name )
       name = 'WPSpacingAlongEmplacementDrift[m]'
       iwpspace  = ispquery( name )
       wpspace  = valuesp( iwpspace )

       call clearchar( 60, name )
       name = 'RNToDetermineCenterOfVolcanicDike[]'
       irnloc = ispquery( name )
cc end scr564;
cc rwj 4-23-05 scr564;
       totdriftlength =  0.0d0
       do idrift = 1, ndrifts
         driftlength = dsqrt(
    &                  (drxy1out(1,idrift)-drxy2out(1,idrift))**2 +
    &                  (drxy1out(2,idrift)-drxy2out(2,idrift))**2 )
         totdriftlength =  totdriftlength + driftlength
       end do

       ikey=30231

     endif
c
c css 04/05/05; SCR 564:  remove Extrusive parameters and add
c     extrusive event flag
cc      pext    = valuesp( iextint )
cc      fext    = valuesp( ifractext )
     extrusive = ivaluesp (iextrusive)
c end change:  SCR564

cc rwj 4-22-05 scr564;

       eventsubarea  = ivaluesp( ieventsubarea )

cc      Check event subarea.
       if (eventsubarea .lt. 1 .or. eventsubarea .gt. nsa) then
          print *, ' ***>>> Error in volcano <<<*** '
          print *, ' eventsubarea .lt.1 .or. .gt. nsa'
          print *, ' eventsubarea = ', eventsubarea
          print *, ' nsa = ', nsa
          STOP
       endif
c
cc get aml as MTU per m2. (convert using acre/m2=2.47105e-4)
      amlperm2 = aml * 2.47105d-4
cc get area of conduit
      conduitarea = pi * diam**2 /4.d0
cc multiply aml*areaofcircle to get amtuejected.
      amtuejected = 0.0d0
      if (extrusive .eq. 1) amtuejected = amlperm2 * conduitarea
      amtuperwp  = valuesp( imtuperwp)
cc End of scr564
cc rwj 4-23-05;scr564
cc        call gsarea( i, area )
cc        call gsamtu( i, amtupersa )
         wpentrained = 0.0d0
         if (i .eq. eventsubarea) then
            wpentrained = amtuejected / amtuperwp
```

```
         end if
cc End of scr564

c
c css 4/20/05; SCR564:  dike width not needed; dike area no
c     longer used
cccc      Find dike area in subarea
cc          call qlhitsa( xyp1, xyp2, i, iflaglhit, alengthinsa )
cc          if (iflaglhit .eq. 1) then
cc              dikeareainsa = alengthinsa * width
cc          else
cc              dikeareainsa = 0.0d0
cc          endif
c end change:  SCR564

cc      If extrusive
c
c css 04/05/05; SCR564:  delete Extrusive parameters and replace
c     with extrusive event flag
cc          if( pext .le. fext ) then
c
cc       if (extrusive .eq. 1) then
c end change:  SCR564

c css 04/20/05; SCR564:  dike area and overlap no longer used
c     just need to calculate amtuejected
cc          if (iflagchit .eq. 1) then
cc             amtuejected = amtupersa * conduitarea / area
cc          end if
cc
cccc        Find overlap between conduit and dike
cccc        Test for conduit in subarea
cc            if( iflagchit .eq. 1 ) then
cc              amtuejected = amtupersa * conduitarea / area
cc
cccc          Test for conduit completely contained in dike.
cc              if (width .ge. diam) then
cc
cccc            Conduit is inside dike
cc                overlaparea= pi*diam**2.d0/4.d0
cc              else
cc
cccc            Conduit exceeds dike width
cccc            Find portion (overlap) of dike inside conduit
cc                overlaparea = pi*diam**2.d0/4.d0 -
cc     &          diam**2.d0/2.d0*dacos(width/diam) +
cc     &          width/2.d0*dsqrt(diam**2.d0 - width**2.d0)
cc              endif
cc            else
cc              conduitarea = 0.d0
cc              overlaparea = 0.d0
cc            endif
cc
cc       endif

cc
cc        dikeonlyarea = dikeareainsa - overlaparea
c end change:  SCR564

cc rwj 4-22-05 scr564
cc amtufailed = amtu released due to intrusive failures in drift
cc wpfailedinsa = intrusive failures in drift
cc wpentrained = wp ejected if event is in this subarea, else 0.
cc failedfraction = intrusive plus extrusive failed fraction for this subarea.
```

Passed - Removed from tpa.inp

```
** 4-5-05  css SCR564: remove current Extrusive parameters and replace
**         with ExtrusiveEventFlag(0=no,1=yes)
**uniform
**RNtoDetermineIfExtrusiveOrIntrusiveVolcanicEvent
**0.0, 1.0
****
**constant
**FractionOfTimeVolcanicEventIsExtrusive
**0.999
**
```

********** end of items tested by Albert Lozano **********

********** beginning of items tested by D. Stead **********

3. In *exec.f*, (approx. line 4235), the number of WPs ejected by the volcanic event was hardcoded to always be reported from subarea 2 for the geometric volcano model. The code was changed to use eventsubarea (variable for input parameter `SubareaOfVolcanicEvent[]`; iuniform; 1,7) to report the ejected WPs, as was already done for the distribution volcano model.

Passed - Verified that the code was changed (to use eventsubarea to report the ejected WPs in the same way for both volcano models) in 'exec.f' as follows:

```
c css 04-21-05; SCR564:  vary the subarea for volmodel = 1
           eventsubarea  = ivaluesp( ieventsubarea )
           if (volmodel .eq. 1) then
cc               if ( isa .eq. 2) then
              if ( isa .eq. eventsubarea) then
                  call gsamtu( isa, amtupersa )
                  releasewpfailedtime(1,3) = DMAX1( 0.0d0,
     &               releasewpfailedtime(1,3) - dble(nwpexhumed) )
                  print *,' *** ejected WPs: ', nwpexhumed
               endif
           else if (volmodel .eq. 2) then
cc               eventsubarea  = ivaluesp( ieventsubarea )
              if ( isa .eq. eventsubarea) then
                 call gsamtu( isa, amtupersa )
                 releasewpfailedtime(1,3) = DMAX1( 0.0d0,
     &              releasewpfailedtime(1,3) - dble(nwpexhumed) )
                 print *,' *** ejected WPs: ', nwpexhumed
              endif
           else
              print *, ' ***>>> Error in exec <<<*** '
              print *, ' volcano model ID is not 1 or 2.'
              print *, ' volmodel = ', volmodel
           endif
```

4. The center of the dike is now calculated using a single random number and the drift end points as found in *drifts.dat*. The AMTU ejected and number of packages entrained are now treated the same for both geometric and distribution models. The methods for determining these values retain their original distinction.

Passed - Verified that the code was changed in subroutine 'volcano' in 'volcano.f' as follows:

```
cc rwj 4-23-05; scr564;
        call clearchar( 60, name )
        name = 'WPSpacingAlongEmplacementDrift[m]'
        iwpspace  = ispquery( name )
        wpspace  = valuesp( iwpspace )

        call clearchar( 60, name )
        name = 'RNToDetermineCenterOfVolcanicDike[]'
```

```
        irnloc = ispquery( name )
cc end scr564;
...

cc rwj 4-22-05 scr564;
cc      Find event position in meters.
        rnloc  = valuesp( irnloc )
        eventposition = rnloc * totdriftlength
        cumdriftlength =  0.0d0
cc sum all drifts until event location is found.
        do idrift = 1, ndrifts
          driftlength = dsqrt(
     &                  (drxy1out(1,idrift)-drxy2out(1,idrift))**2 +
     &                  (drxy1out(2,idrift)-drxy2out(2,idrift))**2 )
          cumdriftlength =  cumdriftlength + driftlength
          if (cumdriftlength .ge. eventposition) go to 200
        end do

        print *, ' ***>>> Error in volcano <<<*** '
        print *, ' Event position not found.'
        print *, ' ndrifts = ', ndrifts
        print *, ' idrift = ', idrift
        print *, ' driftlength = ', driftlength
        print *, ' totdriftlength = ', totdriftlength
        print *, ' eventposition = ', eventposition
        print *, ' cumdriftlength = ', cumdriftlength
        STOP

  200   continue
        feventloc = (cumdriftlength - eventposition) / driftlength
        xlocm = drxy1out(1,idrift) +
     &          (drxy2out(1,idrift)-drxy1out(1,idrift)) * feventloc
        ylocm = drxy1out(2,idrift) +
     &          (drxy2out(2,idrift)-drxy1out(2,idrift)) * feventloc

cc      xlocm   = valuesp( ixloc )
cc      ylocm   = valuesp( iyloc )
CC End scr564

        alength = valuesp( ilength )
        angle   = valuesp( iangle )
c
c css 04/05/05; SCR 564: width of volcanic dike no longer used
cc        width   = valuesp( iwidth )
c end change:  SCR564
        diam    = valuesp( idiam )

        xyp1(1) = xlocm - 0.5d0 *alength * dsin(6.2832*angle/360.0d0)
        xyp1(2) = ylocm - 0.5d0 *alength * dcos(6.2832*angle/360.0d0)
        xyp2(1) = xlocm + 0.5d0 *alength * dsin(6.2832*angle/360.0d0)
        xyp2(2) = ylocm + 0.5d0 *alength * dcos(6.2832*angle/360.0d0)
        xyp(1)  = xlocm
        xyp(2)  = ylocm

        radius = diam / 2.0d0

        pi = 4.d0 * datan(1.d0)

cc rwj 4-22-05 scr564;

        eventsubarea  = ivaluesp( ieventsubarea )

cc      Check event subarea.
        if (eventsubarea .lt. 1 .or. eventsubarea .gt. nsa) then
```

```
          print *, ' ***>>> Error in volcano <<<*** '
          print *, ' eventsubarea .lt.1 .or. .gt. nsa'
          print *, ' eventsubarea = ', eventsubarea
          print *, ' nsa = ', nsa
          STOP
        endif
c
cc get aml as MTU per m2. (convert using acre/m2=2.47105e-4)
       amlperm2 = aml * 2.47105d-4
cc get area of conduit
       conduitarea = pi * diam**2 /4.d0
cc multiply aml*areaofcircle to get amtuejected.
       amtuejected = 0.0d0
       if (extrusive .eq. 1) amtuejected = amlperm2 * conduitarea
       amtuperwp  = valuesp( imtuperwp)
cc End of scr564


cc Loop to calculate failed fraction per subarea.
        do idoloop = 1, nsa
          i = idoloop
          amtufail(i) = 0
cc rwj 4-23-05;scr564
cc        call gsarea( i, area )
cc        call gsamtu( i, amtupersa )
          wpentrained = 0.0d0
          if (i .eq. eventsubarea) then
             wpentrained = amtuejected / amtuperwp
          end if
cc End of scr564


c rwj 8-22-04; SCR 490;
          call gsanwp(i, nwpinsa)
c
c css 4/20/05; SCR564:  dike width not needed; dike area no
c     longer used
cccc      Find dike area in subarea
cc          call qlhitsa( xyp1, xyp2, i, iflaglhit, alengthinsa )
cc          if (iflaglhit .eq. 1) then
cc              dikeareainsa = alengthinsa * width
cc          else
cc              dikeareainsa = 0.0d0
cc          endif
c end change:  SCR564

cc      If extrusive
c
c css 04/05/05; SCR564:  delete Extrusive parameters and replace
c     with extrusive event flag
cc          if( pext .le. fext ) then
c
cc       if (extrusive .eq. 1) then
c end change:  SCR564

cc        Get conduit area
cc          call qchitsa( xyp, radius, i, iflagchit, conduitarea )
c
c css 04/20/05; SCR564:  dike area and overlap no longer used
c     just need to calculate amtuejected
cc          if (iflagchit .eq. 1) then
cc             amtuejected = amtupersa * conduitarea / area
cc          end if
cc
```

```
cccc          Find overlap between conduit and dike
cccc          Test for conduit in subarea
cc              if( iflagchit .eq. 1 ) then
cc                amtuejected = amtupersa * conduitarea / area
cc
cccc            Test for conduit completely contained in dike.
cc                if (width .ge. diam) then
cc
cccc              Conduit is inside dike
cc                  overlaparea= pi*diam**2.d0/4.d0
cc                else
cc
cccc              Conduit exceeds dike width
cccc              Find portion (overlap) of dike inside conduit
cc                  overlaparea = pi*diam**2.d0/4.d0 -
cc     &            diam**2.d0/2.d0*dacos(width/diam) +
cc     &            width/2.d0*dsqrt(diam**2.d0 - width**2.d0)
cc                endif
cc              else
cc                conduitarea = 0.d0
cc                overlaparea = 0.d0
cc              endif
cc
cc        endif

cc
cc         dikeonlyarea = dikeareainsa - overlaparea
c end change:  SCR564

cc rwj 9-25-04; SCR490
          wpfailedinsa = 0.0d0

          do idrift = 1, ndrifts
            driftlength = dsqrt(
     &                    (drxy1out(1,idrift)-drxy2out(1,idrift))**2 +
     &                    (drxy1out(2,idrift)-drxy2out(2,idrift))**2 )

c           Find portion of drift in subarea.
            call qlhitsa(drxy1out(1,idrift), drxy2out(1,idrift),i,
     &                   lhitsa, driftlengthinsa)
            if (driftlengthinsa .gt. 0.0d0) then

c             Check for dike x drift intersection.
              call linehitline(drxy1out(1,idrift), drxy2out(1,idrift),
     &                         xyp1, xyp2, fin1, fin2)

c             Increment number of WP in failed in subarea if drift hits dike.
              if (fin1 .gt. 1.0d-8 .and. fin1 .le. 1.0d0) then
                wpfailedinsa = wpfailedinsa + nWPindrift(idrift) *
     &                         ( driftlengthinsa / driftlength )
              end if
            end if
          end do

cc rwj scr560; prevent wpfailedinsa from exceeding nwpinsa.
          wpfailedinsa = dnint(wpfailedinsa)

          amtufail(i) = wpfailedinsa * amtuperwp
c rwj 8-22-04; SCR 490
cc rwj 4-22-05 scr564
cc amtufailed = amtu released due to intrusive failures in drift
cc wpfailedinsa = intrusive failures in drift
cc wpentrained = wp ejected if event is in this subarea, else 0.
cc failedfraction = intrusive plus extrusive failed fraction for this subarea.
```

```
cc        failedfraction = wpfailedinsa / nwpinsa
          failedfraction = dmin1(wpfailedinsa+wpentrained,nwpinsa) /
     &                     nwpinsa

          if (failedfraction .gt. 1.0d0) then
             print *, ' ***>>> Error in volcano <<<*** '
             print *, ' failedfraction .gt. 1 '
             print *, ' failedfraction = ', failedfraction
             print *, ' conduitarea = ', conduitarea
             print *, ' area = ', area
             print *, ' wpfailedindrift = ', wpfailedindrift
             print *, ' nwpinsa = ', nwpinsa
             print *, ' subarea = ', i
             STOP
           endif
c rwj End of change for SCR 490

             tfail = timeofevent
             fracfailinitial = 0.0d0

cc         Pfail contains both intrusive and extrusive failures to remove
cc         them from consideration for other failures at a later time.
cc         Pfail removes the conduit faiures (which are transported
cc         to the surface) just before calling EBSREL in the executive,
cc         with the aid of the 'amtuejected' argument.

             call maptimeofevent( tfail, fracfailinitial, failedfraction,
     &                            ntim, tim, pfail(1,i) )

         enddo

       else if (volmodel .eq. 2) then

         eventsubarea  = ivaluesp( ieventsubarea )

cc       Check event subarea.
         if (eventsubarea .lt. 1 .or. eventsubarea .gt. nsa) then
            print *, ' ***>>> Error in volcano <<<*** '
            print *, ' eventsubarea .lt.1 .or. .gt. nsa'
            print *, ' eventsubarea = ', eventsubarea
            print *, ' nsa = ', nsa
            STOP
         endif
c
c css 04/05/05; SCR564:  remove Extrusive parameters and replace
c     with extrusive event flag
cc         if( pext .le. fext ) then
         if (extrusive .eq. 1) then
c end change:  SCR564
             lExtrusive = .TRUE.
         else
             lExtrusive = .FALSE.
         end if

         if ( lExtrusive ) then
           wpentrained  = valuesp( iwpentrained )
         else
           wpentrained  = 0.0d0
         end if
```

ATTACHMENT C - Test Plan, PC Platform

Test Plan Name: SCR564 Test Plan, PC

Tested By: David Stead Date: 4/4/2006
TPA Baseline Version: 5.0.0t
TPA Test Version: 5.0.0u

Platform: PC
Host Machines: TPA
Host OS's: Windows Server 2003
Archive of Results: on CD entitled 'SCR564 Test Data'

Path for runs of version 5.0.0t:
`D:\DStead\SCR_564\Runs\Run_500t`
`D:\DStead\SCR_564\Runs\Run_500t`

Environment variables for runs of version 5.0.0t:
`TPA_TEST D:\DStead\TPA_code\TPA_500t`
`TPA_DATA D:\DStead\TPA_code\TPA_500t`

Path for runs of version 5.0.0u (unless otherwise specified):
`D:\DStead\SCR_564\Runs\Run_500u`
`D:\DStead\SCR_564\Runs\Run_500u`

Environment variables for runs of version 5.0.0u:
`TPA_TEST D:\DStead\TPA_code\TPA_500u`
`TPA_DATA D:\DStead\TPA_code\TPA_500u`

Utility codes used to aid in the analysis of the test data: Microsoft Excel 97
Grep32

Notes: References to the `tpa.out` file mean the screen print output, redirected to that file name.

Process Level (PL) Tests

PL-1

Test Objective: Show that intrusive events are absent from some realizations with version 5.0.0t, and that all realizations have an intrusive event with version 5.0.0u.

Test Procedure: Duplicate the base case run (400 realizations, version 5.0.0t) where intrusive events are absent from some realizations. Then run a test case (400 realizations, version 5.0.0u) showing that all realizations have an intrusive event (this is with the new ExtrusiveEventFlag set to 0).

Test Results: In the version 5.0.0t run, realizations 24, 233, and 386 did not report an intrusive event. In the version 5.0.0u run, all realizations reported an intrusive event, except for realizations 264 and 313. Upon examination of *tpa.out*, it was found that the reason for this is that all waste packages had failed in either INITIAL or CORROSION events, so they could not be counted as failed again in a VOLCANIC event.

Paths for Archive of Results:
from_TPA\TPA500t_BaseCase400re_Volc=1
from_TPA\TPA500u_TestCase400re_Volc=1_ExtEvFlag=0

Test Status: **PASSED**

PL-2

Test Objective: Show that with the ExtrusiveEventFlag set to 1, both an extrusive and intrusive event is produced for each realization.

Test Procedure: Run a test case (400 realizations, version 5.0.0u) and analyze results to show that the new ExtrusiveEventFlag, set to 1, produces both an extrusive event and an intrusive event for each realization. (Flag added in 5.0.0u)

Test Results: The test showed that all realizations reported extrusive events, and all realizations except 264 and 313 produced intrusive events. Upon examination of *tpa.out*, it was found that the reason for this is that all waste packages in all subareas had failed in either INITIAL or CORROSION events for these realizations, so they could not be counted as failed again in a VOLCANIC event.

Path for Archive of Results:
from_TPA\TPA500u_TestCase400re_Volc=1_ExtEvFlag=1

Test Status: **PASSED**

PL-3

Test Objective: From the base case run in PL-1, show that extrusive events are always in subarea 2; and from the test case in PL-2, show that all subareas have an extrusive event.

Test Procedure: Using GREP, capture all lines in *tpa.out* from each run that have the words 'realization' or 'ejected' in them, and save the combined results in a text file. Then open the text file in Excel (using the space character as a delimiter, and eliminating column 1) and sort them by the line number column from *tpa.out*. Save the results as an Excel file, and examine the results for the presence of 'ejected' in each realization to determine if extrusive events occurred and in which subarea, as specified in 'Test Objective' above.

Test Results: The base case run in PL-1 shows that extrusive events are always in subarea 2; and the test case in PL-2 shows that all subareas have an extrusive event, as specified. Test shows that every

realization has an extrusive event from one subarea, and every subarea has appeared at least once.

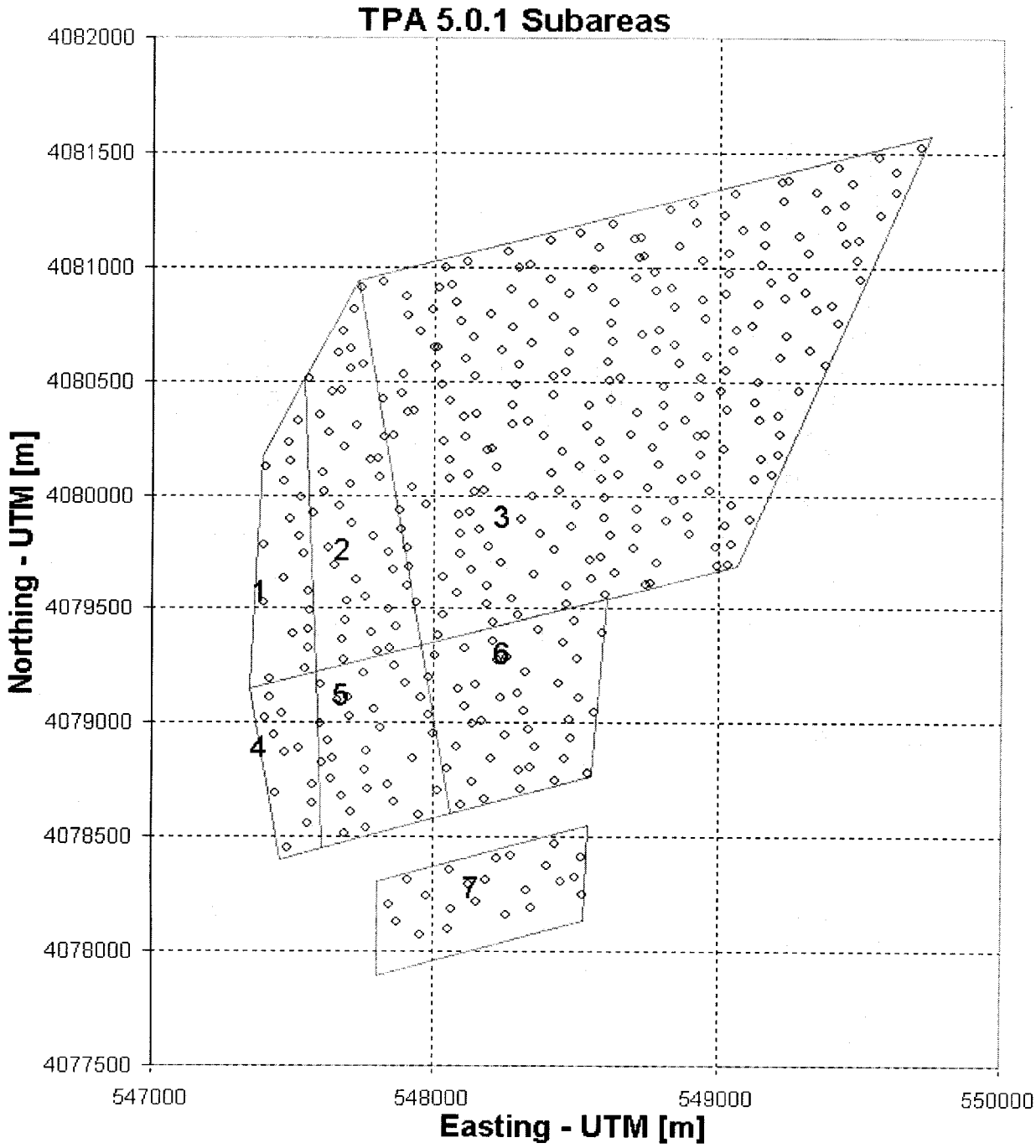
Paths for Archive of Results:
from_TPA\TPA500t_BaseCase400re_Volc=1
from_TPA\TPA500u_TestCase400re_Volc=1_ExtEvFlag=1

Test Status: **PASSED**

PL-4

Test Objective: From the test case in PL-2, show that the dike center is uniformly sampled by plotting the centers on the repository layout diagram.

Test Results: The dike centers were plotted in Excel with the repository subarea diagram, as shown below. They appear to be uniformly sampled.



Path for Archive of Results:
from_TPA\TPA500u_TestCase400re_Volc=1_ExtEvFlag=1_PrtSt-Dike&Ext

Test Status: **PASSED**

ATTACHMENT D - Test Plan, Unix Platform

Test Plan Name: SCR564 Test Plan, PC

Tested By: David Stead Date: 4/4/2006
TPA Baseline Version: 5.0.0t
TPA Test Version: 5.0.0u

Platform: PC
Host Machines: Spock, Texas
Host OS's: Sun OS
Archive of Results: on CD entitled 'SCR564 Test Data'

Path for runs of version 5.0.0t:
`/home/dstead/run_500t`

Environment variables for runs of version 5.0.0t:
```
TPA_TEST    /home/dstead/tpa_500t
TPA_DATA    /home/dstead/tpa_500t
```

Path for runs of version 5.0.0u (unless otherwise specified):
```
/home/dstead/run_500u
/data/dstead/run_500u
```

Environment variables for runs of version 5.0.0u:
```
TPA_TEST    /home/dstead/tpa_500u
TPA_DATA    /home/dstead/tpa_500u
```

Utility codes used to aid in the analysis of the test data: Microsoft Excel 97
Grep32

Notes: References to the *tpa.out* file mean the screen print output, redirected to that file name.

Process Level (PL) Tests

PL-1
Test Objective: Show that intrusive events are absent from some realizations with version 5.0.0t, and that all realizations have an intrusive event with version 5.0.0u.

Test Procedure: Duplicate the base case run (400 realizations, version 5.0.0t) where intrusive events are absent from some realizations. Then run a test case (400 realizations, version 5.0.0u) showing that all realizations have an intrusive event (this is with the new ExtrusiveEventFlag set to 0).

Test Results: In the version 5.0.0t run, realizations 24, 233, and 386 did not report an intrusive event. In the version 5.0.0u run, all realizations reported an intrusive event, except for realizations 264 and 313. Upon examination of *tpa.out*, it was found that the reason for this is that all waste packages had failed in either INITIAL or CORROSION events, so they could not be counted as failed again in a VOLCANIC event.

Paths for Archive of Results:
from_Spock_or_Texas\TPA500t_BaseCase400re_Volc=1
from_Spock_or_Texas\TPA500u_TestCase400re_Volc=1_ExtEvFlag=0

Test Status: **PASSED**

PL-2
Test Objective: Show that with the ExtrusiveEventFlag set to 1, both an extrusive and intrusive event is produced for each realization.

Test Procedure: Run a test case (400 realizations, version 5.0.0u) and analyze results to show that the new ExtrusiveEventFlag, set to 1, produces both an extrusive event and an intrusive event for each realization. (Flag added in 5.0.0u)

Test Results: The test showed that all realizations reported extrusive events, and all realizations except 264 and 313 produced intrusive events. Upon examination of *tpa.out*, it was found that the reason for this is that all waste packages in all subareas had failed in either INITIAL or CORROSION events for these realizations, so they could not be counted as failed again in a VOLCANIC event.

Path for Archive of Results:
from_Spock_or_Texas\TPA500u_TestCase400re_Volc=1_ExtEvFlag=1

Test Status: **PASSED**

PL-3
Test Objective: From the base case run in PL-1, show that extrusive events are always in subarea 2; and from the test case in PL-2, show that all subareas have an extrusive event.

Test Procedure: Using GREP, capture all lines in *tpa.out* from each run that have the words 'realization' or 'ejected' in them, and save the combined results in a text file. Then open the text file in Excel (using the space character as a delimiter, and eliminating column 1) and sort them by the line number column from *tpa.out*. Save the results as an Excel file, and examine the results for the presence of 'ejected' in each realization to determine if extrusive events occurred and in which subarea, as specified in 'Test Objective' above.

Test Results: The base case run in PL-1 shows that extrusive events are always in subarea 2; and the test case in PL-2 shows that all subareas have an extrusive event, as specified. Test shows that every

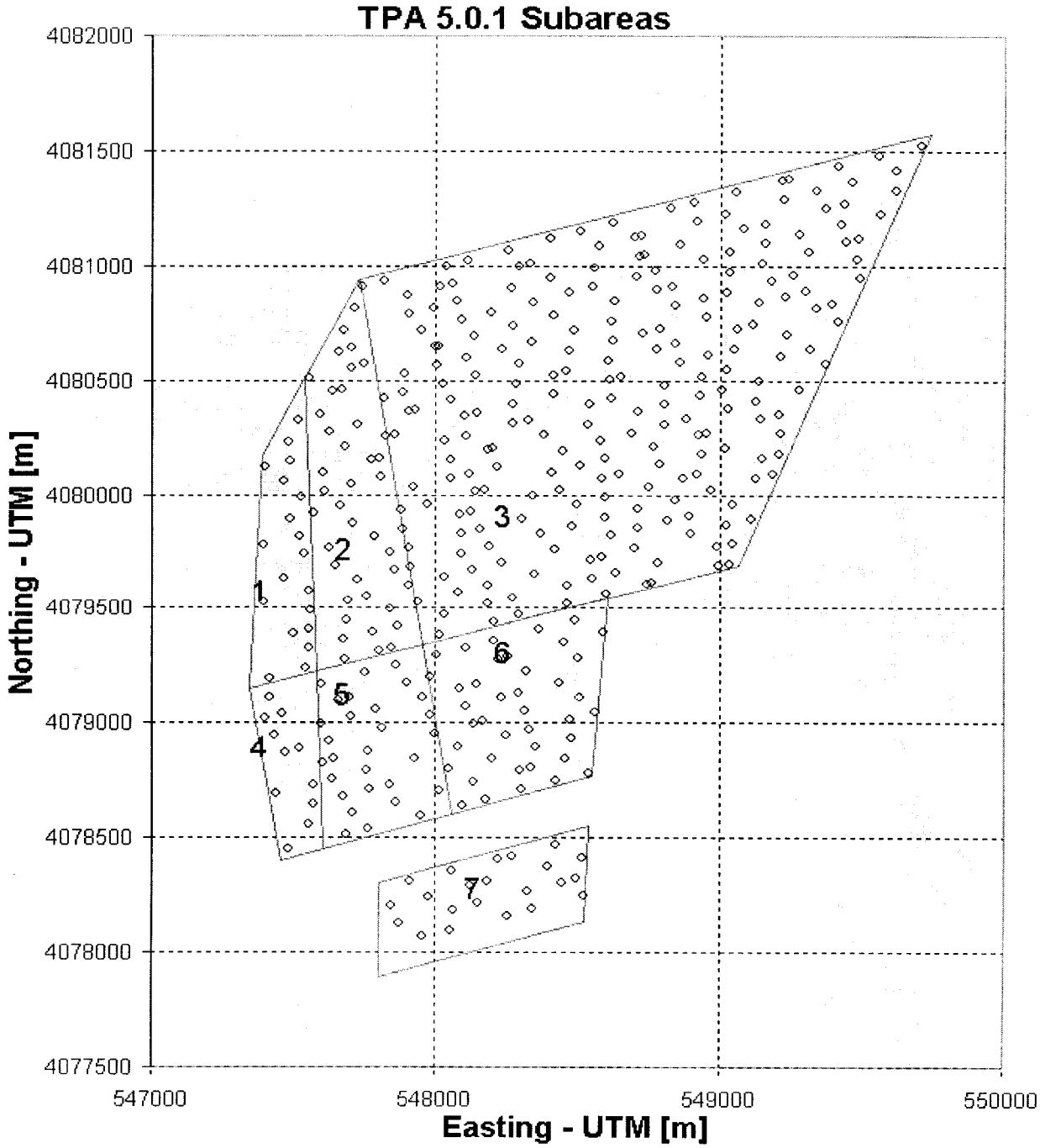
realization has an extrusive event from one subarea, and every subarea has appeared at least once.

Paths for Archive of Results:
from_Spock_or_Texas\TPA500t_BaseCase400re_Volc=1
from_Spock_or_Texas\TPA500u_TestCase400re_Volc=1_ExtEvFlag=1

Test Status: **PASSED**

PL-4
Test Objective: From the test case in PL-2, show that the dike center is uniformly sampled by plotting the centers on the repository layout diagram.

Test Results: The dike centers were plotted in Excel with the repository subarea diagram, as shown below. They appear to be uniformly sampled.



Path for Archive of Results:
from_Spock_or_Texas\TPA500u_TestCase400re_Volc=1_ExtEvFlag=1_PrtSt-Dike&Ext

Test Status: **PASSED**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-570	**2. Software Title and Version:** TPA 5.0.0u	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *exec.f, reader.f, subarea.f, invent.f, sampler.f, driftsa.i, tpa.inp*

A situation occurs in which a subarea that is larger than an emplacement block (i.e., the drift endpoints in *drifts.dat* are inside the subarea) results in the TPA code extending those drifts to intersect the subarea boundaries and thus potentially assign more WPs to the subarea for that particular drift than the number of WPs in the drift as provided in the *drifts.dat* file.
Added print to screen for average linear thermal load of drift.
Miscellaneous cosmetic changes for *invent.f, sampler.f* and *exec.f.*

5. Change Requested by: R. Rice Date: 4-18-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 4-18-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See Attachment A.

8. Implemented by: R. Rice	**Date:** 3-8-05

9. Description of Acceptance Tests:

See Attachment B.

Tests should include volcano dike interaction with drifts.

10. Tested by: J. Menchaca	**Date:** 06-21-05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its funciton in TPA code (calculated from ..., used for calculating..., used to relate... etc)	Distribution	Range	Justificaiton 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source (Initials)

Modify from	Subarea Size		TPA subarea vertices		Subarea 1 (Top Left) 547390., 4080177. 547535., 4080512. 547582., 4079221. 547346., 4079145. 547390., 4080177. Subarea 2 547535., 4080512. 547729., 4080943. 547955., 4079338. 547582., 4079221. 547535., 4080512. Subarea 3 547729., 4080943. 549744., 4081576. 549068., 4079690. 547955., 4079338. 547729., 4080943. Subarea 4 547346., 4079145. 547582., 4079221. 547606., 4078451. 547456., 4078400. 547346., 4079145. Subarea 5 547582., 4079221. 547955., 4079338. 548056., 4078603. 547606., 4078451. 547582., 4079221. Subarea 6 547955., 4079338. 548606., 4079545. 548553., 4078770. 548056., 4078603. 547955., 4079338. Subarea 7 547803., 4078308. 548542., 4078549. 548523., 4078132. 547802., 4077893. 547803., 4078308.	Edges of the subareas were moved outward 2 meters from the edge of their corresponding emplacement block in cases where the edges were nearly co-linear to reduce round off error when calculating the Total Buried Waste	RWJ

Modify to	Subarea Size		TPA subarea vertices		Subarea 1 (Top Left) 547388., 4080177. 547535., 4080514. 547582., 4079221. 547344., 4079145. 547388., 4080177. Subarea 2 547535., 4080514. 547729., 4080945. 547955., 4079338. 547582., 4079221. 547535., 4080512. Subarea 3 547729., 4080945. 549746., 4081578. 549068., 4079692. 547955., 4079338. 547729., 4080945. Subarea 4 547344., 4079145. 547582., 4079221. 547606., 4078449. 547454., 4078398. 547344., 4079145. Subarea 5 547582., 4079221. 547955., 4079338. 548058., 4078605. 547606., 4078453. 547582., 4079221. Subarea 6 547955., 4079338. 548608., 4079543. 548555., 4078768. 548058., 4078601. 547955., 4079338. Subarea 7 547801., 4078310. 548544., 4078551. 548525., 4078130. 547800., 4077891. 547801., 4078306.	Edges of the subareas were moved outward 2 meters from the edge of their corresponding emplacement block in cases where the edges were nearly co-linear to reduce round off error when calculating the Total Buried Waste	RWJ

Attachment A

For *subarea.f*:

Comparing files subarea.f.original and SUBAREA.F.MODIFIED

***** subarea.f.original

```
      if( dabs(quadarea - (a1 + a2 + a3 + a4)) .gt. 0.0001d0 * quadarea)
     &  then
        iflag = 0
```

***** SUBAREA.F.MODIFIED

```
cc rwr 4-19-05 SCR570 - decrease the tolerance so that points
cc                      just outside of a subarea do not get identified
cc                      as inside of the subarea (this can happen when points
cc                      are very close, but outside of the subarea and then
cc                      the qlhitsa subroutine gives incorrect results)
cc      if( dabs(quadarea - (a1 + a2 + a3 + a4)) .gt. 0.0001d0 * quadarea)
cc     &   then
      if(dabs(quadarea-(a1+a2+a3+a4)) .gt. 0.00000001d0*quadarea) then
        iflag = 0
*****
```

For *reader.f*:

The logic for increased accuracy was removed from **fillsubareas**() since it does not apply when multiple east-west emplacement blocks are used.

For *tpa.inp*`:

The edges of the subareas were moved outward about 2 meters from the edge of their corresponding emplacement block in the case where the edges were nearly co-linear. This reduced the round off error when calculating the Total Buried Waste as shoen on the screen print.

Attachment B
Test Plan for TPA SCR#570

Test Plan Name:

Tested By: Jose M. Menchaca

Date: June 01, 2005

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.00u

Test Version: TPA 5.00v

Process Level (PL) Tests

PL-1. Name:
Path for run directory: ~jmench/tpa500v/SCR570/
Path for archive of results: ~jmench/tpa500v/SCR570/
Environment variables: setenv TPA_TEST ~/tpa500v
setenv TPA_DATA ~/tpa500v
Special input files or modifications to input files required :

Pertinent Lines in the tpa.inp file: Changed the vertices for Subareas 2 and 3 as shown

Current Values:

```
Subarea 2
547535., 4080514.
547729., 4080945.
547955., 4079338.
547582., 4079221.
547535., 4080512.
Subarea 3
547729., 4080945.
549746., 4081578.
549068., 4079692.
547955., 4079338.
547729., 4080945.
```

New Values:

```
Subarea 2
547535., 4080514.
547729., 4080943.
547955., 4079338.
547582., 4079221.
547535., 4080512.
Subarea 3
547729., 4080943.
549746., 4081578.
549068., 4079692.
547955., 4079338.
547729., 4080945.
```

Special diagnostic code modifications required :modified fortran files as needed for verification purposes.

Program modes to be used (append flags, scenario/model switches, etc.): Default values

Utility scripts needed to perform the test:

Utility codes needed in the analysis of the test data: Microsoft Excel®

Test Description:

Item 1. TPA code assigning more waste packages to the subarea for subareas larger than the emplacement block.

Execute a TPA 5.0.0u version run with a single large subarea that exceeds the emplacement drift area. Verify that the number of waste packages listed in the REPOSITORY DESIGN INFORMATION section of the screen output exceeds the 8877 waste packages needed to hold 70,040 MTU.

```
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]       [MTU]
   1  18000000.0   129687.9        16437
```

Execute a TPA 5.0.0v version run with a single large subarea that exceeds the emplacement drift area. Verify that the number of waste packages listed in the REPOSITORY DESIGN INFORMATION section of the screen output does not exceed the 8877 waste packages needed to hold 70,040 MTU.

```
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]       [MTU]
   1  18000000.0    70039.5         8877
```

PASS

Volcanic Dike Interaction with Drifts

With the VolcanismDisruptiveScenarioFlag on, volcanic dikes with various locations, lengths and angles will occur in each realization. If a dike intersects a drift, all the waste packages in the drift will fail and be listed in wpsfail.res file in the #igact (igneous activity) column.

To test that only the drifts that are intersected by a dike have failed waste packages, a run with intentionally short dikes (1000 meters or less) was created and the number of waste packages observed.

The number of failed waste packages from volcanic dikes far exceeded the number of waste packages intersected by the volcanic dike.

This problem is addressed in SCR 585.

FAILED

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-571	**2. Software Title and Version:** TPA 5.0.0w	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *failt.f, releaset.f, exec.f*

1) FAILT occasionally produces the following convergence warning message during a run when the time step size is below a certain value.
`"corrosion potential not converging in 10 iterations."`

2) For writing the *relcum.out* file in *releaset.f*, change the header of the third column, named "`Fail Time`", in the first section to "`Start of SF Wet[yr]`". Also remove the last column from the radionuclide section of the *relcum.out* file with the header of "`Fraction Left`".

5. Change Requested by: R. Rice Date: 5-4-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 5-4-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See communication from D. LeNeveu in Attachment A and the difference file in Attachment B for item 1).

The module *releaset.f* was changed as described in item 2).

8. Implemented by: D. Leneveu / R. Janetzke	**Date:** 5-5-05 5-13-05

9. Description of Acceptance Tests: See Attachment C.

10. Tested by: R. Rice	**Date:** 5/31/05 5/31/05

CNWRA Form TOP-5 (05/2000)

SCR571 UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)

Attachment A

I hard coded a value of 1.e-15 for the relative error.

The fix I made does not change the answer it just allows the convergence loop to be terminated properly instead of going on until the maximum of 10 iterations and putting out a warning message.

Look at these lines of code as is:

```
if ( abs(zc).le.1.0e-8 ) go to 150
        eec = eec - zc/dzc
```

This code only works if the value of zc/dzc is much smaller than eec. If the value of eec is for instance 1.e-8 and dzc is around 1.0 and zc is 1.0e-9, the code will terminate the convergence prematurely. In other words the code author chose 1.0e-8 probably because there are 8 significant figures in single precision. This loop should converge when Abs(zc) -> 0 or when zc/dzc is a very small fraction of eec not when abs(zc) is .le. to 1.e-8. So the code author has made a fundamental error here that can cause the loop to be aborted early when eec is very small. Fortunately eec and dzc appear to be larger that 1.0 but if this cannot be guaranteed the code has a real error here that can affect the values.

I added one more fix to get rid of this potential problem with `abs(zc).le.1.0e-8`

This line is now [modified to]:

```
if ( abs(zc) .le. abs(10.D0*relercpass*eec*dzc) ) go to 150
```

This will now work when the increment being added is a very small fraction of ecc no matter the value of eec.

Attachment B

```
***************
*** 1430,1439 ****
      real*8  failtimOL
      common /failuretime /failtimOL

- C*****Code added by D. LeNeveu May 5,2005
-       real*8 relercpass
- C*****End of code added by D.LeNeveu
-
  c-----------------------------------------------------------------
  c       ecrit:  critical potential for localized corrosion (volts she)
  c       refph:  reference ph
--- 1384,1389 ----
***************
*** 1507,1513 ****
  c       dense1, dense2:  inner and outer density [kg/m^3]
  c       wtmol1, wtmol2:  equivalent molecular weight [kg/mol]
  c       failtimOL: time at which the outer layer fails [yr].  Added:
1/17/2000
- c       relercpass: exponent to the base ten of the relative error in cpass
  c-----------------------------------------------------------------

      cfarad = 96485.
--- 1457,1462 ----
***************
*** 1666,1677 ****

  c       ensure that the summation of all currents equal to zero,
  c       newton-raphson method is used as an additional step
! c
! C*****Code added by D. LeNeveu May 5,2005
! c     Set relative precison to one part in ten to the fifteen for ieee
standards
! c     for double precision
!       relercpass=1.D-15
! C*****End of code added by D.LeNeveu
      do 100 i = 1, 10
        yko2 = rkhy * exp(ghy * yyy1)
        curhy = -yko2 * exp( - xxx1 * eec)
--- 1615,1621 ----

  c   ensure that the summation of all currents equal to zero,
  c   newton-raphson method is used as an additional step
!
          do 100 i = 1, 10
            yko2 = rkhy * exp(ghy * yyy1)
            curhy = -yko2 * exp( - xxx1 * eec)
***************
*** 1683,1704 ****
        curox = max(curmax, curox)
        cathod = -(curox + curhy)
        zc = cpass - cathod
- C*****Code added by D. LeNeveu May 5,2005
- c       if zc is of the order of the fractional precision in cpass
- c       then zc cannot get any smaller and is determined by floating point
- c       truncation error
```

```
-         if (abs(zc) .lt. 10.0D0*relercpass*cpass) then
-          zc=0.0d0
-         end if
- C*****End of code added by D. LeNeveu
        dzc = -xxx1 * curhy - xxx3 * curox /
       &          (1 + xxx2 * exp(-xxx3 * eec))
! c     if ( abs(zc).le.1.0e-8 ) go to 150
! C*****Code added by D. LeNeveu May 5,2005
!       if ( abs(zc) .le. abs(10.D0*relercpass*eec*dzc) ) go to 150
! C*****End of code added by D. LeNeveu
         eec = eec - zc/dzc
-
    100     continue

      write (*, *) 'corrosion potential not converging in 10 ',
--- 1627,1636 ----
            curox = max(curmax, curox)
            cathod = -(curox + curhy)
            zc = cpass - cathod
            dzc = -xxx1 * curhy - xxx3 * curox /
       &          (1 + xxx2 * exp(-xxx3 * eec))
!           if ( abs(zc).le.1.0e-8 ) go to 150
              eec = eec - zc/dzc
    100     continue

         write (*, *) 'corrosion potential not converging in 10 ',
***************
```

Attachment C

Test Plan for TPA SCR#571

Test Plan Name: FAILT modifications to output file *failt.out* (screenprint) regarding convergence and RELEASET modifications to *relcum.out* regarding headers/results

Tested By: R. Rice **Date:** May 31, 2005

Host Machine: TPA PC at CNWRA **Host OS:** XP Professional

Baseline Version: 5.0.0w **Test Version:** 5.0.0x

System Level (SL) Tests

SL-1. Name: Test 0 - Basecase

Path for run directory: d:\rrice\tpa500w\test_0_basecase and d:\rrice\tpa500x\test_0_basecase

Path for archive of results: \SCR571\tpa500w\test_0_basecase and \SCR571\tpa500x\test_0_basecase (archived on CD "SCR571 Testing")

Environment variables:

TPA_DATA=d:\rrice\tpa500w\
TPA_TEST=d:\rrice\tpa500w\

and

TPA_TEST=d:\rrice\tpa500x\
TPA_TEST=d:\rrice\tpa500x\

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Using the basecase TPA code for Versions 5.0.0w and 5.0.0x, compare TPA code output to check the impact of modifications made to the FAILT and RELEASET source code to remove statements regarding convergence in the FAILT screenprint (*failt.out*) and the RELEASET output file *relcum.out*.

- Objective: Verify FAILT modifications have no impact on failure

times, releases, and doses using the basecase TPA code. Also, verify changes were made in the header and last column of results in RELEASET output file *relcum.out.*

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *failt.out;* screenprint (i.e., *tpa.out*); *totdose.res*; *rgwnr.tpa; relcum.out*

- Step by step test procedure to be used:

Execute the TPA Versions 5.0.0w and 5.0.0x code using the basecase *tpa.inp* file. Then, perform the following:

1. Compare the *failt.out* files from these two runs
2. Compare the *tpa.out* files from these two runs
3. Compare the *totdose.res* files from these two runs
4. Compare the *rgwnr.tpa* files from these two runs
5. Compare the *relcum.out* files from these two runs

- Pass/Fail criteria:

Criteria 1: For #1 above, any statements in the *relcum.out* file about not converging in the TPA Version 5.0.0w code should not be present in the TPA Version 5.0.0x code; also, the files will show a different time/date of the run

Criteria 2: For #2, #3, and #4 above, the files should be identical except for the time/date of the run

Criteria 3: For #5 above, the file header in *relcum.out* should be changed from "Fail Time[yr]" to "Start SF Wet[yr]"; also, the last column with "Fraction Left" should be removed

Test Results: The *failt.out* files in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\failt.out and
D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\FAILT.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\failt.out
version= 1.0
Tue May 31 10:38:01 2005
nhist3= 201
***** D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\FAILT.OUT
version= 1.0
Tue May 31 10:39:19 2005
nhist3= 201
*****
```

The screenprints (*tpa.out* files) in the run subdirectories for this test are included on the

CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\tpa.out and
D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\TPA.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\tpa.out
      exec: Welcome to TPA Version 5.0.0w
    Job started: Tue May 31 10:37:47 2005
=====================================================================
***** D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\TPA.OUT
      exec: Welcome to TPA Version 5.0.0w
    Job started: Tue May 31 10:39:05 2005
=====================================================================
*****
```

The *totdose.res* files in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\totdose.res and
D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\TOTDOSE.RES
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\totdose.res
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 10:37:47 2005
 Total Dose for All Pathways, All Nuclides, and All Times

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\TOTDOSE.RES
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 10:39:05 2005
 Total Dose for All Pathways, All Nuclides, and All Times

*****
```

The *rgwnr.tpa* files in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\rgwnr.tpa and
D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\RGWNR.TPA
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\rgwnr.tpa
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 10:37:47 2005
 AEDE[rem/yr], GroundWater Pathway  for each nuclide, for each realization

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\RGWNR.TPA
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 10:39:05 2005
 AEDE[rem/yr], GroundWater Pathway  for each nuclide, for each realization

*****
```

The *relcum.out* files (note that these are from the last subarea, Subarea 7, analyzed) in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\relcum.out and D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\RELCUM.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_0_BASECASE\relcum.out

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	4	9.2294E+02	4.3389E+02	9.4686E+02	1.3808E+03
2	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
3	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
4	0	9.9639E+02	0.0000E+00	0.0000E+00	0.0000E+00
5	0	3.4659E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00
8	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00

Radionuclide	Halflife[yr]	xnoloss[ci]	amwp[ci]	xmass[ci]
CM246	4.7310E+03	7.7060E-01	1.5791E-06	2.9116E-04
U238	4.4680E+09	5.4019E+00	5.3436E-05	1.9987E-03
CM245	8.4990E+03	4.3196E+00	8.8518E-06	1.6321E-03
AM241	4.3220E+02	4.5577E+00	9.3397E-06	1.7220E-03
NP237	2.1400E+06	1.9107E+01	3.9153E-05	7.2191E-03
U233	1.5850E+05	7.8742E-01	6.5904E-06	2.9254E-04
TH229	7.3390E+03	2.7226E-01	6.1934E-07	1.0281E-04
AM243	7.3800E+03	2.0424E+02	4.1854E-04	7.7170E-02
PU239	2.4060E+04	4.2193E+03	8.6462E-03	1.5942E+00
PU240	6.5370E+03	3.3310E+03	6.8259E-03	1.2586E+00
U234	2.4450E+05	2.2455E+01	2.2213E-04	8.3082E-03
TH230	7.7000E+04	1.9674E+00	4.2493E-06	7.4313E-04
RA226	1.6000E+03	1.5359E+00	3.1588E-06	5.8029E-04
PB210	2.2300E+01	1.5299E+00	3.1442E-06	5.7802E-04
CS135	2.3000E+06	1.4002E+01	2.7935E-05	3.7466E-01
I129	1.5700E+07	6.3108E-01	1.1765E-06	5.7165E-02
TC99	2.1300E+05	2.5516E+02	5.2190E-04	5.7031E-01
NI59	8.0000E+04	6.7447E+01	1.3821E-04	2.5484E-02
C14	5.7290E+03	3.6883E+00	6.8022E-06	3.7008E-01
SE79	1.1000E+06	1.7465E+00	3.4889E-06	4.4550E-02
NB94	2.0300E+04	1.6888E+01	3.4607E-05	6.3808E-03
CL36	3.0100E+05	2.7352E-01	5.1127E-07	2.4115E-02

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_0_BASECASE\RELCUM.OUT

Type#	Failed	Fail Time[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	4	9.2294E+02	4.3389E+02	9.4686E+02	1.3808E+03
2	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
3	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
4	0	9.9639E+02	0.0000E+00	0.0000E+00	0.0000E+00
5	0	3.4659E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00
8	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00

Radionuclide	Halflife[yr]	xnoloss[ci]	amwp[ci]	xmass[ci]	Fraction Left
CM246	4.7310E+03	7.7060E-01	1.5791E-06	2.9116E-04	9.9962E-01
U238	4.4680E+09	5.4019E+00	5.3436E-05	1.9987E-03	9.9963E-01
CM245	8.4990E+03	4.3196E+00	8.8518E-06	1.6321E-03	9.9962E-01
AM241	4.3220E+02	4.5577E+00	9.3397E-06	1.7220E-03	9.9962E-01
NP237	2.1400E+06	1.9107E+01	3.9153E-05	7.2191E-03	9.9962E-01

U233	1.5850E+05	7.8742E-01	6.5904E-06	2.9254E-04	9.9963E-01
TH229	7.3390E+03	2.7226E-01	6.1934E-07	1.0281E-04	9.9962E-01
AM243	7.3800E+03	2.0424E+02	4.1854E-04	7.7170E-02	9.9962E-01
PU239	2.4060E+04	4.2193E+03	8.6462E-03	1.5942E+00	9.9962E-01
PU240	6.5370E+03	3.3310E+03	6.8259E-03	1.2586E+00	9.9962E-01
U234	2.4450E+05	2.2455E+01	2.2213E-04	8.3082E-03	9.9963E-01
TH230	7.7000E+04	1.9674E+00	4.2493E-06	7.4313E-04	9.9962E-01
RA226	1.6000E+03	1.5359E+00	3.1588E-06	5.8029E-04	9.9962E-01
PB210	2.2300E+01	1.5299E+00	3.1442E-06	5.7802E-04	9.9962E-01
CS135	2.3000E+06	1.4002E+01	2.7935E-05	3.7466E-01	9.7324E-01
I129	1.5700E+07	6.3108E-01	1.1765E-06	5.7165E-02	9.0942E-01
TC99	2.1300E+05	2.5516E+02	5.2190E-04	5.7031E-01	9.9776E-01
NI59	8.0000E+04	6.7447E+01	1.3821E-04	2.5484E-02	9.9962E-01
C14	5.7290E+03	3.6883E+00	6.8022E-06	3.7008E-01	8.9966E-01
SE79	1.1000E+06	1.7465E+00	3.4889E-06	4.4550E-02	9.7449E-01
NB94	2.0300E+04	1.6888E+01	3.4607E-05	6.3808E-03	9.9962E-01
CL36	3.0100E+05	2.7352E-01	5.1127E-07	2.4115E-02	9.1184E-01

*****

- Overall test status: <u>PASS</u>

SL-2. Name: Test 1 - Long Simulation with Outer Overpack Thickness 0.002 m

Path for run directory: d:\rrice\tpa500w\test_1 and d:\rrice\tpa500x\test_1

Path for archive of results: \SCR571\tpa500w\test_1 and
\SCR571\tpa500x\\test_1 (archived on CD "SCR571 Testing")

Environment variables: TPA_DATA=d:\rrice\tpa500w\
TPA_TEST=d:\rrice\tpa500w\

and

TPA_TEST=d:\rrice\tpa500x\
TPA_TEST=d:\rrice\tpa500x\

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Using the basecase TPA code for Versions 5.0.0w and 5.0.0x, but modifying the *tpa.inp* file as follows (i) maximum time of 1,000,000 yr; (ii) 4,800 time steps after the Compliance Period; (iii) 100 realizations, however executing only 1 realization and analyzing Subarea 1 only (i.e., Start and Stop at Subarea 1 and Start and Stop at realization 1); and (iv) Outer Overpack WP thickness equal to 0.002 m, compare TPA code output to check the impact of modifications made to the FAILT and RELEASET source code to remove statements regarding convergence in the FAILT screenprint (*failt.out*) and the RELEASET output file *relcum.out*.

- **Objective:** Verify FAILT modifications have no impact on failure times, releases, and doses using the basecase TPA code. Also, verify changes were made in the header and last column of results in RELEASET output file *relcum.out*.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** *failt.out;* screenprint (i.e., *tpa.out*); *totdose.res*; *rgwnr.tpa; relcum.out*

- **Step by step test procedure to be used:**

Execute the TPA Versions 5.0.0w and 5.0.0x code using the basecase *tpa.inp* file. Then, perform the following:

1. Compare the *failt.out* files from these two runs
2. Compare the *tpa.out* files from these two runs
3. Compare the *totdose.res* files from these two runs
4. Compare the *rgwnr.tpa* files from these two runs
5. Compare the *relcum.out* files from these two runs

- Pass/Fail criteria:

Criteria 1: For #1 above, any statements in the *relcum.out* file about not converging in the TPA Version 5.0.0w code should not be present in the TPA Version 5.0.0x code; also, the files will show a different time/date of the run

Criteria 2: For #2, #3, and #4 above, the files should be identical except for the time/date of the run

Criteria 3: For #5 above, the file header in *relcum.out* should be changed from "Fail Time[yr]" to "Start SF Wet[yr]"; also, the last column with "Fraction Left" should be removed

Test Results: The *failt.out* files in the run subdirectories for this test are included on the CD attached to this test plan. (Note that the WP failure time is 16,393.75 yr with this decreased Outer Overpack thickness.) The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_1\failt.out and
D:\SCR571_TPA_RUNS\TPA500W\TEST_1\FAILT.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_1\failt.out
version= 1.0
Tue May 31 13:42:19 2005
nhist3= 5001
***** D:\SCR571_TPA_RUNS\TPA500W\TEST_1\FAILT.OUT
version= 1.0
Tue May 31 13:45:28 2005
nhist3= 5001
*****

***** D:\SCR571_TPA_RUNS\TPA500X\TEST_1\failt.out
1   16393.75    43.35    2.0878   -0.1181    1   5.0005134E-02  general
failt: Inner overpack LC initiated at 16393.75000000000  years
2   16600.00    43.12  -10.0108   -3.8698    1  -2.0620000E+02  local
***** D:\SCR571_TPA_RUNS\TPA500W\TEST_1\FAILT.OUT
1   16393.75    43.35    2.0878   -0.1181    1   5.0005134E-02  general
corrosion potential not converging in 10 iterations.
failt: Inner overpack LC initiated at 16393.75000000000  years
corrosion potential not converging in 10 iterations.
corrosion potential not converging in 10 iterations.
corrosion potential not converging in 10 iterations.
2   16600.00    43.12  -10.0108   -3.8698    1  -2.0620000E+02  local
*****
```

The screenprints (*tpa.out* files) in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_1\tpa.out and
D:\SCR571_TPA_RUNS\TPA500W\TEST_1\TPA.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_1\tpa.out
      exec: Welcome to TPA Version 5.0.0w
    Job started: Tue May 31 13:42:05 2005
=====================================================================
***** D:\SCR571_TPA_RUNS\TPA500W\TEST_1\TPA.OUT
      exec: Welcome to TPA Version 5.0.0w
    Job started: Tue May 31 13:45:15 2005
=====================================================================
*****
```

The *totdose.res* files in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_1\totdose.res and
D:\SCR571_TPA_RUNS\TPA500W\TEST_1\TOTDOSE.RES
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_1\totdose.res
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 13:42:05 2005
 Total Dose for All Pathways, All Nuclides, and All Times

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_1\TOTDOSE.RES
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 13:45:15 2005
 Total Dose for All Pathways, All Nuclides, and All Times

*****
```

The *rgwnr.tpa* files in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_1\rgwnr.tpa and
D:\SCR571_TPA_RUNS\TPA500W\TEST_1\RGWNR.TPA
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_1\rgwnr.tpa
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 13:42:05 2005
 AEDE[rem/yr], GroundWater Pathway  for each nuclide, for each realization

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_1\RGWNR.TPA
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 13:45:15 2005
 AEDE[rem/yr], GroundWater Pathway  for each nuclide, for each realization

*****
```

The *relcum.out* files (note that these are from the last subarea, Subarea 7, analyzed) in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_1\relcum.out and
D:\SCR571_TPA_RUNS\TPA500W\TEST_1\RELCUM.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_1\relcum.out

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	4	9.2294E+02	5.4025E+02	9.4686E+02	1.4871E+03
2	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
3	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
4	0	9.9639E+02	0.0000E+00	0.0000E+00	0.0000E+00
5	0	3.4659E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	5.0500E+05	0.0000E+00	0.0000E+00	0.0000E+00
8	448	1.6394E+04	0.0000E+00	1.6600E+04	1.6600E+04

Radionuclide	Halflife[yr]	xnoloss[ci]	amwp[ci]	xmass[ci]
CM246	4.7310E+03	9.5814E-27	0.0000E+00	2.0009E-11
U238	4.4680E+09	2.6298E+02	2.7629E-04	1.6456E-01
CM245	8.4990E+03	2.8051E-26	0.0000E+00	3.1024E-11
AM241	4.3220E+02	1.7581E-22	0.0000E+00	5.5026E-11
NP237	2.1400E+06	6.7575E+02	7.0995E-04	4.2283E-01
U233	1.5850E+05	7.1706E+02	7.5334E-04	4.4868E-01
TH229	7.3390E+03	7.1895E+02	7.5533E-04	4.4986E-01
AM243	7.3800E+03	1.5009E-24	0.0000E+00	2.6989E-11
PU239	2.4060E+04	8.6173E-08	0.0000E+00	2.3467E-10
PU240	6.5370E+03	2.7630E-23	0.0000E+00	2.4516E-11
U234	2.4450E+05	6.6050E+01	6.9393E-05	4.1329E-02
TH230	7.7000E+04	9.6211E+01	1.0108E-04	6.0202E-02
RA226	1.6000E+03	9.6842E+01	1.0174E-04	6.0596E-02
PB210	2.2300E+01	9.6851E+01	1.0175E-04	6.0602E-02
CS135	2.3000E+06	5.0590E+02	5.1569E-04	1.5358E+01
I129	1.5700E+07	2.9414E+01	2.7265E-05	3.4782E+00
TC99	2.1300E+05	4.9557E+02	5.1993E-04	9.9603E-01
NI59	8.0000E+04	6.1826E-01	6.4954E-07	3.8686E-04
C14	5.7290E+03	3.5529E-26	0.0000E+00	3.8295E-10
SE79	1.1000E+06	4.5571E+01	4.6536E-05	1.3046E+00
NB94	2.0300E+04	1.7149E-12	0.0000E+00	1.9419E-10
CL36	3.0100E+05	1.3625E+00	1.2832E-06	1.4192E-01

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_1\RELCUM.OUT

Type#	Failed	Fail Time[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	4	9.2294E+02	5.4025E+02	9.4686E+02	1.4871E+03
2	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
3	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
4	0	9.9639E+02	0.0000E+00	0.0000E+00	0.0000E+00
5	0	3.4659E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	5.0500E+05	0.0000E+00	0.0000E+00	0.0000E+00
8	448	1.6394E+04	0.0000E+00	1.6600E+04	1.6600E+04

Radionuclide	Halflife[yr]	xnoloss[ci]	amwp[ci]	xmass[ci]	Fraction Left
CM246	4.7310E+03	9.5814E-27	0.0000E+00	2.0009E-11	-2.0883E+15
U238	4.4680E+09	2.6298E+02	2.7629E-04	1.6456E-01	9.9937E-01
CM245	8.4990E+03	2.8051E-26	0.0000E+00	3.1024E-11	-1.1060E+15
AM241	4.3220E+02	1.7581E-22	0.0000E+00	5.5026E-11	-3.1299E+11
NP237	2.1400E+06	6.7575E+02	7.0995E-04	4.2283E-01	9.9937E-01

U233	1.5850E+05	7.1706E+02	7.5334E-04	4.4868E-01	9.9937E-01
TH229	7.3390E+03	7.1895E+02	7.5533E-04	4.4986E-01	9.9937E-01
AM243	7.3800E+03	1.5009E-24	0.0000E+00	2.6989E-11	-1.7982E+13
PU239	2.4060E+04	8.6173E-08	0.0000E+00	2.3467E-10	9.9728E-01
PU240	6.5370E+03	2.7630E-23	0.0000E+00	2.4516E-11	-8.8729E+11
U234	2.4450E+05	6.6050E+01	6.9393E-05	4.1329E-02	9.9937E-01
TH230	7.7000E+04	9.6211E+01	1.0108E-04	6.0202E-02	9.9937E-01
RA226	1.6000E+03	9.6842E+01	1.0174E-04	6.0596E-02	9.9937E-01
PB210	2.2300E+01	9.6851E+01	1.0175E-04	6.0602E-02	9.9937E-01
CS135	2.3000E+06	5.0590E+02	5.1569E-04	1.5358E+01	9.6964E-01
I129	1.5700E+07	2.9414E+01	2.7265E-05	3.4782E+00	8.8175E-01
TC99	2.1300E+05	4.9557E+02	5.1993E-04	9.9603E-01	9.9799E-01
NI59	8.0000E+04	6.1826E-01	6.4954E-07	3.8686E-04	9.9937E-01
C14	5.7290E+03	3.5529E-26	0.0000E+00	3.8295E-10	-1.0779E+16
SE79	1.1000E+06	4.5571E+01	4.6536E-05	1.3046E+00	9.7137E-01
NB94	2.0300E+04	1.7149E-12	0.0000E+00	1.9419E-10	-1.1223E+02
CL36	3.0100E+05	1.3625E+00	1.2832E-06	1.4192E-01	8.9584E-01

*****

- Overall test status: <u>PASS</u>

SL-3. Name: Test 2 - Long Simulation with Outer Overpack Thickness 0.0000002 m

Path for run directory: d:\rrice\tpa500w\test_2 and d:\rrice\tpa500x\test_2

Path for archive of results: \SCR571\tpa500w\test_2 and
\SCR571\tpa500x\\test_2 (archived on CD "SCR571 Testing")

Environment variables: TPA_DATA=d:\rrice\tpa500w\
TPA_TEST=d:\rrice\tpa500w\

and

TPA_TEST=d:\rrice\tpa500x\
TPA_TEST=d:\rrice\tpa500x\

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Using the basecase TPA code for Versions 5.0.0w and 5.0.0x, but modifying the *tpa.inp* file as follows (i) maximum time of 1,000,000 yr; (ii) 4,800 time steps after the Compliance Period; (iii) 100 realizations, however executing only 1 realization and analyzing Subarea 1 only (i.e., Start and Stop at Subarea 1 and Start and Stop at realization 1); and (iv) Outer Overpack WP thickness equal to 0.0000002 m, compare TPA code output to check the impact of modifications made to the FAILT and RELEASET source code to remove statements regarding convergence in the FAILT screenprint (*failt.out*) and the RELEASET output file *relcum.out*.

- **Objective:** Verify FAILT modifications have no impact on failure times, releases, and doses using the basecase TPA code. Also, verify changes were made in the header and last column of results in RELEASET output file *relcum.out*.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** *failt.out;* screenprint (i.e., *tpa.out*); *totdose.res*; *rgwnr.tpa; relcum.out*

- **Step by step test procedure to be used:**

Execute the TPA Versions 5.0.0w and 5.0.0x code using the basecase *tpa.inp* file. Then, perform the following:

1. Compare the *failt.out* files from these two runs
2. Compare the *tpa.out* files from these two runs
3. Compare the *totdose.res* files from these two runs
4. Compare the *rgwnr.tpa* files from these two runs
5. Compare the *relcum.out* files from these two runs

- Pass/Fail criteria:

Criteria 1: For #1 above, any statements in the *relcum.out* file about not converging in the TPA Version 5.0.0w code should not be present in the TPA Version 5.0.0x code; also, the files will show a different time/date of the run

Criteria 2: For #2, #3, and #4 above, the files should be identical except for the time/date of the run

Criteria 3: For #5 above, the file header in *relcum.out* should be changed from "Fail Time[yr]" to "Start SF Wet[yr]"; also, the last column with "Fraction Left" should be removed

Test Results: The *failt.out* files in the run subdirectories for this test are included on the CD attached to this test plan. (Note that the WP failure time is 16,393.75 yr with this decreased Outer Overpack thickness.) The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_2\failt.out and
D:\SCR571_TPA_RUNS\TPA500W\TEST_2\FAILT.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_2\failt.out
version= 1.0
Tue May 31 13:20:19 2005
nhist3= 5001
***** D:\SCR571_TPA_RUNS\TPA500W\TEST_2\FAILT.OUT
version= 1.0
Tue May 31 13:17:46 2005
nhist3= 5001
*****
```

Note that the following lines regarding convergence are present in both of these files and they occur during "hmd oxd" calculations. These statements were intended to be removed by the changes introduced in this SCR.

```
2    899.57    136.69    0.0000    0.0000    0   4.9995782E-02  hmd oxd
2    922.94    135.25    0.0000    0.0000    0   4.9995198E-02  hmd oxd
corrosion potential not converging in 10 iterations.
corrosion potential not converging in 10 iterations.
corrosion potential not converging in 10 iterations.
corrosion potential not converging in 10 iterations.
corrosion potential not converging in 10 iterations.
2    946.86    133.83   -10.0502   -10.7396    1   -3.2079206E+01  general
```

The screenprints (*tpa.out* files) in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_2\tpa.out and
D:\SCR571_TPA_RUNS\TPA500W\TEST_2\TPA.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_2\tpa.out
      exec: Welcome to TPA Version 5.0.0w
    Job started: Tue May 31 13:20:06 2005
==========================================================================
***** D:\SCR571_TPA_RUNS\TPA500W\TEST_2\TPA.OUT
      exec: Welcome to TPA Version 5.0.0w
    Job started: Tue May 31 13:17:32 2005
==========================================================================
*****
```

The *totdose.res* files in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_2\totdose.res and
D:\SCR571_TPA_RUNS\TPA500W\TEST_2\TOTDOSE.RES
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_2\totdose.res
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 13:20:06 2005
 Total Dose for All Pathways, All Nuclides, and All Times

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_2\TOTDOSE.RES
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 13:17:32 2005
 Total Dose for All Pathways, All Nuclides, and All Times

*****
```

The *rgwnr.tpa* files in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

```
Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_2\rgwnr.tpa and
D:\SCR571_TPA_RUNS\TPA500W\TEST_2\RGWNR.TPA
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_2\rgwnr.tpa
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 13:20:06 2005
 AEDE[rem/yr], GroundWater Pathway  for each nuclide, for each realization

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_2\RGWNR.TPA
 Base case.
 TPA 5.0.0w, Job started: Tue May 31 13:17:32 2005
 AEDE[rem/yr], GroundWater Pathway  for each nuclide, for each realization

*****
```

The *relcum.out* files (note that these are from the last subarea, Subarea 7, analyzed) in the run subdirectories for this test are included on the CD attached to this test plan. The file comparison between these two files is listed below.

Comparing files D:\SCR571_TPA_RUNS\TPA500X\TEST_2\relcum.out and
D:\SCR571_TPA_RUNS\TPA500W\TEST_2\RELCUM.OUT
***** D:\SCR571_TPA_RUNS\TPA500X\TEST_2\relcum.out

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	4	9.2294E+02	5.4025E+02	9.4686E+02	1.4871E+03
2	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
3	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
4	0	9.9639E+02	0.0000E+00	0.0000E+00	0.0000E+00
5	0	3.4659E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	5.0500E+05	0.0000E+00	0.0000E+00	0.0000E+00
8	448	9.2294E+02	5.4025E+02	9.4686E+02	1.4871E+03

Radionuclide	Halflife[yr]	xnoloss[ci]	amwp[ci]	xmass[ci]
CM246	4.7310E+03	9.5814E-27	0.0000E+00	2.0009E-11
U238	4.4680E+09	2.6298E+02	2.9137E-04	1.8828E-01
CM245	8.4990E+03	2.8051E-26	0.0000E+00	3.1024E-11
AM241	4.3220E+02	1.7581E-22	0.0000E+00	5.5026E-11
NP237	2.1400E+06	6.7575E+02	7.4869E-04	4.8379E-01
U233	1.5850E+05	7.1706E+02	7.9446E-04	5.1337E-01
TH229	7.3390E+03	7.1895E+02	7.9655E-04	5.1472E-01
AM243	7.3800E+03	1.5009E-24	0.0000E+00	2.6989E-11
PU239	2.4060E+04	8.6173E-08	0.0000E+00	2.4175E-10
PU240	6.5370E+03	2.7630E-23	0.0000E+00	2.4516E-11
U234	2.4450E+05	6.6050E+01	7.3180E-05	4.7288E-02
TH230	7.7000E+04	9.6211E+01	1.0660E-04	6.8881E-02
RA226	1.6000E+03	9.6842E+01	1.0730E-04	6.9333E-02
PB210	2.2300E+01	9.6851E+01	1.0731E-04	6.9339E-02
CS135	2.3000E+06	5.0590E+02	5.4383E-04	1.5402E+01
I129	1.5700E+07	2.9414E+01	2.8753E-05	3.4806E+00
TC99	2.1300E+05	4.9557E+02	5.4830E-04	1.0407E+00
NI59	8.0000E+04	6.1826E-01	6.8499E-07	4.4263E-04
C14	5.7290E+03	3.5529E-26	0.0000E+00	3.8295E-10
SE79	1.1000E+06	4.5571E+01	4.9075E-05	1.3086E+00
NB94	2.0300E+04	1.7149E-12	0.0000E+00	1.9402E-10
CL36	3.0100E+05	1.3625E+00	1.3532E-06	1.4203E-01

***** D:\SCR571_TPA_RUNS\TPA500W\TEST_2\RELCUM.OUT

Type#	Failed	Fail Time[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	4	9.2294E+02	5.4025E+02	9.4686E+02	1.4871E+03
2	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
3	0	9.2294E+02	0.0000E+00	0.0000E+00	0.0000E+00
4	0	9.9639E+02	0.0000E+00	0.0000E+00	0.0000E+00
5	0	3.4659E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	5.0500E+05	0.0000E+00	0.0000E+00	0.0000E+00
8	448	9.2294E+02	5.4025E+02	9.4686E+02	1.4871E+03

Radionuclide	Halflife[yr]	xnoloss[ci]	amwp[ci]	xmass[ci]	Fraction Left
CM246	4.7310E+03	9.5814E-27	0.0000E+00	2.0009E-11	-2.0883E+15
U238	4.4680E+09	2.6298E+02	2.9137E-04	1.8828E-01	9.9928E-01
CM245	8.4990E+03	2.8051E-26	0.0000E+00	3.1024E-11	-1.1060E+15
AM241	4.3220E+02	1.7581E-22	0.0000E+00	5.5026E-11	-3.1299E+11
NP237	2.1400E+06	6.7575E+02	7.4869E-04	4.8379E-01	9.9928E-01

U233	1.5850E+05	7.1706E+02	7.9446E-04	5.1337E-01	9.9928E-01
TH229	7.3390E+03	7.1895E+02	7.9655E-04	5.1472E-01	9.9928E-01
AM243	7.3800E+03	1.5009E-24	0.0000E+00	2.6989E-11	-1.7982E+13
PU239	2.4060E+04	8.6173E-08	0.0000E+00	2.4175E-10	9.9719E-01
PU240	6.5370E+03	2.7630E-23	0.0000E+00	2.4516E-11	-8.8729E+11
U234	2.4450E+05	6.6050E+01	7.3180E-05	4.7288E-02	9.9928E-01
TH230	7.7000E+04	9.6211E+01	1.0660E-04	6.8881E-02	9.9928E-01
RA226	1.6000E+03	9.6842E+01	1.0730E-04	6.9333E-02	9.9928E-01
PB210	2.2300E+01	9.6851E+01	1.0731E-04	6.9339E-02	9.9928E-01
CS135	2.3000E+06	5.0590E+02	5.4383E-04	1.5402E+01	9.6956E-01
I129	1.5700E+07	2.9414E+01	2.8753E-05	3.4806E+00	8.8167E-01
TC99	2.1300E+05	4.9557E+02	5.4830E-04	1.0407E+00	9.9790E-01
NI59	8.0000E+04	6.1826E-01	6.8499E-07	4.4263E-04	9.9928E-01
C14	5.7290E+03	3.5529E-26	0.0000E+00	3.8295E-10	-1.0779E+16
SE79	1.1000E+06	4.5571E+01	4.9075E-05	1.3086E+00	9.7128E-01
NB94	2.0300E+04	1.7149E-12	0.0000E+00	1.9402E-10	-1.1214E+02
CL36	3.0100E+05	1.3625E+00	1.3532E-06	1.4203E-01	8.9576E-01

*****

- Overall test status: <u>FAIL (see bold above)</u>

<u>FAILT convergence will be addressed in SCR-577</u>

That is, removing statements regarding convergence in the FAILT output (which are found in the FAILT screenprint in standalone mode or *failt.out* from a TPA code simulation) during humid oxidation calculations in FAILT will be addressed in SCR-577.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-574	**2. Software Title and Version:** TPA 5.0.0	**3. Project No:** 20.06002.01.354
4. Affected Software Module(s), Description of Problem(s): *volcano.f, tpa.inp* The volcano input parameters for the geometric model do not permit the adjustment of the MTU ejected in a straight forward, physically intuitive way.		
5. Change Requested by: B. Hill Date: 5-11-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 5-11-05	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment A		
8. Implemented by: Jose M. Menchaca	**Date:** 05/13/05	
9. Description of Acceptance Tests: Tests were carried out in accordance with the test plan tp_scr574.wpd (see Attachment B), which also includes the test report. All tests passed. Test directories are archived on the CD entitled "TPA SCR #574 - Test Directories".		
10. Tested by: Carol S. Scherer	**Date:** December 8, 2005	

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
modify from	volcano	DiameterOfVolcanicConduit[m]	used for calculating amtuejected	uniform	28., 280.		

modify to	volcano	DiameterOfVolcanicConduit[m]	used for calculating amtuejected	uniform	5., 50.	Subsurface conduits for basaltic scoria cone volcanoes have roughly cylindrical conduits with these diameters at depths comparable to the potential repository drifts (NRC, 1999; Doubik and Hill, 1999).Used to calculate number of waste packages ejected for extrusive event in geometric model; applies when AshEvolutionMode = 0 only)	B. Hill

Attachment A

The current method of calculating MTU ejected in a volcanic event is a complicated calculation using the area of the volcanic conduit, waste package payload and areal mass loading. A simpler method was needed to be able to calculate the MTU ejected in a simpler straightforward way.

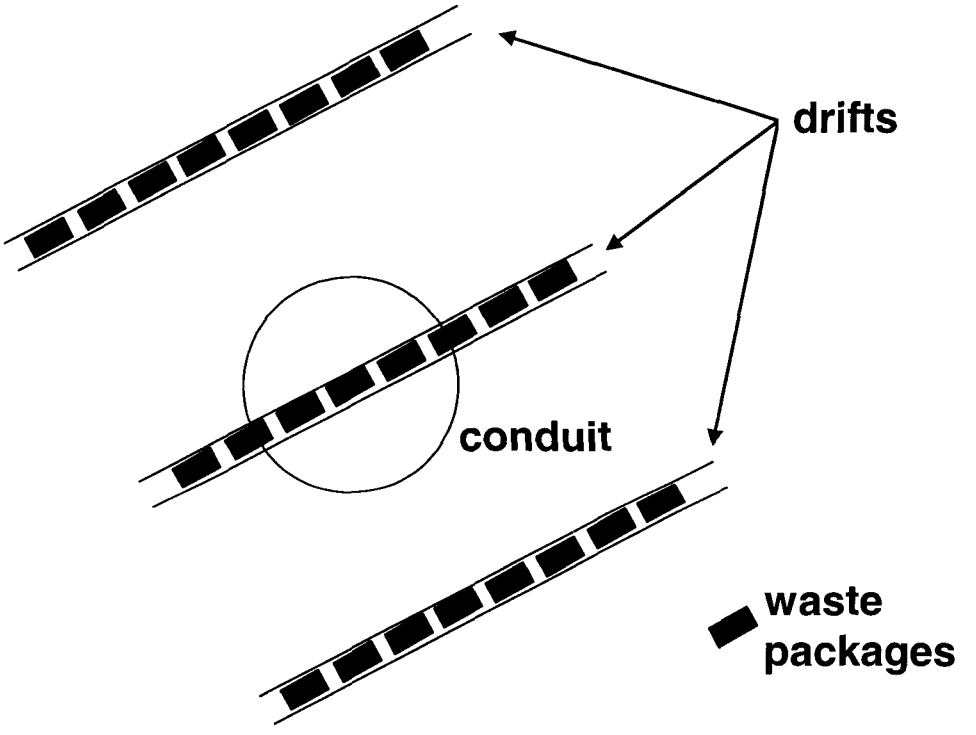


Figure 1

Figure 1 is a schematic representation demonstrating the concept used for determining the number of waste packages ejected by a volcanic event. The conduit diameter now has a range of 5 to 50 meters, less than the 81 meter spacing between drifts, therefore the conduit is only expected to intercept a single drift. The new equation for calculating the MTU ejected is as follows,

$$MTU\ ejected = \frac{conduit\ diameter}{waste\ package\ spacing} \times MTU/WP$$

where *conduit diameter* and *waste package spacing* have units of meters. The equation is implemented in the code as follows (Note: the code is not shown in the actual context as it appears in the code but the sequence of the commands is shown correctly):

```
 name = 'DiameterOfVolcanicConduit[m]'
 idiam = ispquery( name )
 diam    = valuesp( idiam )

 name = 'WastePackagePayload[MTU]'
 imtuperwp = ispquery( name )

 name = 'WPSpacingAlongEmplacementDrift[m]'
 iwpspace  = ispquery( name )
 wpspace  = valuesp( iwpspace )

amtuejected = 0.0d0
amtuperwp  = valuesp( imtuperwp)
if (extrusive .eq. 1) amtuejected = (diam / wpspace) * amtuperwp
```

ATTACHMENT B

Test Plan/Report for TPA SCR #574

Test Plan Name: Test Modifications to VOLCANO to Calculate MTU Ejected in a More Straightforward Manner

Tested By: Carol S. Scherer **Date:** December 8, 2005

Host Machine: SUN Ultra-4 server: Spock **Host OS:** Sun Solaris 5.8

Baseline Version: **TPA** 5.0.0y **Test Version:** **TPA** 5.0.0beta

Testing Setup:

Directories/paths used for testing:
$HOME = spock/home/cscherer
Path for run directory: ***$HOME/scr574***

Environment variables:

TPA_TEST = $HOME /
TPA_DATA = $HOME /

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 574 - Test Directories*" (attached).

Test preparation instructions:

1. Copy **TPA** version 5.0.1beta to ***$HOME/scr574***. Compile *tpa.e*.

Function Level Tests:

These tests are designed to demonstrate the functionality of the specified module.

1. Name: Visual Inspection of *tpa.inp* for **TPA**5.0.0beta.

   Paths for archives of results: none.

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: none.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that specified changes have been made to *tpa.inp*.
   - assumptions: all setup instructions have been carried out.
   - constraints: none.
   - output files to compare or examine: none.
   - step by step test procedure to be used:
     1. look at *tpa.inp* 5.0.0beta and verify that the changes specified in the scr document have been made, i.e., the range of values for the sampled parameter DiameterOfVolcanicConduit[m] has been changed from "28.0, 280.0" to "5.0, 50.0".
   - pass/fail criteria: the test passes if:
     1. Specified changes have been made.

   Results of running test:

   PASSED.

2. Name: Determine That Modified Code Calculates Ejected MTU As Specified.

Paths for archives of results: ***$HOME /scr574***

Special input files or modifications to input files required: none.

Special diagnostic code modifications required: add the following print statements to *volcano.f* after the if block where wpentrained is calculated.

```
        if (i .eq. eventsubarea) then
           wpentrained = amtuejected / amtuperwp
        end if

c test SCR574
        print *, 'TEST574'
        print *, 'TEST574  diam          = ', diam
        print *, 'TEST574  wpspace       = ', wpspace
        print *, 'TEST574  amtuperperwp  = ', amtuperwp
        print *, 'TEST574  amtuejected   = ', amtuejected
        print *, 'TEST574  wpentrained   = ', wpentrained
c end test
```

Program modes to be used: use base case *tpa.inp* (TPA5.0.1beta) and make the following changes:

```
set NumberOfRealizations                          to 425
set StopAtRealization                             to 10
set VolcanismDisruptiveScenarioFlag(yes=1,no=0)   to 1
set LengthOfVolcanicDike[m]                       to 200.0, 1000.0
```

Utility scripts needed to perform the test: none.

Utility codes needed in the analysis of the test data: none.

Test description:

- objective: to show that the modified **TPA** code calculates ejected MTU as expected.

- assumptions: all setup instructions have been carried out.

- constraints: none.

- output files to compare or examine:

- step by step test procedure to be used:
  1. —> change directory to <<run directory>>

2. run *tpa.e* using command "***tpa.e > tpa_testcalc.out.out***"
3. copy the data values printed out in *tpa_testcalc.out.out* by the print statements added as specified above to the spreadsheet *calculations-tpa501beta.xls*.
4. compare the expected values with the actual values for MTU ejected

- pass/fail criteria: the test passes if:

1. The **TPA** run completes successfully.

2. In the spreadsheet, *calculations-tpa501beta.xls*, the values for actual MTU ejected are within 5% of the expected values. The following table shows the calculations from the spreadsheet.

realization	conduit diameter	WP space	MTU / WP	MTU ejected	subarea	WP entrained	% diff expected - actual TPA	Expected MTU ejected
1	46.8391	5.265	7.89	70.19193	4	8.896315	-5.06E-13	70.19193
2	22.99375	5.265	7.89	34.45787	5	4.367284	1.07E-12	34.45787
3	47.26233	5.265	7.89	70.82617	1	8.976701	-3.61E-13	70.82617
4	23.99224	5.265	7.89	35.95418	6	4.556931	3.95E-14	35.95418
5	31.11605	5.265	7.89	46.62975	4	5.909981	3.05E-13	46.62975
6	34.81718	5.265	7.89	52.17617	1	6.61295	-2.32E-13	52.17617
7	36.34875	5.265	7.89	54.47135	5	6.903846	3E-13	54.47135
8	26.3603	5.265	7.89	39.5029	4	5.006705	-7.37E-13	39.5029
9	35.85351	5.265	7.89	53.72919	5	6.809783	-7.01E-13	53.72919
10	36.57286	5.265	7.89	54.80719	5	6.946412	-1.82E-13	54.80719

Results of running test:

PASSED.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-574	**2. Software Title and Version:** TPA 5.0.0	**3. Project No:** 20.06002.01.354
4. Affected Software Module(s), Description of Problem(s): *volcano.f, tpa.inp* The volcano input parameters for the geometric model do not permit the adjustment of the MTU ejected in a straight forward, physically intuitive way.		
5. Change Requested by: B. Hill Date: 5-11-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 5-11-05	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment A		
8. Implemented by: Jose M. Menchaca	**Date:** 05/13/05	
9. Description of Acceptance Tests:		
10. Tested by:	**Date:**	

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Parameter Name**	**Description 1. definition of parameter in terms of its function in TPA code (calculated from ..., used for calculating..., used to relate... etc)**	**Distribution**	**Range**	**Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions**	Source (Initials)
modify from	volcano	DiameterOfVolcanicConduit[m]	used for calculating amtuejected	uniform	28., 280.		

modify to	volcano	DiameterOfVolcanicConduit[m]	used for calculating amtuejected	uniform	5., 50.	Subsurface conduits for basaltic scoria cone volcanoes have roughly cylindrical conduits with these diameters at depths comparable to the potential repository drifts (NRC, 1999; Doubik and Hill, 1999).Used to calculate number of waste packages ejected for extrusive event in geometric model; applies when AshEvolutionMode = 0 only)	B. Hill

Attachment A

The current method of calculating MTU ejected in a volcanic event is a complicated combination of area of the volcanic conduit, waste package payload and areal mass loading. A simpler method was needed to be able to calculate the MTU ejected in a simpler straightforward way.

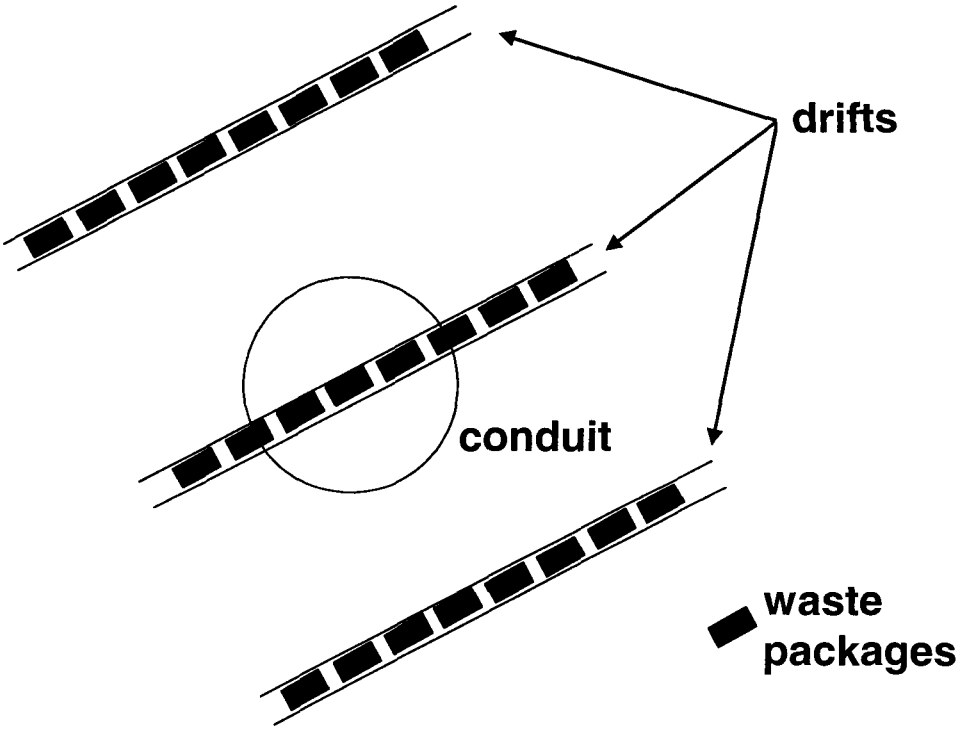


Figure 1

Figure 1 is a schematic representation of the concept used for determining the number of waste packages ejected by a volcanic event. The conduit diameter now has a range of 5 to 50 meters, less than the 81 meter spacing between drifts, therefore the conduit is only expected to intercept a single drift. The new equation for calculating the MTU ejected is as follows.

$$MTU\ ejected = \frac{conduit\ diameter\,[m]}{waste\ package\ spacing\,[m]} \times MTU/WP$$

The equation is implemented in the code as follows (Note: the code is not shown in the actual context as it appears in the code but the sequence of the commands is shown correctly):

```
 name = 'DiameterOfVolcanicConduit[m]'
 idiam = ispquery( name )
 diam    = valuesp( idiam )

 name = 'WastePackagePayload[MTU]'
 imtuperwp = ispquery( name )

 name = 'WPSpacingAlongEmplacementDrift[m]'
 iwpspace  = ispquery( name )
 wpspace  = valuesp( iwpspace )

amtuejected = 0.0d0
amtuperwp  = valuesp( imtuperwp)
if (extrusive .eq. 1) amtuejected = (diam / wpspace) * amtuperwp
```

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-576	**2. Software Title and Version:** TPA 5.0.0y	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *ashplumo.f, seismo2.f, uzft.f, ebsfail.f, ebsrel.f*

Some auxiliary codes to not have a "successfully completed" flag to permit the detection of failed execution of the standalone code.

5. Change Requested by: R. Rice 5-12-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 5-12-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Modifications were made to the affected modules to delete the major output file before the modules are executed, so that an error would be generated upon accessing a non-existent or incomplete file if the module experienced an unsuccessful run.

8. Implemented by: R. Janetzke	**Date:** 5-16-05

9. Description of Acceptance Tests:

See Attachment A, also named "Test_Plan_SCR576.wpd" on the CD labeled "Detecting Stand-alone Code Failed Execution", that contains a description of the Acceptance Tests for the change listed above in Box #4.

10. Tested by: R. Rice	**Date:** 10-12-05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 576

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	Module	Parameter Name	Description 1. definition of parameter in terms of its function in TPA code (calculated from . . ., used for calculating . . ., used to relate . . . etc.)	Distribution	Range	Justification 1. site references (journals, sci. notebooks, publishings) 2. is uncertainty covered by the distribution / range ? 3. explain why you chose this range / distribution vs. other possible values / methods / distributions	Source

Attachment A

Test Plan for TPA SCR#576

Test Plan Name: Detect Unsuccessful Completion of TPA Executables

Tested By: R. Rice

Date: October 12, 2005

Host Machine: "TPA" machine

Host OS: MS Windows Server 2003

Baseline Version: 5.0.0y

Test Version: 5.0.1beta

System Level (SL) Tests

SL-1. Name: Detect Execution Failure

Path for run directory:
d:\rrice\SCR576\tpa500y\runs*
d:\rrice\SCR576\tpa501beta\runs*
(where * = 10 standalone code names)

Path for archive of results:
\SCR576\tpa500y\runs* (archived on CD)
\SCR576\tpa500y\runs* (archived on CD)
(where * = 10 standalone code names)

(Note that the 10 standalone codes, in order of TPA code execution, are: SNLLHS, DSFAILT, MECHFAIL, FAILT, RELEASET, EBSFILT, NEFMKS, ENVIN, ENV, and ASHPLUME.)

Environment variables:
TPA_DATA=d:\rrice\SCR576\tpa500y
TPA_DATA=d:\rrice\SCR576\tpa501beta

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only and with VOLCANO activated)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: In the TPA code, it may happen that the execution of a standalone code is unsuccessful and the TPA code will continue to run. This continuation occurs because files from previous subarea calculations remain in the run directory and those files are read and values incorrectly used in the calculations for the

current subarea. To avoid this situation, the major output file from each standalone code (i.e., a file whose values are read and used in calculations) should be deleted, thereby when execution of the standalone code is unsuccessful, the TPA code execution will stop because it will not be able to open and read from this major output file.

- Objective: Verify that the TPA Version 5.0.1beta code execution stops in all cases when execution is unsuccessful for the 10 standalone codes.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: screenprint

- Step by step test procedure to be used:

1. Create "runs" subdirectories in both the TPA Versions 5.0.0y and 5.0.1beta main source code directory.
2. In each of these run directories, create a subdirectory for each of the 10 standalone codes. These subdirectories are labeled according to the name of the standalone code.
3. Execute the TPA Versions 5.0.0y and 5.0.1beta code using the basecase *tpa.inp* file (with VOLCANO activated and for Subarea 1 only) and capture the screenprint in the *tpa.inp* file.
4. Copy the output files from the TPA Versions 5.0.0y code runs in #3 into each of the 10 subdirectories created in #2 for he TPA Version 5.0.0y code.
5. Copy the output files from the TPA Versions 5.0.1beta code runs in #3 into each of the 10 subdirectories created in #2 for he TPA Version 5.0.1beta code.
6. Create 10 codes subdirectories in both the TPA Versions 5.0.0y and 5.0.1beta main directories. The files contained in these subdirectories should be the same as the files in the "codes" subdirectory. In each of the 10 subdirectories, replace that subdirectories standalone executable with a "stub" executable program. This stub executable has the same name as the standalone code executable it replaces. (Note that upon execution, this stub executable prints to the screen "Executing empty program").
7. In each of the the ten subdirectories in #6, delete all executables called by the TPA code after this stub.
8. Repeat steps #6 and #7 for the TPA Version 5.0.1beta subdirectory.
9. Run the TPA in the 10 subdirectories for both Versions 5.0.0y and 5.0.1beta.
10. Review screenprint in the *tpa.inp* file and determine whether the TPA code execution stopped as a result of unsuccessful execution of a standalone code.

- Pass/Fail criteria:

Criteria 1: The TPA Version 5.0.1beta code executions should be stopped for all cases when the TPA code execution stopped for the TPA Version 5.0.0y code.

Criteria 2: For instances when the TPA Version 5.0.0y code execution continued (when it shouldn't have done so), the TPA Version 5.0.1beta code execution should stop.

Test Results: The files in the \SCR576\tpa500y\runs* and \SCR576\tpa500y\runs* subdirectories (where * = 10 standalone code names) contains results for this test. The results in these subdirectories indicate that the Pass/Fail Criteria for "Criteria 2" listed above were **NOT** met. That is, when FAILT did not successfully complete execution, the TPA Version 5.0.1beta did not stop execution. The following table summarizes the test results.

Standalone Code	Execution of the TPA Version 5.0.0y code	Execution of the TPA Version 5.0.0y code	TEST STATUS
SNLLHS	TPA code stops	TPA code stops	passes Crit. 1
DSFAILT	TPA code stops	TPA code stops	passes Crit. 1
MECHFAIL	TPA code stops	TPA code stops	passes Crit. 1
FAILT	TPA code CONTINUES	**TPA code CONTINUES - FAIL CRIT. 2**	
RELEASET	TPA code CONTINUES	TPA code stops	passes Crit. 2
EBSFILT	TPA code CONTINUES	TPA code stops	passes Crit. 2
NEFMKS	TPA code stops	TPA code stops	passes Crit. 1
ENVIN	TPA code stops	TPA code stops	passes Crit. 1
ENV	TPA code stops	TPA code stops	passes Crit. 1
ASHPLUME	TPA code stops	TPA code stops	passes Crit. 1

- Overall test status: FAIL

The failure of the FAILT portion of this test will be addressed in SCR593.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 597	**2. Software Title and Version:** TPA Version 5.0.2i	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *exec.f, ebsrel.f*

The glass release data from *relcum.out* is not transferred to the *ebsrel.rlt* file.

5. Change Requested by: T. McCartin Date: 2-27-06	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 2-27-06

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The transfer of data is performed in a two step process. After the glass run of *releaset.e* has completed, the *relcum.out* file is copied to *relcumglass.out* in *ebsrel.f*, then the *relcumglass.out* file is copied to the *ebsrel.rlt* file in *exec.f.*

The code for these changes is structurally and logically similar, and positioned immediately after the existing code that handles the data from the *relcum.out* file for the spent fuel run of *releaset.e.*

8. Implemented by: R. Janetzke	**Date:** 3-3-06

9. Description of Acceptance Tests:
Tests were carried out in accordance with the test plan tp_scr597.wpd (see Attachments A and B), which also includes the test report. All tests passed. Test directories are archived on the attached CD entitled "TPA SCR #597 - Test Directories".

10. Tested by: C. Scherer	**Date:** 3-30-06

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 597

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
No Change to any TPA.INP parameter							

ATTACHMENT A

Test Plan/Report for TPA SCR #597

Test Plan Name: Test Changes to Actinide Kd/Rd Calculations

Tested By: Carol S. Scherer

Date: March 30, 2006

Host Machine: AMD Opteron PC: TPA

Host OS: MS Windows Server 2003 Version 5.2

Baseline Version: TPA 5.0.2i

Test Version: TPA 5.0.2j

Testing Setup:

Directories\paths used for testing:
$HOME = d:\CScherer
Path for run directory: ***$HOME\scr597***

Environment variables:

to run **TPA5.0.2j**:
TPA_TEST = **$HOME*SCR597***
TPA_DATA = **$HOME*SCR597***

to run **TPA5.0.2i** :
TPA_TEST = **$HOME*SCR597*\tpa502i**
TPA_DATA = **$HOME*SCR597*\tpa502i**

Disposition of documentation of results: All modified\new source code files, all executables used in testing, and all input\output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 597 - Test Directories*" (attached). PC versions of the test directories will follow the paths indicated under a root directory called scr597-pc.

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***SCR597***, ***SCR597\tpa502i***, ***SCR597\plt1***, ***SCR597\plt1\tpa502i***, ***SCR597\plt2***, and ***SCR597\plt2\tpa502i***

2. Copy **TPA** version 5.0.2j to ***$HOME\SCR597***. Compile *tpa.exe*.

3. Copy **TPA** version 5.0.2i to ***$HOME\SCR597\tpa502i***. Compile *tpa.exe*.

Process Level Tests:

These tests are designed to demonstrate the functionality of the specified module.

1. Name: Visual Inspection of Directory and Output Files After Running **TPA5.0.2i** and **TPA5.0.2j** with All Subareas and All Appended Files.

   Paths for archives of results: ***$HOME \SCR597\plt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use base case *tpa.inp* for each version and set OutputMode to 1.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that specified changes have been made to **TPA** and that the changes do not affect Peak Mean Dose.

   - assumptions: all setup instructions have been carried out.

   - constraints: none.

   - output files to compare or examine: *relcumglass.out*, *relcumsf.out*, and *ebsrel.rlt*.

   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>***\tpa502i***
     2. run *tpa.exe* using command "***%TPA_TEST%\tpa.exe > tpa_basecase-AF.out***"
     3. copy *tpa_basecase-AF.out* to ***$HOME\SCR597\plt1****tpa_basecase502i-AF.out*
     4. copy *ebsrel.rlt* and *relcum.out* to ***$HOME\SCR597\plt1\tpa502i***
     5. —> change directory to <<run directory>>
     6. run *tpa.exe* using command "***%TPA_TEST%\tpa.exe > tpa_basecase-AF.out***"

7. copy *tpa_basecase-AF.out* to ***$HOME\SCR597\plt1****tpa_basecase502j-AF.out*
8. copy *ebsrel.rlt, relcum.out, relcumsf.out,* and *relcumglass.out* to ***$HOME\SCR597\plt1***

- pass\fail criteria: the test passes if:

  1. Both **TPA** runs complete successfully.

  2. The files relcumsf.out and relcumglass.out appear in the directory ***$HOME \SCR597*** after running **TPA5.0.2j** but do not appear in the directory ***$HOME\SCR597\tpa502i***.

  3. The information contained in *relcumglass.out* and *relcumsf.out* appears in *ebsrel.rlt* for subarea 10 for the **TPA5.0.2j** run.

  4. Peak Mean Dose is the same in both *tpa_basecase502j-AF.out* and *tpa_basecase502i-AF.out*.

Results of running test:

PASSED.

2. Name: Visual Inspection of Directory and Output Files After Running **TPA5.0.2i** and **TPA5.0.2j** with One Subarea and All Appended Files.

   Paths for archives of results: ***$HOME \SCR597****plt2*

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use base case *tpa.inp* for each version, set StartAtSubarea to 4, StopAtSubarea to 4, and OutputMode to 1.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that specified changes have been made to **TPA** and that the changes do not affect Peak Mean Dose.

   - assumptions: all setup instructions have been carried out.

   - constraints: none.

   - output files to compare or examine: *relcumglass.out*, *relcumsf.out*, and *ebsrel.rlt*.

   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>***\tpa502i***
     2. run *tpa.exe* using command "***%TPA_TEST%\tpa.exe > tpa_basecase-sa4-AF.out***"
     3. copy *tpa_basecase-AF.out* to ***$HOME\SCR597\plt1****tpa_basecase502i-AF.out*
     4. copy *ebsrel.rlt* and *relcum.out* to ***$HOME\SCR597\plt1\tpa502i***
     5. —> change directory to <<run directory>>
     6. run *tpa.exe* using command "***%TPA_TEST%\tpa.exe > tpa_basecase-sa4-AF.out***"
     7. copy *tpa_basecase-AF.out* to ***$HOME\SCR597\plt1****tpa_basecase502j-AF.out*
     8. copy *ebsrel.rlt, relcum.out, relcumsf.out,* and *relcumglass.out* to ***$HOME\SCR597\plt1***

   - pass\fail criteria: the test passes if:

1. Both **TPA** runs complete successfully.

2. The files relcumsf.out and relcumglass.out appear in the directory ***$HOME \SCR597*** after running **TPA5.0.2j** but do not appear in the directory ***$HOME\SCR597\tpa502i***.

3. The information contained in *relcumglass.out* and *relcumsf.out* appears in *ebsrel.rlt* for subarea 4 for the **TPA5.0.2j** run.

4. Peak Mean Dose is the same in both *tpa_basecase502j-AF.out* and *tpa_basecase502i-AF.out*.

Results of running test:

PASSED.

NOTES:

ATTACHMENT B

Test Plan/Report for TPA SCR #597

Test Plan Name: Test Changes to Actinide Kd/Rd Calculations

Tested By: Carol S. Scherer **Date:** March 30, 2006

Host Machine: SUN Ultra-4 server: Spock **Host OS:** Sun Solaris 5.8

Baseline Version: TPA 5.0.2i **Test Version: TPA** 5.0.2j

Testing Setup:

Directories/paths used for testing:
$HOME = spock/home/cscherer
Path for run directory: ***$HOME/scr597***

Environment variables:

to run **TPA5.0.2j**:
TPA_TEST = $HOME/*SCR597*
TPA_DATA = $HOME/*SCR597*

to run **TPA5.0.2i** :
TPA_TEST = $HOME/*SCR597*/tpa502i
TPA_DATA = $HOME/*SCR597* tpa502i

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 597 - Test Directories*" (attached). UNIX versions of the test directories will follow the paths indicated under a root directory called scr597-unix.

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***SCR597***, ***SCR597/tpa502i***, ***SCR597/plt1***, ***SCR597/plt1/tpa502i***, ***SCR597/plt2***, and ***SCR597/plt2/tpa502i***

2. Copy **TPA** version 5.0.2j to ***$HOME/SCR597***. Compile *tpa.e*.

3. Copy **TPA** version 5.0.2i to ***$HOME/SCR597/tpa502i***. Compile *tpa.e*.

Process Level Tests:

These tests are designed to demonstrate the functionality of the specified module.

1. Name: Visual Inspection of Directory and Output Files After Running **TPA5.0.2i** and **TPA5.0.2j** with All Subareas and All Appended Files.

   Paths for archives of results: ***$HOME /SCR597/plt1***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use base case *tpa.inp* for each version and set OutputMode to 1.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that specified changes have been made to **TPA** and that the changes do not affect Peak Mean Dose.

   - assumptions: all setup instructions have been carried out.

   - constraints: none.

   - output files to compare or examine: *relcumglass.out*, *relcumsf.out*, and *ebsrel.rlt*.

   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>***/tpa502i***
     2. run *tpa.e* using command "***tpa.e > tpa_basecase-sa4-AF.out***"
     3. copy *tpa_basecase-AF.out* to ***$HOME/SCR597/plt1/****tpa_basecase502i-AF.out*
     4. copy *ebsrel.rlt* and *relcum.out* to ***$HOME/SCR597/plt1/tpa502i***
     5. —> change directory to <<run directory>>
     6. run *tpa.e* using command "***tpa.e > tpa_basecase-sa4-AF.out***"
     7. copy *tpa_basecase-AF.out* to ***$HOME/SCR597/plt1/****tpa_basecase502j-AF.out*
     8. copy *ebsrel.rlt, relcum.out, relcumsf.out,* and *relcumglass.out* to ***$HOME/SCR597/plt1***

- pass/fail criteria: the test passes if:

  1. Both **TPA** runs complete successfully.

  2. The files relcumsf.out and relcumglass.out appear in the directory ***$HOME /SCR597*** after running **TPA5.0.2j** but do not appear in the directory ***$HOME/SCR597/tpa502i***.

  3. The information contained in *relcumglass.out* and *relcumsf.out* appears in *ebsrel.rlt* for subarea 10 for the **TPA5.0.2j** run.

  4. Peak Mean Dose is the same in both *tpa_basecase502j-AF.out* and *tpa_basecase502i-AF.out*.

Results of running test:

PASSED.

2. Name: Visual Inspection of Directory and Output Files After Running **TPA5.0.2i** and **TPA5.0.2j** with One Subarea and All Appended Files.

   Paths for archives of results: ***$HOME /SCR597/plt2***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use base case *tpa.inp* for each version, set StartAtSubarea to 4, StopAtSubarea to 4, and OutputMode to 1.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that specified changes have been made to **TPA** and that the changes do not affect Peak Mean Dose.

   - assumptions: all setup instructions have been carried out.

   - constraints: none.

   - output files to compare or examine: *relcumglass.out*, *relcumsf.out*, and *ebsrel.rlt*.

   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>***/tpa502i***
     2. run *tpa.e* using command "***tpa.e > tpa_basecase-AF.out***"
     3. copy *tpa_basecase-AF.out* to ***$HOME/SCR597/plt1****/tpa_basecase502i-AF.out*
     4. copy *ebsrel.rlt* and *relcum.out* to ***$HOME/SCR597/plt1/tpa502i***
     5. —> change directory to <<run directory>>
     6. run *tpa.e* using command "***tpa.e > tpa_basecase-AF.out***"
     7. copy *tpa_basecase-AF.out* to ***$HOME/SCR597/plt1****/tpa_basecase502j-AF.out*
     8. copy *ebsrel.rlt*, *relcum.out, relcumsf.out,* and *relcumglass.out* to ***$HOME/SCR597/plt1***

   - pass/fail criteria: the test passes if:

     1. Both **TPA** runs complete successfully.

2. The files relcumsf.out and relcumglass.out appear in the directory ***$HOME /SCR597*** after running **TPA5.0.2j** but do not appear in the directory ***$HOME/SCR597/tpa502i.***

3. The information contained in *relcumglass.out* and *relcumsf.out* appears in *ebsrel.rlt* for subarea 4 for the **TPA5.0.2j** run.

4. Peak Mean Dose is the same in both *tpa_basecase502j-AF.out* and *tpa_basecase502i-AF.out.*

Results of running test:

PASSED.

NOTES:

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 598	**2. Software Title and Version:** TPA 5.0.2o	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *tpa_include.inp*

The west end point of the boundary line between subareas 3 and 4/5 falls slightly west of the boundary line between subareas 2 and 3/4, causing subareas 3 and 4 to overlap slightly with subarea 2, which results in one too many waste packages being reported by the TPA code.

5. Change Requested by:	**6. Change Authorized by** (*Software Developer*):
D. Stead Date: 3-22-06	R. Janetzke Date: 3-22-06

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The end points (and the point of intersection with the boundary line between subareas 4 and 5) of the boundary line between subareas 3 and 4/5 have been adjusted to prevent subarea overlap, and to make the line parallel to adjacent drifts.

See page 2 for a listing of coordinate changes.

See Attachment A for a plot of the subareas and drifts.

The Southeast corner of subarea 5 was approximately 2 meters to the east of where it should be to get a waste package count that yielded all 70,040 MTU of waste. The southeast vertex coordinates of subarea 5 were adjusted so that the subarea border maintains a uniform distance from the eastmost drift edges.

8. Implemented by:	**Date:**
D. Stead / J. Menchaca	4-11-06 / 4-21-06

9. Description of Acceptance Tests:

See Attachment B (PC platform test - J. Menchaca).
See Attachment C (Unix platform test - J. Menchaca).
See Attachment D (PC platform test 2 - D. Stead).
See Attachment E (Unix platform test 2 - D. Stead).

10. Tested by:	**Date:**
J. M. Menchaca / D. Stead	4-12-06 / 4-26-06

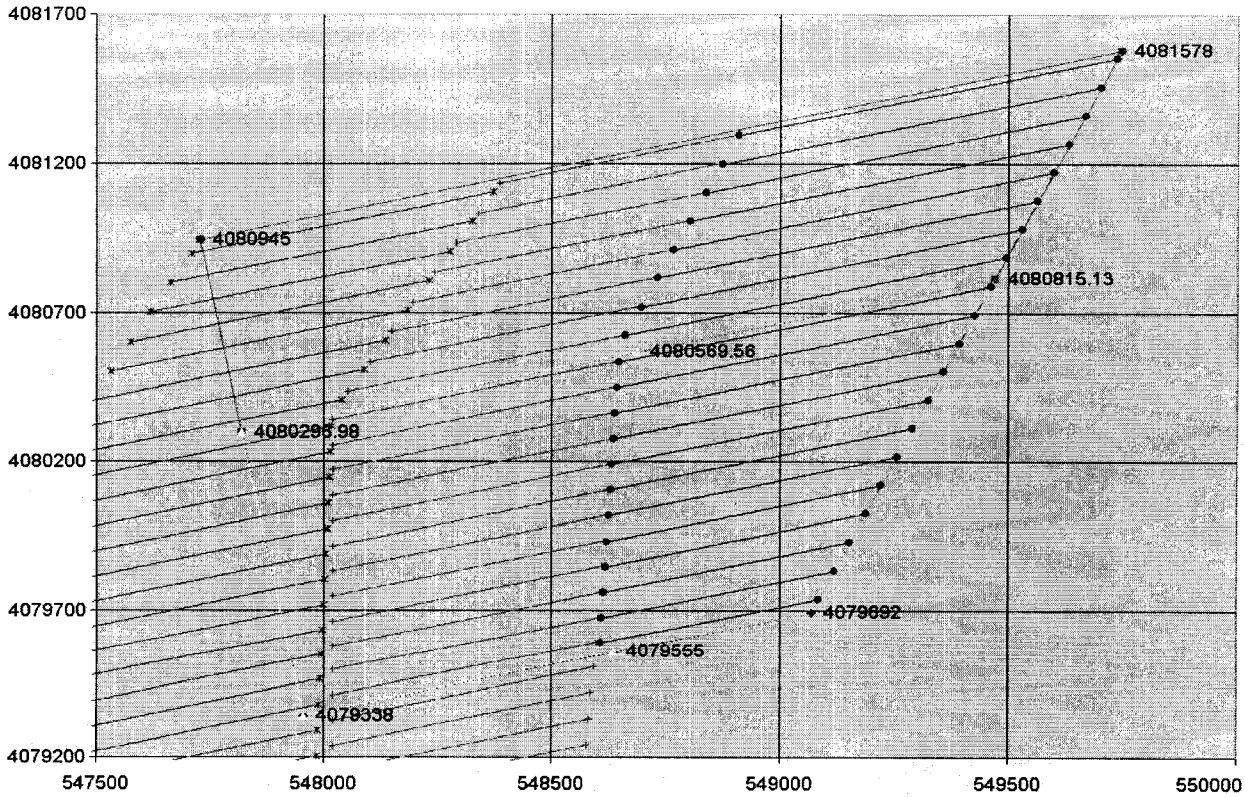
UPDATE REQUIREMENTS for TPA_INCLUDE.INP

SCR 598

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
Modify from	reader	Subarea 3		none	547729., 4080945. 549746., 4081578. 549485., 4080850. 547820., 4080296. 547729., 4080945.	Avoid subarea overlap.	SCR598
Modify to	reader	Subarea 3		none	547729., 4080945. 549746., 4081578. 549471.76, 4080815.13 547820.1, 4080296.98 547729., 4080945.	Avoid subarea overlap.	SCR598

Modify from	reader	Subarea 4		none	547820., 4080296. 548690., 4080586. 548638., 4079555. 547955., 4079338. 547820., 4080296.	Avoid subarea overlap.	SCR598
Modify to	reader	Subarea 4		none	547820.1, 4080296.98 548689., 4080569.56 548638., 4079555. 547955., 4079338. 547820.1, 4080296.98	Avoid subarea overlap.	SCR598
Modify from	reader	Subarea 5		none	548690., 4080586. 549485., 4080850. 549068., 4079692. 548638., 4079555. 548690., 4080586.	Avoid subarea and drift overlap.	SCR598
Modify to	reader	Subarea 5		none	548689., 4080569.56 549471.76, 4080815.13 549070., 4079692. 548638., 4079555. 548689., 4080569.56	Avoid subarea and drift overlap.	SCR598

ATTACHMENT A



Subareas 3, 4, 5, with revised SA3 / 4 & 5 boundary line, and Drifts shown

Attachment B
PC Based Test Plan for TPA SCR#598

Test Plan Name: Subarea Waste Package Count Test

Tested By: Jose M. Menchaca Date: March 7, 2006

Host Machine: AMD Opteron PC Host OS: MS Windows Server 2003 Version 5.2

Baseline Version: TPA 5.0.2o Test Version: TPA 5.0.2p

Process Level (PL) Tests

PL-1. Name: Test of WP count with revised subarea vertices

Path for run directory: D:\Public\jmenchaca\tpa502p\basecaseRuns\singleVector
Note: This is the D: drive on the "TPA" computer.

Path for archive of results: R:\pc_tpa502p\basecaseRuns\singleVector
Note: The R: drive is the designated CD drive for stu2560.

Environment variables: set TPA_TEST=D:\Public\jmenchaca\pc_tpa502p
set TPA_DATA=D:\Public\jmenchaca\pc_tpa502p
Note: This is the D: drive on the "TPA" computer.

Special input files or modifications to input files required : N/A

Pertinent Lines in the tpa.inp file: N/A

Special diagnostic code modifications required: N/A

Program modes to be used (append flags, scenario/model switches, etc.): N/A

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data: N/A

Test 1 description:

- objective:
The objective of this test is to verify that the correct number of waste packages is being counted for subarea 3. The revised subarea coordinates were duplicating a single waste package count because the western edges of subareas 3 and 4 intruded into the eastern edge of subarea 2. SCR 598 corrected this overlap.

- assumptions: N/A

- constraints: N/A

- output files to compare or examine: tpa.out (screen output redirected to tpa.out file)

- step by step test procedure to be used:
Execute a single realization run of the prior version's (tpa502o) standard tpa.inp file. Verify that subarea 3 reports 2905 waste packages. Execute a single realization run of the current version's (tpa502p) standard tpa.inp file. Verify that subarea 3 reports 2904 waste packages.

- pass fail criteria
The pass criteria is achieved if the correct number of waste packages is reported.

Test Results:

- disposition of output and supporting files:
Portion of previous tpa.out file:

```
d:\Public\jmenchaca\pc_tpa502o\basecaseRuns\singleVector>more tpa.out
=====================================================================
         exec: Welcome to TPA Version 5.0.2o
       Job started: Fri Mar 31 16:31:58 2006
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]       [MTU]
   1     224091.0     3025.5         526
   2     448476.0     6108.4        1062
   3    1217081.0    16709.1        2905
   4     782749.5    10313.0        1793
   5     623364.0     8345.9        1451
   6     152357.0     1972.9         343
   7     318122.0     4003.3         696
   8     439350.0     5355.0         931
   9     305880.0     4158.6         723
  10     747165.5    10048.4        1747

Total Area [acre]          =  1299.391153941191
        .
        .
        .
```

Portion of current tpa.out file:

```
d:\Public\jmenchaca\pc_tpa502p\basecaseRuns\singleVector>more tpa.out
=====================================================================
         exec: Welcome to TPA Version 5.0.2p
       Job started: Wed Apr 12 14:36:09 2006
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]      [MTU]
   1     224091.0     3025.5         526
   2     448476.0     6108.4        1062
   3    1241313.5    16703.3        2904
   4     775953.1    10313.0        1793
   5     604631.8     8345.9        1451
   6     152357.0     1972.9         343
   7     318122.0     4003.3         696
   8     439350.0     5355.0         931
   9     305880.0     4158.6         723
  10     747165.5    10048.4        1747

Total Area [acre]          =  1299.070915221193
```

.

.

.

- overall test status (PASS/FAIL): **PASS**

ATTACHMENT C

Unix Based Test Plan for TPA SCR#598

Test Plan Name: Subarea Waste Package Count Test

Tested By: Jose M. Menchaca Date: April 6, 2006

Host Machine: SUN Ultra-4 server: Spock Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0.2o Test Version: TPA 5.0.2p

Process Level (PL) Tests

PL-1. Name: Test of WP count with revised subarea vertices

Path for run directory: ~jmench/unix_tpa502p/basecaseRuns/singleVector

Path for archive of results: R:\unix_tpa502o\basecaseRuns\singleVector
Note: The R: drive is the designated CD drive for stu2560.

Environment variables: setenv TPA_TEST ~/unix_tpa502p
setenv TPA_DATA ~/unix_tpa502p

Special input files or modifications to input files required : N/A

Pertinent Lines in the tpa.inp file: N/A

Special diagnostic code modifications required: N/A

Program modes to be used (append flags, scenario/model switches, etc.): N/A

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data: N/A

Test 1 description:

- objective:
The objective of this test is to verify that the correct number of waste packages is being counted for subarea 3. The revised subarea coordinates were duplicating a single waste package count because the western edges of subareas 3 and 4 intruded into the eastern edge of subarea 2. SCR 598 corrected this overlap.

- assumptions: N/A

- constraints: N/A

- output files to compare or examine: tpa.out (screen output redirected to tpa.out file)

- step by step test procedure to be used:
Execute a single realization run of the prior version's (tpa502o) standard tpa.inp file. Verify that subarea 3 reports 2905 waste packages. Execute a single realization run of the current version's (tpa502p) standard tpa.inp file. Verify that subarea 3 reports 2904 waste packages.

- pass fail criteria
The pass criteria is achieved if the correct number of waste packages is reported.

Test Results:

- disposition of output and supporting files:
Portion of previous version tpa.out file:

```
=====================================================================
          exec: Welcome to TPA Version 5.0.2o
        Job started: Mon Apr  3 10:23:36 2006
=====================================================================
 REPOSITORY DESIGN INFORMATION
 Subarea    Area       Waste    Number of WP
    #      [m^2]      [MTU]
    1    224091.0     3025.5         526
    2    448476.0     6108.4        1062
    3   1217081.0    16709.1        2905
    4    782749.5    10313.0        1793
    5    623364.0     8345.9        1451
    6    152357.0     1972.9         343
    7    318122.0     4003.3         696
    8    439350.0     5355.0         931
    9    305880.0     4158.6         723
   10    747165.5    10048.4        1747

 Total Area [acre]          =     1299.3911539412
       .
       .
       .
```

Portion of current version tpa.out file:

```
==========================================================================
          exec: Welcome to TPA Version 5.0.2p
        Job started: Wed Apr 12 13:34:42 2006
==========================================================================
 REPOSITORY DESIGN INFORMATION
 Subarea    Area       Waste    Number of WP
    #      [m^2]       [MTU]
    1     224091.0     3025.5         526
    2     448476.0     6108.4        1062
    3    1241313.5    16703.3        2904
    4     775953.1    10313.0        1793
    5     604631.8     8345.9        1451
    6     152357.0     1972.9         343
    7     318122.0     4003.3         696
    8     439350.0     5355.0         931
    9     305880.0     4158.6         723
   10     747165.5    10048.4        1747

 Total Area [acre]          =     1299.0709152212
        .
        .
        .
```

- overall test status (PASS/FAIL): **PASS**

Attachment D
PC Based Test Plan 2 for TPA SCR#598

Test Plan Name:	Total MTU and Subarea 5 Waste Package Count Test
Tested By: D. Stead	Date: April 26, 2006
Host Machine: AMD Opteron PC: "TPA"	Host OS: MS Windows Server 2003 Version 5.2
Baseline Version: TPA 5.1 Beta	Test Version: TPA 5.1 Beta A

Process Level (PL) Tests

PL-1. Name: Test of WP count with revised subarea vertices

Path for run directory: D:\DStead\Runs\Run_51b
D:\DStead\Runs\Run_51bA
Note: This is the D: drive on the "TPA" computer.

Path for archive of results: from_TPA\Run_TPA51beta (v. 5.1 Beta)
from_TPA\Run_TPA51betaA (v. 5.1 BetaA)
Note: These paths are relative to the root of the CD.

Environment variables: set TPA_TEST=D:\DStead\TPA_code\TPA_51b (v. 5.1 Beta)
set TPA_DATA=D:\DStead\TPA_code\TPA_51b (v. 5.1 Beta)
set TPA_TEST=D:\DStead\TPA_code\TPA_51bA (v. 5.1 Beta A)
set TPA_DATA=D:\DStead\TPA_code\TPA_51bA (v. 5.2 Beta A)
Note: This is the D: drive on the "TPA" computer.

Special input files or modifications to input files required : N/A

Pertinent Lines in the tpa.inp file: N/A

Special diagnostic code modifications required: N/A

Program modes to be used (append flags, scenario/model switches, etc.): N/A

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data: N/A

Test 1 description:

- objective:
The objective of this test is to verify that the total Buried Waste (MTU) is being reported and that the correct number of waste packages is being counted for subarea 5. The subarea coordinates were causing an error of one waste package because the eastern boundary of subareas 5 cut off the southernmost drift on its eastern end. SCR 598 moved the southeastern boundary point for subarea 5 east by two meters to avoid this error.

- assumptions: N/A

- constraints: N/A

- output files to compare or examine: tpa.out (screen output redirected to tpa.out file)

- step by step test procedure to be used:
1) Execute a single realization run of the prior version (TPA5.1 Beta) with the standard tpa.inp file. Verify that subarea 5 reports 1451 waste packages and that the *Total Buried Waste [MTU]* is 70034.248...

2) Execute a single realization run of the current version (TPA 5.1 Beta A) with the standard tpa.inp file. Verify that subarea 5 reports 1452 waste packages and that the *Total Buried Waste [MTU]* is exactly 70040.

- pass fail criteria
The pass criteria is achieved if the correct number of waste packages and MTU are reported.

Test Results:

- disposition of output and supporting files:
Portion of previous tpa.out file:

```
=====================================================================
         exec: Welcome to TPA Version 5.1beta
       Job started: Wed Apr 26 15:51:36 2006
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]       [MTU]
   1     224091.0     3025.5         526
   2     448476.0     6108.4        1062
   3    1241313.5    16703.3        2904
   4     775953.1    10313.0        1793
   5     604631.8     8345.9        1451
   6     152357.0     1972.9         343
   7     318122.0     4003.3         696
   8     439350.0     5355.0         931
   9     305880.0     4158.6         723
  10     747165.5    10048.4        1747
```

```
Total Area [acre]          =  1299.070915221193
Total Buried Waste [MTU]   =  70034.24817278476
```

Portion of current tpa.out file:

```
=====================================================================
         exec: Welcome to TPA Version 5.1betaA
       Job started: Wed Apr 26 15:13:22 2006
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area       Waste   Number of WP
   #     [m^2]       [MTU]
   1    224091.0     3025.5         526
   2    448476.0     6108.4        1062
   3   1241313.5    16703.3        2904
   4    775953.1    10313.0        1793
   5    605892.0     8351.7        1452
   6    152357.0     1972.9         343
   7    318122.0     4003.3         696
   8    439350.0     5355.0         931
   9    305880.0     4158.6         723
  10    747165.5    10048.4        1747

Total Area [acre]          =  1299.382289078371
Total Buried Waste [MTU]   =  70040.00000000000
```

- overall test status (PASS/FAIL): **PASS**

ATTACHMENT E

Unix Based Test Plan 2 for TPA SCR#598

Test Plan Name: Total MTU and Subarea 5 Waste Package Count Test

Tested By: D. Stead Date: April 26, 2006

Host Machine: SUN SunFire V880: "Texas" Host OS: Sun Solaris 5.9

Baseline Version: TPA 5.1 Beta Test Version: TPA 5.1 Beta A

Process Level (PL) Tests

PL-1. Name: Test of MTU and WP count with revised subarea vertices

Path for run directory: data/dstead/run_51b (v. 5.1 Beta)
data/dstead/run_51ba (v. 5.1 Beta A)

Path for archive of results: from_Texas\Run_TPA51beta (v. 5.1 Beta)
from_Texas\Run_TPA51betaA (v. 5.1 Beta A)
Note: These paths are relative to the root of the CD.

Environment variables: setenv TPA_TEST data/dstead/tpa51b (v. 5.1 Beta)
setenv TPA_DATA data/dstead/tpa51b (v. 5.1 Beta)
setenv TPA_TEST data/dstead/tpa51ba (v. 5.1 Beta A)
setenv TPA_DATA data/dstead/tpa51ba (v. 5.1 Beta A)

Special input files or modifications to input files required : N/A

Pertinent Lines in the tpa.inp file: N/A

Special diagnostic code modifications required: N/A

Program modes to be used (append flags, scenario/model switches, etc.): N/A

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data: N/A

Test 1 description:

- objective:
The objective of this test is to verify that the total Buried Waste (MTU) is being reported and that the correct number of waste packages is being counted for subarea 5. The subarea coordinates were causing an error of one waste package because the eastern boundary of subareas 5 cut off the southernmost drift on its eastern end. SCR 598 moved the southeastern boundary point for subarea 5 east by two meters to avoid this error.

- assumptions: N/A

- constraints: N/A

- output files to compare or examine: tpa.out (screen output redirected to tpa.out file)

- step by step test procedure to be used:
1) Execute a single realization run of the prior version (TPA5.1 Beta) with the standard tpa.inp file. Verify that subarea 5 reports 1451 waste packages and that the *Total Buried Waste [MTU]* is 70034.248...

2) Execute a single realization run of the current version (TPA 5.1 Beta A) with the standard tpa.inp file. Verify that subarea 5 reports 1452 waste packages and that the *Total Buried Waste [MTU]* is exactly 70040.

- pass fail criteria
The pass criteria is achieved if the correct number of waste packages and MTU are reported.

Test Results:

- disposition of output and supporting files:
Portion of previous version tpa.out file:

```
=====================================================================
         exec: Welcome to TPA Version 5.1beta
       Job started: Wed Apr 26 16:09:42 2006
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]      [MTU]
   1     224091.0     3025.5         526
   2     448476.0     6108.4        1062
   3    1241313.5    16703.3        2904
   4     775953.1    10313.0        1793
   5     604631.8     8345.9        1451
   6     152357.0     1972.9         343
   7     318122.0     4003.3         696
   8     439350.0     5355.0         931
   9     305880.0     4158.6         723
  10     747165.5    10048.4        1747
```

```
Total Area [acre]          =     1299.0709152212
Total Buried Waste [MTU]   =     70034.248172785
```

Portion of current version tpa.out file:

```
=====================================================================
         exec: Welcome to TPA Version 5.1betaA
       Job started: Wed Apr 26 15:56:12 2006
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area       Waste   Number of WP
   #      [m^2]      [MTU]
   1    224091.0     3025.5         526
   2    448476.0     6108.4        1062
   3   1241313.5    16703.3        2904
   4    775953.1    10313.0        1793
   5    605892.0     8351.7        1452
   6    152357.0     1972.9         343
   7    318122.0     4003.3         696
   8    439350.0     5355.0         931
   9    305880.0     4158.6         723
  10    747165.5    10048.4        1747

Total Area [acre]          =     1299.3822890784
Total Buried Waste [MTU]   =     70040.000000000
```

- overall test status (PASS/FAIL): **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 599	**2. Software Title and Version:** TPA Version 5.0.2l	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *condxyzt.f, exec.f, failt.f.*

1) The TPA code produces a NaN in several output files when the ventilation end time is the same as a TPA time step.

2) When **AshEvolutionMode** is set to 0 the *ashremob.out* file should be cleared and NOT included as output.

3) Corrosion credit is not restricted to the outer package, but includes the inner also. This is not conservative and should be changed in *failt.f.*

5. Change Requested by:	**6. Change Authorized by** (*Software Developer*):
A. Simpkins, R. Rice Date: 3-15-06	R. Janetzke Date: 3-15-06

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

1) Put an "`if then`" test in **tempgl()** function of *condxyzt.f* to prevent division by zero.

2) Added an "`inquire`" "`rm`" combination to remove existing *ashremob.out* files.

3) Removed InnerWPThickness corrosion credit from total thickness calculations.

See Attachment A for details.

8. Implemented by:	**Date:**
J. Menchaca	3-22-06

9. Description of Acceptance Tests:

See Attachment B for the Windows test plan.

See Attachment C for the Unix test plan.

10. Tested by:	**Date:**
J. Mancillas	4-27-06

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 598

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
No Change to any TPA.INP parameter							

ATTACHMENT A

1) If the **RatioOfLastToFirstTimeStepInCompliancePeriod** is changed such that a time step coincides with the ventilation end time a `NaN` error occurs in several files. An "`if then`" test in the **tempgl()** function of *condxyzt.f* was inserted to prevent division by zero.

```
483c483,490
< cjmm SCR599 20060322 To remove NaN errors when tend = t
---
>       tempgl =  qpp / ( 4.0d0 * rho * cp * dsqrt(3.14159265359d0) ) *
>      &  ( 1.0d0 / dsqrt( 4.0d0 * alpha * (tend - t ) ) ) *
>      &  ( zportderf((aL - x)/dsqrt(4.0d0 * alpha * (tend - t))) +
>      &    zportderf((aL + x)/dsqrt(4.0d0 * alpha * (tend - t))) ) *
>      &  ( zportderf((aB - y)/dsqrt(4.0d0 * alpha * (tend - t))) +
>      &    zportderf((aB + y)/dsqrt(4.0d0 * alpha * (tend - t))) ) *
>      &  ( dmyexp( - z**2 / ( 4.0d0 * alpha * (tend-t) ) )  -
>      &    dmyexp( - (z-2.0 * aH)**2/ ( 4.0d0 * alpha * (tend-t) ) )  )
485,499d491
<       if (tend .eq. t) then
<          tempgl = 0
<       else
<          tempgl =  qpp / ( 4.0d0 * rho * cp * dsqrt(3.14159265359d0) ) *
<      &     ( 1.0d0 / dsqrt( 4.0d0 * alpha * (tend - t ) ) ) *
<      &     ( zportderf((aL - x)/dsqrt(4.0d0 * alpha * (tend - t))) +
<      &       zportderf((aL + x)/dsqrt(4.0d0 * alpha * (tend - t))) ) *
<      &     ( zportderf((aB - y)/dsqrt(4.0d0 * alpha * (tend - t))) +
<      &       zportderf((aB + y)/dsqrt(4.0d0 * alpha * (tend - t))) ) *
<      &     ( dmyexp( - z**2 / ( 4.0d0 * alpha * (tend-t) ) )  -
<      &       dmyexp( - (z-2.0 * aH)**2/ ( 4.0d0 * alpha * (tend-t) ) ))
<       endif
<
< cjmm end SCR 599
<
```

2) If **AshEvolutionMode** is set to 0 and run in the same directory as a previous run with the **AshEvolutionMode** is set to 1, the *ashremob.out* file is not cleared and remains as an output file. Adding an "`inquire`" "`rm`" combination in *exec.f* to remove any pre-existing *ashremob.out* file solved the problem.

```
9596,9600d9595
< cjmm 20060321 SCR599 clear ashremob.out if it exists
<         inquire( file='ashremob.out', EXIST=lexist)
<         if (lexist) istatus = zportsh( 'rm ashremob.out' )
< cjmm end SCR599
<
```

3) Corrosion credit is given to both the inner package (**InnerWPThickness[m]**) and the outer package (**OuterWPThickness[m]**). To be conservative, restrict the corrosion to the outer package only in *failt.f.*

```
440,444c440
< cjmm SCR599 20060322 To restrict corrosion credit to OuterWPThickness (cthick1)
< cjmm                 remove InnerWPThickness corrosion credit (cthick2).
< cjmm      thicktot = cthick1 + cthick2
<           thicktot = cthick1
< cjmm end SCR599
---
>           thicktot = cthick1 + cthick2
```

Attachment B
Test Plan for TPA SCR599

Test Plan Name: SCR599 Testing for Windows XP

Tested By: J. Mancillas | Date: 04-27-2006

Host Machine: TPA | Host OS: Win XP

Baseline Version: TPA 5.0.2l | Test Version: TPA 5.0.2m

Process Level (PL) Tests

PL-1. Name: Comparison between baseline and test versions of the TPA code for SCR599

Path for run directory: None

Path for archive of results: CD titled: SCR599 Testing: \SCR599\files_fc\

Environment variables: None

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Compare baseline and test versions of the file modified by SCR599. These files are *condxyzt.f, exec.f* and *failt.f.*

- objective: The objective of this test is to verify that the requested modifications were included into the test version of the TPA code, and that no other inadvertent changes were made.

- assumptions: None

- constraints: None

- output files to compare or examine: Examine the baseline and test versions of the modified files and examine the results of a file comparison between the baseline and test versions of the modified

files.

- step by step test procedure to be used

1) perform a file comparison between the baseline and test versions of the modified files: *condxyz.f, exec.f* and *failt.f* using the windows system command 'fc'. The output of the file comparisons will be saved as: *condxyz_fc, exec_fc* and *failt_fc*.
2) Examine the differences between the versions of the code, looking for extraordinary code changes not defined by SCR599.
3) Examine the test version of the code for proper code syntax and logic changes

- pass fail criteria

The changes made to the TPA test version are consistent with those requested by SCR599

Test Results:

The following text is an excerpt from \SCR599\files_fc*condxyzt_fc*, which is a file comparison between the baseline and test versions of *condxyzt.f*. This excerpt shows the functional differences between the two versions.

```
***** TPA502M\condxyzt.f

cjmm SCR599 20060322 To remove NaN errors when tend = t

      if (tend .eq. t) then
         tempgl = 0
      else
         tempgl =  qpp / ( 4.0d0 * rho * cp * dsqrt(3.14159265359d0) ) *
     &      ( 1.0d0 / dsqrt( 4.0d0 * alpha * (tend - t ) ) ) *
     &      ( zportderf((aL - x)/dsqrt(4.0d0 * alpha * (tend - t))) +
     &        zportderf((aL + x)/dsqrt(4.0d0 * alpha * (tend - t))) ) *
     &      ( zportderf((aB - y)/dsqrt(4.0d0 * alpha * (tend - t))) +
     &        zportderf((aB + y)/dsqrt(4.0d0 * alpha * (tend - t))) ) *
     &      ( dmyexp( - z**2 / ( 4.0d0 * alpha * (tend-t) ) )  -
     &        dmyexp( - (z-2.0 * aH)**2/ ( 4.0d0 * alpha * (tend-t) ) ))
      endif

cjmm end SCR 599

***** TPA502L\CONDXYZT.F

      tempgl =  qpp / ( 4.0d0 * rho * cp * dsqrt(3.14159265359d0) ) *
     &  ( 1.0d0 / dsqrt( 4.0d0 * alpha * (tend - t ) ) ) *
     &  ( zportderf((aL - x)/dsqrt(4.0d0 * alpha * (tend - t))) +
     &    zportderf((aL + x)/dsqrt(4.0d0 * alpha * (tend - t))) ) *
     &  ( zportderf((aB - y)/dsqrt(4.0d0 * alpha * (tend - t))) +
     &    zportderf((aB + y)/dsqrt(4.0d0 * alpha * (tend - t))) ) *
     &  ( dmyexp( - z**2 / ( 4.0d0 * alpha * (tend-t) ) )  -
     &    dmyexp( - (z-2.0 * aH)**2/ ( 4.0d0 * alpha * (tend-t) ) )  )

*****
```

The functional difference between the two codes is the inclusion of a conditional statement which prevents the possible division by zero and return of a NaN.
This is presented as evidence that SCR599 was properly implemented.

The following text is an excerpt from \SCR599\files_fc*exec_fc*, which is a file comparison between the baseline and test versions of *exec.f*. This excerpt shows the functional differences between the two versions.

```
***** TPA502M\exec.f

cjmm 20060321 SCR599 clear ashremob.out if it exists
        inquire( file='ashremob.out', EXIST=lexist)
        if (lexist) istatus = zportsh( 'rm ashremob.out' )
cjmm end SCR599
```

The functional difference between the two versions of *exec.f* is the conditional check for a previously existing ashremob.out file. If the file exists then it is removed to prevent its use in the current TPA realization.
This is presented as evidence that SCR599 was properly implemented.

The following text is an excerpt from \SCR599\files_fc*failt_fc*, which is a file comparison between the baseline and test versions of *fail.f*. This excerpt shows the functional differences between the two versions.

```
***** TPA502M\CODES\failt.f

cjmm SCR599 20060322 To restrict corrosion credit to OuterWPThickness (cthick1)
cjmm                 remove InnerWPThickness corrosion credit (cthick2).
cjmm      thicktot = cthick1 + cthick2
          thicktot = cthick1
cjmm end SCR599

***** TPA502L\CODES\FAILT.F

          thicktot = cthick1 + cthick2

*****
```

The functional difference between the two versions of failt.f is the value for thicktot. In the test version this value is initially set to cthick1, which corresponds to the WP outer barrier thickness. In the baseline version thicktot is initially set to the sum of cthick1 and cthick2, which are the inner and outer WP barrier thickness (these values are read from the data file *ebsfail.inp*).

This is presented as evidence that SCR599 was properly implemented.

- overall test status: **PASS**

System Level (SL) Tests

SL-1. Name: NaN generated when TPA time step equals end of active ventilation

Path for run directory:

Baseline: [TPA] D:\Mancillas\tpa502l\test1\L
Test : [TPA] D:\Mancillas\tpa502m\test1\M

Path for archive of results:

Baseline: CD[Titled: SCR599 Testing] :SCR599\test1\L
Test : CD[Titled: SCR599 Testing] :SCR599\test1\M

Environment variables:

Baseline: TPA_DATA=D:\Mancillas\tpa502l
TPA_TEST =D:\Mancillas\tpa502l

Test : TPA_DATA=D:\Mancillas\tpa502m
TPA_TEST =D:\Mancillas\tpa502m

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: When the time for end of ventilation corresponds to a TPA time step a NaN value is generated by the **tempgl()** function of *condxyzt.f*. This results in a crash of the TPA code. This has been corrected in the test version of the TPA.

- objective: Verify that when the TPA time step corresponds to the end of active ventilation a NaN is not generated.

- assumptions None other than those made within the TPA code

- constraints None

- output files to compare or examine screen capture of TPA execution

- step by step test procedure to be used

1) Set the ratio of first and last time steps during the compliance period to 1.00 (in the *tpa.inp* file) for a baseline and test version TPA realizations. This will result in TPA time steps with equal spacings of 50 yrs. The default time for the end of active

ventilation is 50yrs.
2)Examine the screen captures of the baseline and test TPA code realizations

- pass fail criteria
  1) This conditions should result in the crash of the baseline TPA code, and the test version of the TPA code should execute properly

Test Results:

During the execution of the baseline TPA code, the code crashed during a call to the module ebsfail.
The screen capture of this realization is *SCR599\test1\L\out.*

During the execution of the test TPA code, the code successfully executed.
The screen capture of this realization is *SCR599\test1\M\out.*

The crash of the basecase and the successful execution of the test case are presented as evidence that SCR599 has been properly implemented.

- overall test status: **PASS**

SL-2. Name: Ensure that the file ashremob.out which might be present from a previous realization is removed.

Path for run directory:
Baseline: [TPA] D:\Mancillas\tpa502l\test2\L

Path for archive of results:
Baseline: CD[Titled: SCR599 Testing] :SCR599\test2

Environment variables:

Test : TPA_DATA=D:\Mancillas\tpa502m
TPA_TEST =D:\Mancillas\tpa502m

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Append all, activate Volcanism disruptive event

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: With the **VolcanismDisruptiveScenarioFlag(yes=1,no=0)** parameter set to 1 and the **AshEvolutionMode** set to 1, the TPA code will generate the file *ashremob.out.* In the previous version of the TPA code (TPA 502l), the file ashremob.out would persist if a subsequent TPA run were performed in the same directory, even if this module was not used (either **VolcanismDisruptiveScenarioFlag(yes=1,no=0)** set to 0 or **AshEvolutionMode** set to 0). This test is developed to verify that the file ashremob.out was removed if it existed from a previous TPA realization.

- objective Ensure that if the file ashremob.out which exists in a run directory from a previous realization exists that it is removed.

- assumptions None other than those made in the TPA code

- constraints None

- output files to compare or examine List of files in a run directory

- step by step test procedure to be used
  1) In directory *Mancillas\test2\M1* perform a single realization of the TPA code for subarea 1, with **VolcanismDisruptiveScenarioFlag(yes=1,no=0)** parameter set to 1 and **AshEvolutionMode** set to 1, and Append all .
  2) copy all the files generated by the TPA execution into a second directory named *Mancillas\test2\M2*

3) In directory *Mancillas\test2\M2* perform a single realization of the TPA code for subarea 1,with **VolcanismDisruptiveScenarioFlag(yes=1,no=0)** parameter set to 1 and **AshEvolutionMode** set to 0, and Append all

4) Compare the directory contents of *Mancillas\test2\M1* and *Mancillas\test2\M2* .

- pass fail criteria

1) If SCR599 has been properly implemented then the directory *Mancillas\test2\M2* should not contain a copy of the file *ashremob.out* which was copied into that directory from *Mancillas\test2\M1*.

Test Results:

The following text are excerpts from the files *Mancillas\test2\yes_ashremob.out* and *Mancillas\test2\no_ashremob.out*. These two files are the directory listings of *Mancillas\test2\M1* and *Mancillas\test2\M2* , respectively.

Volume in drive D is Data
Volume Serial Number is E88F-D312

The following is the first several files which are in *Mancillas\test2\M1*, which are archived into the directory [CD: SCR599]: *SCR599\test2\M1*

```
 Directory of D:Mancillas\test2\M1

04/27/2006  12:17 PM    <DIR>          .
04/27/2006  12:17 PM    <DIR>          ..
04/27/2006  12:14 PM             2,753 airpkdos.res
04/27/2006  12:14 PM             2,753 arpkds_c.res
04/27/2006  12:14 PM               794 ashout.res
04/27/2006  12:14 PM            53,066 ashremob.out
03/23/2006  05:43 PM             1,736 burnup.dat
04/27/2006  12:14 PM             5,250 chlrdmf.dat
03/23/2006  05:43 PM           900,000 climato1.dat
03/23/2006  05:43 PM             3,645 climato2.dat
```

The following is the first several files which are in *Mancillas\test2\M2,* which are archived into the directory [CD: SCR599]: *SCR599\test2\M2*

```
 Directory of D:\Mancillas\test2\M2

04/27/2006  12:17 PM    <DIR>          .
04/27/2006  12:17 PM    <DIR>          ..
04/27/2006  12:16 PM             2,753 airpkdos.res
04/27/2006  12:16 PM             2,753 arpkds_c.res
04/27/2006  12:16 PM             3,655 ashcmd.out
04/27/2006  12:16 PM               921 ashout.res
03/23/2006  05:50 PM           653,596 ashplume.exe
04/27/2006  12:16 PM             1,643 ashplume.in
04/27/2006  12:16 PM             2,114 ashplume.out
03/23/2006  05:43 PM             1,736 burnup.dat
04/27/2006  12:16 PM             5,250 chlrdmf.dat
03/23/2006  05:43 PM           900,000 climato1.dat
```

```
03/23/2006  05:43 PM            3,645 climato2.dat
```

The file ashremob.out has been removed during the execution of the TPA code in the directory *SCR599\test2\M2*. This is the expected behavior of the TPA code. These results area presented as evidence that SCR599 has been properly implemented.

- overall test status **PASS**

SL-3. Name: WP initial thickness for corrosion analysis

Path for run directory:

Baseline: [TPA] D:\Mancillas\tpa502l\test3\L
Test : [TPA] D:\Mancillas\tpa502m\test3\M

Path for archive of results:

Baseline: CD[Titled: SCR599 Testing] :SCR599\test3\L
Test : CD[Titled: SCR599 Testing] :SCR599\test3\M

Environment variables:

Baseline: TPA_DATA=D:\Mancillas\tpa502l
TPA_TEST =D:\Mancillas\tpa502l

Test : TPA_DATA=D:\Mancillas\tpa502m
TPA_TEST =D:\Mancillas\tpa502m

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Append All

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: The WP thickness used to determine failure by corrosion is recorded in the append file *corrode.out.*. The WP thickness in this file should have an initial value for the WP thickness equal to the WP outer barrier thickness defined in the *tpa.inp* file. A comparison between the baseline and test versions of the corrode.out WP thicknesses should show that in the baseline case the WP thickness is equal to the total thickness of the WP barriers and in the test case the WP thickness is equal to the WP outer barrier thickness. (Note: The outer barrier provides substantial corrosion resistance because it is made of alloy-22, while the inner barrier is made of SS-316 which is significantly less corrosion resistant.)

- objective Verify that the WP thickness used to evaluate corrosion life of the WP is only the outer barrier thickness

- assumptions None other than those made within the TPA code

- constraints None

- output files to compare or examine *corrode.out, tpa.inp*

- step by step test procedure to be used

1) Examine the WP thickness in the append files *corrode.out* for the baseline and test

versions of the TPA code and compare those thicknesses to the thicknesses defined in the *tpa.inp* files

- pass fail criteria

  1) The WP thicknesses in the test version of the corrode.out should initially begin at the WP outer barrier thickness given in the *tpa.inp* file

Test Results:

The following text are excerpts from the baseline *tpa.inp* file and the *corrode.out* file.

CD:\SCR599\test3\L\tpa.inp

```
constant
OuterWPThickness[m]
0.02
**
constant
InnerWPThickness[m]
0.05
```

CD:\SCR599\test3\L\corrode.out

```
 ilayer  tstop      tcan      ecrit      ecorr   chloride   rthick      mode
         [yr]       [C]       [vshe]     [vshe]    flag       [m]
=================================================================================
 1        2.31      63.92     0.0000     0.0000     0    7.0000000E-02  dry oxd
```

These excerpt show that the total thickness of the WP is 0.07m. This total thickness is the value used in the corrosion analysis for the initial value of *rthick* is 0.07m, which is the total thickness. This result is inconsistent with the TPA abstraction of WP corrosion failure analysis

The following text are excerpts from the test version *tpa.inp* file and the *corrode.out* file.

CD:\SCR599\test3\M\tpa.inp

```
constant
OuterWPThickness[m]
0.02
**
constant
InnerWPThickness[m]
0.05
```

CD:\SCR599\test3\M\corrode.out

```
 ilayer  tstop      tcan      ecrit      ecorr   chloride   rthick      mode
         [yr]       [C]       [vshe]     [vshe]    flag       [m]
=================================================================================
 1        2.31      63.92     0.0000     0.0000     0    2.0000000E-02  dry oxd
```

These excerpt show that the total thickness of the WP is 0.07m. This total thickness is the value used in the corrosion analysis for the initial value of *rthick* is 0.02m. This is the correct value and is consistent with the TPA abstraction of WP corrosion failure analysis.

These results are presented as evidence that SCR599 has been properly implemented.

- overall test status **PASS**

Attachment C
Test Plan for TPA SCR599

Test Plan Name: SCR599 Comparison between Windows and Unix results

Tested By: J. Mancillas

Date: 04-27-2006

Host Machine:
Baseline: TPA
Test : spock

Host OS:
Baseline: Windows XP
Test : Unix SunOS 5.9

Baseline Version: TPA 502m

Test Version: TPA 502m

System Level (SL) Tests

SL-1. Name: Comparison between Windows and Unix platform results for TPA502m

Path for run directory:
Baseline: [TPA]D:\Mancillas\meanrun
Test : [spock]:home/jmancillas/TPA/meanrun

Path for archive of results:
Baseline: [CD: Titled: SCR599 Testing]:SCR599\meanrun
Test : [CD: Titled: SCR599 Testing]:SCR599\Unix\meanrun

Environment variables:
Baseline: TPA_DATA=D:\Mancillas\tpa502m
TPA_TEST =D:\Mancillas\tpa502m

Test : TPA_DATA=//home/jmancillas/TPA/tpa502m/
TPA_TEST =//home/jmancillas/TPA/tpa502m/

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): mean value case

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Compare the time and the value of the peak mean dose for the Windows platform TPA502m and the Unix platform TPA502m.

- objective Ensure that the two versions of TPA502m generate the same results and are consistent

with each others calculations

- assumptions None

- constraints None

- output files to compare or examine Screen capture of TPA execution

- step by step test procedure to be used
  1) execute the TPA code on both OS platforms using the mean value case.

- pass fail criteria
  1) the time and values for the peak mean dose should be the same

Test Results: The mean peak values calculated by the baseline (Windows) and test (Unix) TPA502m versions are presented bellow.

The following text excerpt shows the peak mean dose calculated by the baseline TPA502m.
SCR599\Mancillas\meanrun\out

```
exec: end realizations

exec: Peak Mean Dose is 5.51830E-04 rem/yr at    1994.7 yr, based on     1
realizations.

exec:  Run Successfully Completed
```

And the following text excerpt shows the peak mean dose calculated by the test TPA502m
SCR599\Unix\meanrun\out

```
exec: end realizations

 exec: Peak Mean Dose is 5.51830E-04 rem/yr at    1994.7 yr, based on     1
realizations.

 exec:  Run Successfully Completed
```

The peak mean dose for both TPA platform calculation have the same time of 1994.7 yrs and value of 5.51830E-04 rem/yr. These results are presented as evidence that SCR599 has been properly implemented for both operating platforms.

- overall test status **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 600	2. Software Title and Version: TPA 5.0.2c	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *tpa.inp, tpa_include.inp, exec.f sampler.f*

I) The Repository Block is currently divided into 8 subareas to allow for consideration of differences in spatial infiltration patterns, and rock types. A report by Fedors et al (2005) documents the basis for the 8 subareas. The subarea identified as subarea 3 in that report is much larger than all of the other subareas, and there is a concern that dose estimates are being dominated by this subarea when certain combinations of stochastic parameters occur that are applied over such a large area, when, in fact, these parameter combinations should be much more spatially variable.

Reference: Fedors, R.F, et al. "Updates to Hydrology-Related Abstractions and Inputs for the Total-System Performance Assessment Version 5.0.1 Code." CNWRA Letter Report. 2005.

II) The use of the *tpameans.out* file as a TPA input file produces an error when the number of realizations is not set to 1.

5. Change Requested by: James Winterle Date: 10-31-05	6. Change Authorized by (*Software Developer*): Ron Janetzke Date: 11-4-05

7. Description of Change(s) or Problem Resolution:

See Attachment A.

8. Implemented by: James Winterle	Date: 12/08/2005

9. Description of Acceptance Tests:

See Attachment C for PC platform tests.

See Attachment D for Unix platform tests.

10. Tested by: D. Stead	Date: 03/29/2006

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 600

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
(ADD, DELETE, MODIFY TO, MODIFY FROM)			***(Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)*** **Distribution, Range**			***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	
Add	SEISMO	StartingBlockPointerOne_9[] StartingBlockPointerOne_10[]		uniform	1, 10000	Adds two subareas. Same values used as for the other 8 subareas.	SCR600

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Add	SEISMO	StartingBlockPointerTwo_9[] StartingBlockPointerTwo_10[]		uniform	1, 10000	Adds two subareas. Same values used as for the other 8 subareas.	SCR600
Add	SEISMO	FractionRockTypeOneInSubarea_9[] FractionRockTypeOneInSubarea_10[]		constant	0.85	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	SEISMO	BulkingFactorRockTypeOneSubarea_9[] BulkingFactorRockTypeOneSubarea_10[]		uniform	1.15, 1.25	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	SEISMO	BulkingFactorRockTypeTwoSubarea_9[] BulkingFactorRockTypeTwoSubarea_10[]		uniform	1.15, 1.25	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	SEISMO	DegradationTimeRockTypeOneSubarea_9[yr] DegradationTimeRockTypeOneSubarea_10[yr]		beta	250.0, 1000.0, 3.25842, 1.82124	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	SEISMO	DegradationTimeRockTypeTwoSubarea_9[yr] DegradationTimeRockTypeTwoSubarea_10[yr]		beta	250.0, 1000.0, 3.25842, 1.82124	Add two subareas. Same values used as for the other 8 subareas.	SCR600

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Add	SEISMO	GroundAccelerationInitialRockTypeOneSubarea_9[pga] GroundAccelerationInitialRockTypeOneSubarea_10[pga]		beta	0.2, 0.3, 2.21348, 5.85392	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	SEISMO	GroundAccelerationInitialRockTypeTwoSubarea_9[pga] GroundAccelerationInitialRockTypeTwoSubarea_10[pga]		beta	0.2, 0.3, 2.21348, 5.85392	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	SEISMO	GroundAccelerationMaximumlRockTypeOneSubarea_9[pga] GroundAccelerationMaximumlRockTypeOneSubarea_10[pga]		beta	1.0, 2.0, 2.79439, 17.1495	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	SEISMO	GroundAccelerationMaximumlRockTypeTwoSubarea_9[pga] GroundAccelerationMaximumlRockTypeTwoSubarea_10[pga]		beta	1.0, 2.0, 2.79439, 17.1495	Add two subareas. Same values used as for the other 8 subareas.	SCR600

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Add	SEISMO	DripShieldBucklingLoadSubarea_9[kg/m] DripShieldBucklingLoadSubarea_10[kg/m]		beta	25000.0, 150000.0, 2.08134, 8.92986	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	EBSREL	SFWettedFraction_Initial_9 SFWettedFraction_Initial_10		uniform	0,1	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	EBSREL	SFWettedFraction_Seismo1_9 SFWettedFraction_Seismo1_10		uniform	0,1	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	EBSREL	SFWettedFraction_Seismo2_9 SFWettedFraction_Seismo2_10		uniform	0,1	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	EBSREL	SFWettedFraction_Seismo3_9 SFWettedFraction_Seismo3_10		uniform	0,1	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	EBSREL	SFWettedFraction_Seismo4_9 SFWettedFraction_Seismo4_10		uniform	0,1	Add two subareas. Same values used as for the other 8 subareas.	SCR600

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Add	EBSREL	SFWettedFraction_Corrosion_9 SFWettedFraction_Corrosion_10		uniform	0,1	Add two subareas. Same values used as for the other 8 subareas.	SCR600
Add	EBSREL	InletArea_9Subarea[m2] InletArea_10Subarea[m2]		constant	5.4e5	Add two subareas. Same values used as for the other 8 subareas.	SCR600

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Modify from	UZFT	TSw_Thickness_4SubArea[m]		constant	68.0	(Apply throughout) Values for old subarea 4 are now the values for subarea 6; old subarea 5 becomes subarea 7; old subarea 6 becomes subarea 8; old subarea 7 becomes subarea 9, and old subarea 8 becomes subarea 10. New values will need to be estimated for subareas 3, 4, and 5; in the interim, however, old values for subarea 3 are assigned to subareas 3, 4 and 5 because they are all within the domain of old subarea 3.	
Modify to	UZFT	TSw_Thickness_4SubArea[m]		constant	111.4		

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Modify from	UZFT	CHnvThickness_4SubArea[m]		triangular	51.7, 55.5, 62.1		
Modify to	UZFT	CHnvThickness_4SubArea[m]		triangular	0.0, 4.2, 9.1		
Modify from	UZFT	CH_Total_Thickness_4SubArea[m]		constant	89.2		
Modify to	UZFT	CH_Total_Thickness_4SubArea[m]		constant	157.4		
Modify from	UZFT	PPw_Thickness_4SubArea[m]		constant	47.7		
Modify to	UZFT	PPw_Thickness_4SubArea[m]		constant	10.0		
Modify from	UZFT	UCF_Thickness_4SubArea[m]		constant	52.2		
Modify to	UZFT	UCF_Thickness_4SubArea[m]		constant	0.0		
Modify from	UZFT	BFw_Thickness_4SubArea[m]		constant	15.0		
Modify to	UZFT	BFw_Thickness_4SubArea[m]		constant	0.0		

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Modify from	UZFT	TSw_Thickness_5SubArea[m]		constant	112.6		
Modify to	UZFT	TSw_Thickness_5SubArea[m]		constant	111.4		
Modify from	UZFT	CHnvThickness_5SubArea[m]		triangular	3.2, 49.5, 62.7		
Modify to	UZFT	CHnvThickness_5SubArea[m]		triangular	0.0, 4.2, 9.1		
Modify from	UZFT	CH_Total_Thickness_5SubArea[m]		constant	101.2		
Modify to	UZFT	CH_Total_Thickness_5SubArea[m]		constant	157.4		
Modify from	UZFT	PPw_Thickness_5SubArea[m]		constant	45.7		
Modify to	UZFT	PPw_Thickness_5SubArea[m]		constant	10.0		
Modify from	UZFT	UCF_Thickness_5SubArea[m]		constant	37.1		
Modify to	UZFT	UCF_Thickness_5SubArea[m]		constant	0.0		

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Modify from	UZFT	BFw_Thickness_5SubArea[m]		constant	3.0		
Modify to	UZFT	BFw_Thickness_5SubArea[m]		constant	0.0		
Modify from	UZFT	TSw_Thickness_6SubArea[m]		constant	170.1		
Modify to	UZFT	TSw_Thickness_6SubArea[m]		constant	68.0		
Modify from	UZFT	CHnvThickness_6SubArea[m]		triangular	2.4, 16.7, 71.2		
Modify to	UZFT	CHnvThickness_6SubArea[m]		triangular	51.7, 55.5, 62.1		
Modify from	UZFT	CH_Total_Thickness_6SubArea[m]		constant	119.3		
Modify to	UZFT	CH_Total_Thickness_6SubArea[m]		constant	89.2		
Modify from	UZFT	PPw_Thickness_6SubArea[m]		constant	31.7		
Modify to	UZFT	PPw_Thickness_6SubArea[m]		constant	47.7		

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Modify from	UZFT	UCF_Thickness_6SubArea[m]		constant	3.0		
Modify to	UZFT	UCF_Thickness_6SubArea[m]		constant	52.2		
Modify from	UZFT	BFw_Thickness_6SubArea[m]		constant	0.0		
Modify to	UZFT	BFw_Thickness_6SubArea[m]		constant	15.0		
Modify from	UZFT	TSw_Thickness_7SubArea[m]		constant	140.4		
Modify to	UZFT	TSw_Thickness_7SubArea[m]		constant	112.6		
Modify from	UZFT	CHnvThickness_7SubArea[m]		triangular	2.4, 38.5, 104.0		
Modify to	UZFT	CHnvThickness_7SubArea[m]		triangular	3.2, 49.5, 62.7		
Modify from	UZFT	CH_Total_Thickness_7SubArea[m]		constant	104.0		
Modify to	UZFT	CH_Total_Thickness_7SubArea[m]		constant	101.2		

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Modify from	UZFT	PPw_Thickness_7SubArea[m]		constant	46.2		
Modify to	UZFT	PPw_Thickness_7SubArea[m]		constant	45.7		
Modify from	UZFT	UCF_Thickness_7SubArea[m]		constant	33.0		
Modify to	UZFT	UCF_Thickness_7SubArea[m]		constant	37.1		
Modify from	UZFT	BFw_Thickness_7SubArea[m]		constant	5.0		
Modify to	UZFT	BFw_Thickness_7SubArea[m]		constant	3.0		
Modify from	UZFT	TSw_Thickness_8SubArea[m]		constant	116.5		
Modify to	UZFT	TSw_Thickness_8SubArea[m]		constant	170.0		
Modify from	UZFT	CHnvThickness_8SubArea[m]		triangular	3.9, 65.0, 96.0		
Modify to	UZFT	CHnvThickness_8SubArea[m]		triangular	2.4, 16.7, 71.2		

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Modify from	UZFT	CH_Total_Thickness_8SubArea[m]		constant	97.0		
Modify to	UZFT	CH_Total_Thickness_8SubArea[m]		constant	119.3		
Modify from	UZFT	PPw_Thickness_8SubArea[m]		constant	57.5		
Modify to	UZFT	PPw_Thickness_8SubArea[m]		constant	31.7		
Modify from	UZFT	UCF_Thickness_8SubArea[m]		constant	58.3		
Modify to	UZFT	UCF_Thickness_8SubArea[m]		constant	3.0		
Modify from	UZFT	BFw_Thickness_8SubArea[m]		constant	15.0		
Modify to	UZFT	BFw_Thickness_8SubArea[m]		constant	0.0		
Add	UZFT	TSw_Thickness_9SubArea[m]		constant	140.4		
Add	UZFT	CHnvThickness_9SubArea[m]		triangular	2.4, 38.5, 104.0		

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Add	UZFT	CH_Total_Thickness_9SubArea[m]		constant	104.0		
Add	UZFT	PPw_Thickness_9SubArea[m]		constant	46.2		
Add	UZFT	UCF_Thickness_9SubArea[m]		constant	33.0		
Add	UZFT	BFw_Thickness_9SubArea[m]		constant	5.0		
Add	UZFT	UFZ_Thickness_9SubArea[m]		constant	0.0		
Add	UZFT	TSw_Thickness_10SubArea[m]		constant	116.5		
Add	UZFT	CHnvThickness_10SubArea[m]		triangular	3.9, 65.0, 96.0		
Add	UZFT	CH_Total_Thickness_10SubArea[m]		constant	97.0		
Add	UZFT	PPw_Thickness_10SubArea[m]		constant	57.5		
Add	UZFT	UCF_Thickness_10SubArea[m]		constant	58.3		

Status	Module	Parameter Name	Description	Distribution	Range	Justification	Source
Add	UZFT	BFw_Thickness_10SubArea[m]		constant	15.0		
Add	UZFT	UFZ_Thickness_10SubArea[m]		constant	0.0		

ATTACHMENT A

The following changes were made:

Part I)

(1) Two additional subareas were added by splitting old subarea 3 into three parts. The Attachment B on the following page shows a picture of this revised subarea layout and the new numbering system. This change is implemented in the file *tpa_include.inp*, which resides in the data directory, by specifying new subareas.

(2) For *tpa.inp*, numerous changes were also made to the tpa.inp file. Basically, for all subarea specific parameters, new parameters had to be added for the two new subareas. Also, subarea-specific parameter values were changed to reflect renumbering of subareas. Values for old subarea 4 are now the values for subarea 6; old subarea 5 becomes subarea 7; old subarea 6 becomes subarea 8; old subarea 7 becomes subarea 9, and old subarea 8 becomes subarea 10.

(3) Parameter values for UZ layer thicknesses are duplicated for new subareas 3, 4, and 5, which reflect the splitting of old subarea 3.

Preliminary testing was done by running the TPA version 5.0.2a with the revised *tpa.inp* file and *tpa_include.inp* file in the data directory. This run was in stochastic mode for a single realization, no volcano or faulting were selected. The model ran successfully. I then ran the code using the *tpameans.out* file as the input file and compared results with a run of the *tpameans.out* file from a run with the previous 8-subarea version of the input file. Both runs resulted in peak mean dose of 3.2E-4 rem/yr at 1994.7 yr.

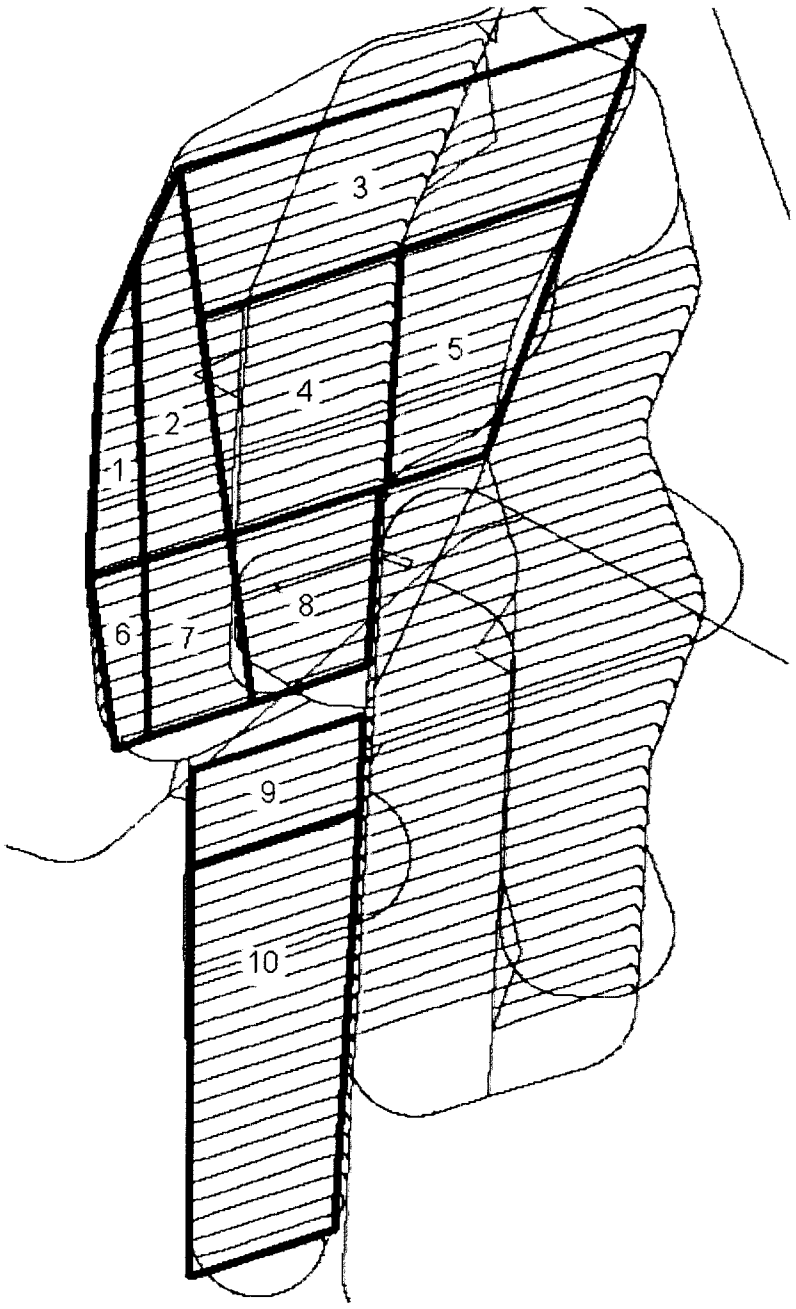
Part II)

The handling in *sampler.f* of runs that do not contain any sampled parameters (e.g. mean, maximum and minimum value runs) was changed to provide a warning message if the number of realizations is not 1, instead of the original error message.

The call to **newrealization()** in *exec.f* was limited to only those realizations that occur at or before the stop realization number. This will prevent the *sampler.f* warning message about non-sampled runs from appearing needlessly.

ATTACHMENT B

Description of Revised Repository Subareas
The following picture shows the new numbering and layout for TPA version 5.1, implemented by SCR600.



ATTACHMENT C: Test Plan for PC platform

Test Plan Name: SCR600 Test Plan, PC

Tested By: David Stead Date: 3/7/2006
TPA Baseline Version: 5.02c
TPA Test Version: 5.02d

Platform: PC
Host Machines: TPA
Host OS's: Windows Server 2003
Archive of Results: on CD entitled 'SCR600 Test Data'

Path for runs of version 5.0.2c:
`D:\DStead\SCR_600\Runs\Run_502c`
`D:\DStead\SCR_600\Runs\Run_502c`

Environment variables for runs of version 5.0.2c:
`TPA_TEST D:\DStead\TPA_code\TPA_502c`
`TPA_DATA D:\DStead\TPA_code\TPA_502c`

Path for runs of version 5.0.2d (unless otherwise specified):
`D:\DStead\SCR_600\Runs\Run_502d`
`D:\DStead\SCR_600\Runs\Run_502d`

Environment variables for runs of version 5.0.2d:
`TPA_TEST D:\DStead\TPA_code\TPA_502d`
`TPA_DATA D:\DStead\TPA_code\TPA_502d`

Utility codes used to aid in the analysis of the test data: Microsoft Excel 97
Microsoft WinDiff

Notes: References to the `tpa.out` file mean the screen print output, redirected to that file name.

Process Level (PL) Tests

PART I

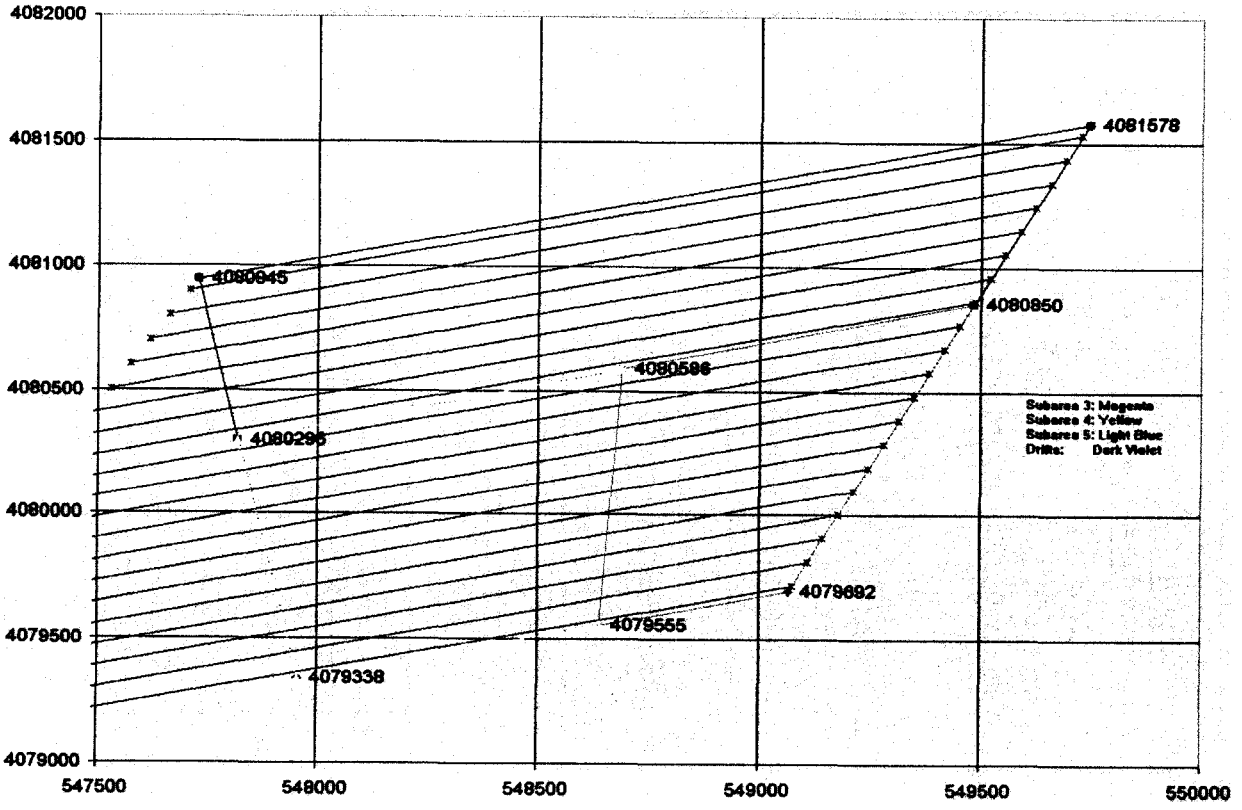
PL-1
Test objective: Verify that coincident corner coordinates among subareas 3, 4, and 5, and their neighboring subareas, are the same numerically.

Test Procedure: Obtain the coordinates from the *tpa_include.inp* files and compare the numbers visually.
Results: The coordinates of the four corner match exactly. They were plotted in Excel for visual

clarity (in `SCR600_SubAreaDetail_Final.xls`). A plot from this file appears below.

Corner Coordinates:

Version 5.0.2c [all subarea (SA) 3]	Version 5.0.2d [subareas 3,4,5]	New subarea
547729., 4080945.	547729., 4080945.	3
549746., 4081578.	549746., 4081578.	3
549068., 4079692.	549068., 4079692.	5
547955., 4079338.	547955., 4079338.	4



plot of new subareas 3, 4, and 5, from the file `SCR600_SubAreaDetail_Final.xls`

Paths for archive of results:
`from_TPA\TPA_502c`
`from_TPA\TPA_502d`
`Analysis\SCR600_SubAreaDetail_Final.xls`

Test Status: **Passed**

PL-2

Test Description: Verify that the number of waste packages in subareas 3, 4, & 5 is equal to the old subarea 3 count, and justify any differences.

Test Procedure: Make base case runs of both versions of the code, and compare the number of waste packages reported by each version in the *`tpa.out`* files.

Excerpt from *tpa.out*, for version 5.0.2c:

```
=====================================================================
         exec: Welcome to TPA Version 5.0.2c
       Job started: Mon Feb 27 21:33:50 2006
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area       Waste   Number of WP
   #      [m^2]      [MTU]
   1    224091.0     3025.5         526
   2    448476.0     6108.4        1062
   3   2621741.5    35362.2        6148
   4    152357.0     1972.9         343
   5    318122.0     4003.3         696
   6    439350.0     5355.0         931
   7    305880.0     4158.6         723
   8    747165.5    10048.4        1747
```

Excerpt from *tpa.out*, for version 5.0.2d:

```
=====================================================================
         exec: Welcome to TPA Version 5.0.2d
       Job started: Mon Mar 27 14:24:14 2006
=====================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area       Waste   Number of WP
   #      [m^2]      [MTU]
   1    224091.0     3025.5         526        Test Results
   2    448476.0     6108.4        1062        Number of WPs, in new SAs
   3   1217081.0    16709.1        2905        2905 \
   4    782749.5    10313.0        1793        1793 |-> total 6149
   5    623364.0     8345.9        1451        1451 /
   6    152357.0     1972.9         343
   7    318122.0     4003.3         696
   8    439350.0     5355.0         931
   9    305880.0     4158.6         723
  10    747165.5    10048.4        1747
```

The sum of the Number of WPs in Subareas 3,4, and 5 for the v. 5.0.2d run is 6149, which is one more than the result for the old Subarea 3 for the v. 5.0.2c run. This is due to a slight overlap of the subareas, which will be addressed in SCR598.

Paths for archive of results:
`from_TPA\TPA502c_BaseLine`
`from_TPA\TPA502d_BaseCase`

Test Results: **Failed**

PL-3

Test Description: Verify that the total area displayed on the screen is within 0.5 percent of what it was with the baseline version.

Test Procedure: Make base case runs of both versions of the code, and compare the total area reported by each version in the *tpa.out* files.

Test Results: The total area reported in *tpa.out* for version 5.0.2d is 1299.391153941191

acres, which is about 0.03% greater than the total area reported for version 5.0.2c, which is 1299.032122559921 acres.

Paths for archive of results:
`from_TPA\TPA502c_BaseLine`
`from_TPA\TPA502d_BaseCase`

Test Status: **Passed**

PL-4
Test Description: Verify (may be done graphically with high enough resolution) that the new subareas do not overlap any other subareas.

Test Procedure: Compare the subarea coordinates from the *tpa_include.inp* files and plot in Excel. In the Excel file *SCR600_SubAreaDetail_Final.xls*, graph *lt. ctr SA3,4* shows that the dividing point between the new subareas 3 and 4 falls west of the old subarea 3 boundary line, causing a slight overlap of new subareas 3 and 4 with subarea 2.

Test Results: The new subareas slightly overlap other subareas. The coordinates were compared numerically and graphically in Excel to verify this. This discrepancy will be addressed in SCR598.

Paths for archive of results:
`from_TPA\TPA_502c`
`from_TPA\TPA_502d`

Test Status: **Failed**

PL-5
Test Description: Verify that the volcanic dike appears in all subareas with a dike length of a constant 100m and with the dike location range set to appropriate values.

Special diagnostic code modifications required: Add print statement to *volcano.f*, within the 'if' block whose criteria is that a drift hit the volcanic dike (~line 728).

Test Procedure: Set volcanic dike length in *tpa.inp* to a constant 100m and the dike location range to cover all subareas, and make a 20-realization run of the version 5.02d code. Verify that the dike appears in all subareas by confirming the appearance of the inserted print statement in the *tpa.out* file at least once for each subarea.

Test Results: The volcanic dike appeared at least once for each subarea.

Path for runs:
`D:\DStead\SCR_600\Runs\RunD502d`

Path for archive of results:
`from_TPA\TPA502d_20re_100mDL_F&V_Geom_EEF=1_wPrtDriftHitDike`

Test Status:: **Passed**

PL-6
Test Description: Verify that the volcanic conduit appears in all subareas with the conduit location range set to appropriate values.

Test Procedure: Set the volcanic conduit location range in *tpa.inp* to cover all subareas, and make a 400-realization run of the version 5.0.2d code. Verify that the conduit appears in all subareas, as indicated by nonzero values of '#ign_act' in the *wpsfail.res* file appearing at least once for each subarea.

Test Results: The *wpsfail.res* file was opened in Excel and column was added to show the subarea number when a nonzero value of '#ign_act' was detected, and saved as *Analysis\wpsfail_TPAxp-400re-100mDL&FTLen_F&V_Geom_EEF=1.xls*.
The volcanic conduit appeared in all subareas as specified.

Path for archive of results:
`from_TPA\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1`

Test Status: **Passed**

PL-7
Test Description: Verify that the fault appears in all subareas with both the NW and NE fault trace lengths to 100m, and the fault location range set to appropriate values.

Test Procedure: Set both the NW and NE fault trace lengths to 100m, and set the fault location range to cover all subareas, and make a 400-realization run of the version 5.0.2d code. Verify that the fault appears in all subareas, as indicated by nonzero values of '#fault' in the *wpsfail.res* file appearing at least once for each subarea.

Test Results The *wpsfail.res* file was opened in Excel and column was added to show the subarea number when a nonzero value of '#fault' was detected, and saved as *Analysis\wpsfail_TPAxp-400re-100mDL&FTLen_F&V_Geom_EEF=1.xls*.
The fault appeared in all subareas as specified.

Path for archive of results:
`from_TPA\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1`

Test Status: **Passed**

PL-8
Test Description: Verify that the code will perform 400 realizations with the new subareas.

Test Procedure: Make a 400-realization run of the version 5.0.2d code, and verify that it ran to

completion by appearance of the statement '`exec: Run Successfully Completed`' at the end of the *tpa.out* file.

Test Results: The version 5.0.2d code completed 400 realizations with the new subareas.

Path for archive of results:
`from_TPA\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1`

Test Status: **Passed**

PL-9
Test Description: Verify that the *tpa.inp* values listed in the SCR table are the only values that have changed in the new *tpa.inp* file.

Test Results: The version 5.0.2c and version 5.0.2d tpa.inp files were compared in WinDiff, and
the version 5.02d file contains the new values as specified in the table entitled ***UPDATE REQUIREMENTS for TPA.INP***.

Paths for archive of results:
`from_TPA\TPA_502c`
`from_TPA\TPA_502d`

Test Status: **Passed**

PART II

PL-10

Test Description: Verify that the code runs to completion with 1 realization, using the *tpameans.out*, *tpamin.out*, and *tpamax.out* files from the 400 realization run (from PL-6 and PL-7, above) as input files.

Test Procedure: Take the *tpameans.out*, *tpamin.out*, and *tpamax.out* files from the 400 realization run from tests PL-6 and PL-7 and edit the stop realization to 1, change the filenames to *tpa.inp* one at a time, and verify that the code runs to completion with these input files by appearance of the statement '`exec: Run Successfully Completed`' at the end of the *tpa.out* file.

Test Results: The version 5.0.2d code ran to completion in all three cases.

Path for runs:
`D:\DStead\SCR_600\Runs\Runm502d`

Paths for archive of results:
`from_TPA\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1\TPA502d_400re_TPAmin`
`from_TPA\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1\TPA502d_400re_TPAmeans`
`from_TPA\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1\TPA502d_400re_TPAmax`

Test Status: **Passed**

PL-11

Test Description: Verify that the code runs to completion using the *tpameans.out*, *tpamin.out*, and *tpamax.out* files from the base case run (from PL-2, above) as input files.

Test Procedure: Take the *tpameans.out*, *tpamin.out*, and *tpamax.out* files from the base case run from test PL-2, change the filenames to *tpa.inp* one at a time, and verify that the code runs to completion with these input files by appearance of the statement '`exec: Run Successfully Completed`' at the end of the *tpa.out* file.

Test Results: The version 5.0.2d code ran to completion in all three cases with files from the base case run.

Path for runs:
`D:\DStead\SCR_600\Runs\Runm502d`

Paths for archive of results:
`from_TPA\TPA502d_BaseCase\TPA502d_TPAminBC`
`from_TPA\TPA502d_BaseCase\TPA502d_TPAmeansBC`
`from_TPA\TPA502d_BaseCase\TPA502d_TPAmaxBC`

Test Status: **Passed**

ATTACHMENT D: Test Plan, Unix Platform

Test Plan Name: SCR600 Test Plan, Unix

Tested By: David Stead Date: 3/7/2006

Platform: Unix
Host Machines: Spock, Texas
Host OS's: Sun OS

Baseline Version: 5.02c Test Version: 5.02d

Path for runs of version 5.0.2c:
`/home/dstead/run_502c`

Environment variables for runs of version 5.0.2c:
`TPA_TEST /home/dstead/tpa_502c`
`TPA_DATA /home/dstead/tpa_502c`

Path for runs of version 5.0.2d (unless otherwise specified):
`/home/dstead/run_502d`

Environment variables for runs of version 5.0.2d:
`TPA_TEST /home/dstead/tpa_502c`
`TPA_DATA /home/dstead/tpa_502c`

Utility codes used to aid in the analysis of the test data: Microsoft Excel 97
Microsoft WinDiff

Notes: References to the *tpa.out* file mean the screen print output, redirected to that file name.

Process Level (PL) Tests

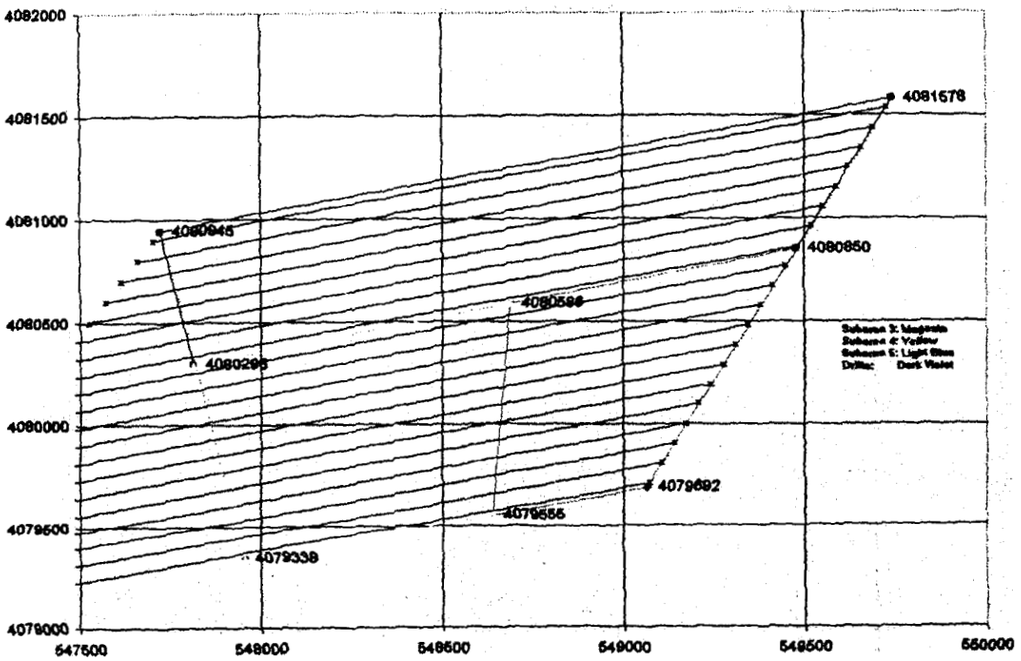
PART I

PL-1
Test Objective: Verify that coincident corner coordinates among subareas 3, 4, and 5, and their neighboring subareas, are the same numerically.

Test Procedure: Obtain the coordinates from the *tpa_include.inp* files and compare the numbers visually.
Results: The coordinates of the four corner match exactly. They were plotted in Excel for visual clarity (in `SCR600_SubAreaDetail_Final.xls`). A plot from this file appears below.

Corner Coordinates:	Version 5.0.2c	Version 5.0.2d	
	[all subarea (SA) 3]	[subareas 3,4,5]	New subarea
	547729., 4080945.	547729., 4080945.	3

```
549746., 4081578.        549746., 4081578.        3
549068., 4079692.        549068., 4079692.        5
547955., 4079338.        547955., 4079338.        4
```



plot of new subareas 3, 4, and 5, from the file `SCR600_SubAreaDetail_Final.xls`

Paths for archive of results:
`from_Spock_or_Texas\TPA_502c`
`from_Spock_or_Texas\TPA_502d`
`Analysis\SCR600_SubAreaDetail_Final.xls`

Test Status: **Passed**

PL-2
Test Description: Verify that the number of waste packages in subareas 3, 4, & 5 is equal to the old subarea 3 count, and justify any differences.

Test Procedure: Make base case runs of both versions of the code, and compare the number of waste packages reported by each version in the *tpa.out* files.

Excerpt from *tpa.out*, for version 5.0.2c:

```
=================================================================
        exec: Welcome to TPA Version 5.0.2c
      Job started: Mon Jan 16 18:17:55 2006
```

```
=========================================================================
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]       [MTU]
   1     224091.0     3025.5         526
   2     448476.0     6108.4        1062
   3    2621741.5    35362.2        6148
   4     152357.0     1972.9         343
   5     318122.0     4003.3         696
   6     439350.0     5355.0         931
   7     305880.0     4158.6         723
   8     747165.5    10048.4        1747
```

Excerpt from `tpa.out`, for version 5.0.2d:

```
=========================================================================
         exec: Welcome to TPA Version 5.0.2d
       Job started: Tue Mar 28 13:53:11 2006
=========================================================================
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]       [MTU]
   1     224091.0     3025.5         526
   2     448476.0     6108.4        1062
   3    1217081.0    16709.1        2905
   4     782749.5    10313.0        1793
   5     623364.0     8345.9        1451
   6     152357.0     1972.9         343
   7     318122.0     4003.3         696
   8     439350.0     5355.0         931
   9     305880.0     4158.6         723
  10     747165.5    10048.4        1747
```

Test Results
Number of WPs, in new SAs
**2905 **
1793 |-> total 6149
1451 /

The sum of the Number of WPs in Subareas 3,4, and 5 for the v. 5.0.2d run is 6149, which is one more than the result for the old Subarea 3 for the v. 5.0.2c run. This is due to a slight overlap of the subareas, which will be addressed in SCR598.

Paths for archive of results:
`from_Spock_or_Texas\TPA502c_BaseLine`
`from_Spock_or_Texas\TPA502d_BaseCase_Texas`

Test Results: **Failed**

PL-3
Test Description: Verify that the total area displayed on the screen is within 0.5 percent of what it was with the baseline version.

Test Procedure: Make base case runs of both versions of the code, and compare the total area reported by each version in the `tpa.out` files.

Test Results: The total area reported for version 5.0.2d is 1299.3911539412 acres, which is about 0.03% greater than the total area reported for version 5.0.2c, which is 1299.0321225599 acres (refer to excerpts from `tpa.out`, in item 2, above).

Paths for archive of results:
`from_Spock_or_Texas\TPA502c_BaseLine`
`from_Spock_or_Texas\TPA502d_BaseCase_Texas`

Test Status: **Passed**

PL-4
Test Description: Verify (may be done graphically with high enough resolution) that the new subareas do not overlap any other subareas.

Test Procedure: Compare the subarea coordinates from the *tpa_include.inp* files and plot in Excel. In the Excel file *SCR600_SubAreaDetail_Final.xls*, graph *lt. ctr SA3,4* shows that the dividing point between the new subareas 3 and 4 falls west of the old subarea 3 boundary line, causing a slight overlap of new subareas 3 and 4 with subarea 2.

Test Results: The new subareas slightly overlap other subareas. The coordinates were compared numerically and graphically in Excel to verify this. This discrepancy will be addressed in SCR598.

Paths for archive of results:
`from_Spock_or_Texas\TPA_502c`
`from_Spock_or_Texas\TPA_502d`

Test Status: **Failed**

PL-5
Test Description: Verify that the volcanic dike appears in all subareas with a dike length of a constant 100m and with the dike location range set to appropriate values.
Special diagnostic code modifications required: Add print statement to *volcano.f,* within the 'if' block whose criteria is that a drift hit the volcanic dike (~line 728).

Test Procedure: Set volcanic dike length in *tpa.inp* to a constant 100m and the dike location range to cover all subareas, and make a 20-realization run of the version 5.02d code. Verify that the dike appears in all subareas by confirming the appearance of the inserted print statement in the *tpa.out* file at least once for each subarea.

Test Results: The volcanic dike appeared at least once for each subarea.

Path for runs:
`/home/dstead/rund502d`

Path for archive of results:
`from_Spock_or_Texas\TPA502d_20re_100mDL_F&V_Geom_EEF=1_wPrtDriftHitDike`

Test Status:: **Passed**

PL-6
Test Description: Verify that the volcanic conduit appears in all subareas with the conduit location range set to appropriate values.

Test Procedure: Set the volcanic conduit location range in *tpa.inp* to cover all subareas, and make a 400-realization run of the version 5.0.2d code. Verify that the conduit appears in all subareas, as indicated by nonzero values of '#ign_act' in the *wpsfail.res* file appearing at least once for each subarea.

Test Results: The *wpsfail.res* file was opened in Excel and column was added to show the subarea number when a nonzero value of '#ign_act' was detected, and saved as *Analysis\wpsfail_Unix-400re-100mDL&FTLen_F&V_Geom_EEF=1.xls*.
The volcanic conduit appeared in all subareas as specified.

Path for runs:
`/data/dstead/run_502d`

Path for archive of results:
`from_Spock_or_Texas\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1`

Test Status: **Passed**

PL-7
Test Description: Verify that the fault appears in all subareas with both the NW and NE fault trace lengths to 100m, and the fault location range set to appropriate values.

Test Procedure: Set both the NW and NE fault trace lengths to 100m, and set the fault location range to cover all subareas, and make a 400-realization run of the version 5.0.2d code. Verify that the fault appears in all subareas, as indicated by nonzero values of '#fault' in the *wpsfail.res* file appearing at least once for each subarea.

Test Results The *wpsfail.res* file was opened in Excel and column was added to show the subarea number when a nonzero value of '#fault' was detected, and saved as *Analysis\wpsfail_Unix-400re-100mDL&FTLen_F&V_Geom_EEF=1.xls*.
The fault appeared in all subareas as specified.

Path for runs:
`/data/dstead/run_502d`

Path for archive of results:
`from_Spock_or_Texas\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1`

Test Status: **Passed**

PL-8
Test Description: Verify that the code will perform 400 realizations with the new subareas.

Test Procedure: Make a 400-realization run of the version 5.0.2d code, and verify that it ran to completion by appearance of the statement '`exec: Run Successfully Completed`' at the end of the *`tpa.out`* file.

Test Results: The version 5.0.2d code completed 400 realizations with the new subareas.

Path for archive of results:
`from_Spock_or_Texas\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1`

Test Status: **Passed**

PL-9
Test Description: Verify that the *`tpa.inp`* values listed in the SCR table are the only values that have changed in the new *`tpa.inp`* file.

Test Results: The version 5.0.2c and version 5.0.2d tpa.inp files were compared in WinDiff, and
the version 5.02d file contains the new values as specified in the table entitled ***UPDATE REQUIREMENTS for TPA.INP***.

Paths for archive of results:
`from_Spock_or_Texas\TPA_502c`
`from_Spock_or_Texas\TPA_502d`

Test Status: **Passed**

PART II

PL-10

Test Description: Verify that the code runs to completion with 1 realization, using the *tpameans.out*, *tpamin.out*, and *tpamax.out* files from the 400 realization run (from PL-6 and PL-7, above) as input files.

Test Procedure: Take the *tpameans.out*, *tpamin.out*, and *tpamax.out* files from the 400 realization run from tests PL-6 and PL-7 and edit the stop realization to 1, change the filenames to *tpa.inp* one at a time, and verify that the code runs to completion with these input files by appearance of the statement '`exec: Run Successfully Completed`' at the end of the *tpa.out* file.

Test Results: The version 5.0.2d code ran to completion in all three cases.

Path for runs:
`/home/dstead/runm502d`

Paths for archive of results:
`from_Spock_or_Texas\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1_Texas\TPA502d_400re_TPAmin`
`from_Spock_or_Texas\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1_Texas\TPA502d_400re_TPAmeans`
`from_Spock_or_Texas\TPA502d_400re_100mDL&FTL_F&V_Geom_EEF=1_Texas\TPA502d_400re_TPAmax`

Test Status: **Passed**

PL-11

Test Description: Verify that the code runs to completion using the *tpameans.out*, *tpamin.out*, and *tpamax.out* files from the base case run (from PL-2, above) as input files.

Test Procedure: Take the *tpameans.out*, *tpamin.out*, and *tpamax.out* files from the base case run from test PL-2, change the filenames to *tpa.inp* one at a time, and verify that the code runs to completion with these input files by appearance of the statement '`exec: Run Successfully Completed`' at the end of the *tpa.out* file.

Test Results: The version 5.0.2d code ran to completion in all three cases with files from the base case run.

Path for runs:
`/home/dstead/runm502d`

Paths for archive of results:
`from_Spock_or_Texas\TPA502d_BaseCase_Texas\TPA502d_TPAminBC`
`from_Spock_or_Texas\TPA502d_BaseCase_Texas\TPA502d_TPAmeansBC`
`from_Spock_or_Texas\TPA502d_BaseCase_Texas\TPA502d_TPAmaxBC`

Test Status: **Passed**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 602	**2. Software Title and Version:** TPA 5.0.2g	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *exec.f*

The infiltration/flow intermediate data file does not contain all of the TPA time steps, and some of the values are not in convenient physical units. A list of current parameters to be maintained and newly proposed parameters is provided in Attachment A.

5. Change Requested by: R. Fedors Date: 11-7-05	**6. Change Authorized by** (*Software Developer*): Ron Janetzke Date: 11-7-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

All occurrences of averaging over the number of subareas are removed and the subarea index for the **percinfil()** array was removed. Five new intermediate flow values were added to the *infilper.res* file. These values are described in Attachment A.

Factors fr, fd, and fw are hardwired to values fo 1.0 until SCR608 is completed.

8. Implemented by: Ron Janetzke	**Date:** 2-11-06

9. Description of Acceptance Tests:

See attachment B for Acceptance Test (unix platform)

See attachment C for Acceptance Test (PC platform)

10. Tested by: Jose M. Menchaca	**Date:** **March 7, 2006**

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 602

Status (*ADD, DELETE, MODIFY TO, MODIFY FROM)*	Module	Parameter Name	Description (*Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)*	Distribution	Range	Justification *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	Source

ATTACHMENT A

TPA Intermediate Flow Parameters

Abstraction ID	TPA ID	Description	Units	Location	Comments
	AAP(time)	Average annual precipitation at YM.	mm/yr	*dcagw.ech*	Available in V5.0.1
	Σ(qm3peryrinsa(time) over subareas) / Σ(subarea areas)	Flow rate of water percolating toward all analyzed subareas.	mm/yr		Not required
q_{in_sa}	percinfil(time,1)	Flow rate of water percolating toward subarea.	mm/yr	*infilper.res*	Implement.
q_{perc}	QinSA(time); qm3peryrinsa(time)	Subarea volumetric flow rate of water percolating toward the subarea.	m^3/yr	*uzflow.rlt; exec.f*	Available in V5.0.1
	qm3peryrperwpinsahitwp(time) / (WP footprint); [percinfil(time,2)]	Subarea flow rate of water percolating toward the drifts after reflux.	mm/yr	*infilper.res*	Implement.
q_1;q_{hit}	qm3peryrperwpinsahitwp(time)	Volumetric flow rate per WP of water percolating toward the drift after reflux.	m^3/yr	*nfenv.rlt*	Available in V5.0.1
q_{miss}	qm3peryrperwpinsamisswp(time)	Volumetric flow rate per WP of water percolating away from the drift after reflux.	m^3/yr	*nfenv.rlt*	Available in V5.0.1
q_2	f_{ow}(time) x f_{wet}(time) x qm3peryrperwpinsahitwp(time) / (WP footprint);[percinfil(time,3)]	Subarea focused flow rate toward drift after considering diversion (f_{ow}) and non-flowing fractures (f_{wet}).	mm/yr	*infilper.res*	Implement.
q_{5a}	f_{mult}(time) x f_{ow}(time) x f_{wet}(time) x qm3peryrperwpinsahitwp(time) / (WP footprint); [percinfil(time,4)]	Near-field focused flow rate toward drip shield after f_{mult}.	mm/yr	*infilper.res*	Implement.

Abstraction ID	TPA ID	Description	Units	Location	Comments
q_{5b}	wpflow x f_{mult}(time) x f_{ow}(time) x f_{wet}(time) x qm3peryrperwpinsahitwp(time) / (WP footprint); [percinfil(time,5)]	Drift focused flow rate hitting drip shield after flow multiplication factor (wpflow).	mm/yr	*infilper.res*	Implement.
qfr	fr x wpflow x f_{mult}(time) x f_{ow}(time) x f_{wet}(time) x qm3peryrperwpinsahitwp(time) / (WP footprint); [percinfil(time,6)]	Flow rate after factor fr is applied. (Seepage rubble factor)	mm/yr	*infilper.res*	Implement to accommodate upcoming modifications in SCR608.
qfd	fd x fr x wpflow x f_{mult}(time) x f_{ow}(time) x f_{wet}(time) x qm3peryrperwpinsahitwp(time) / (WP footprint); [percinfil(time,7)]	Flow rate after factor fd is applied. (Seepage drip shield factor)	mm/yr	*infilper.res*	Implement to accommodate upcoming modifications in SCR608.
qfw	fw x fd x fr x wpflow x f_{mult}(time) x f_{ow}(time) x f_{wet}(time) x qm3peryrperwpinsahitwp(time) / (WP footprint); [percinfil(time,8)]	Flow rate after factor fw is applied. (Seepage waste package protection factor)	mm/yr	*infilper.res*	Implement to accommodate upcoming modifications in SCR608.

Attachment B
Test Plan for TPA SCR#602

Test Plan Name: Infilper.res test

Tested By: Jose M. Menchaca | Date: March 7, 2006

Host Machine: SUN Ultra-4 server: Spock | Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0.2g | Test Version: TPA 5.0.2j

Process Level (PL) Tests

PL-1. Name: Test of infilper.res results

Path for run directory: ~jmench/tpa502j/basecaseRuns/singleVector (for Test 1)
~jmench/tpa502j/SCR602/singleVector3 (for Test 2)

Path for archive of results: R:\unix_tpa502j\basecaseRuns\singleVector (for Test 1)
R:\unix_tpa502j\SCR602\singleVector3 (for Test 2)
Note: The R: drive is the designated CD drive for stu2560.

Environment variables: setenv TPA_TEST ~/tpa502j
setenv TPA_DATA ~/tpa502j

Special input files or modifications to input files required :
For testing the flow rate factors for rubble, drip shield, and waste package, (fr, fd, and fw respectively) change the hardcoded values in the ebsrel.f file to test if they get propagated through to the infilper.res file.

Pertinent Lines in the tpa.inp file:

Special diagnostic code modifications required:

Program modes to be used (append flags, scenario/model switches, etc.):

Utility scripts needed to perform the test:

Utility codes needed in the analysis of the test data:

Test 1 description:

- objective:
The objective of this test is to verify that the data is correctly being written to the infilper.res file, including intermediate flow values, fow, fmult, fr, fd, fw, and wpflow.

- assumptions:
The current tests are only testing for position and header consistency as the calculations are still being coded at this time. The intermediate flow values of fr, fd, and fw are being finalized in SCR608.

- constraints:

- output files to compare or examine: infliper.res

- step by step test procedure to be used:
Execute a single realization run of the standard tpa.inp file. Verify that there are data for each column for the 2010 time steps (201 time steps × 10 subareas = 2010 total time steps).

- pass fail criteria
The pass criteria is achieved if each data column reflects the label header information in the time steps and subarea order as expected.

Test Results:

- disposition of output and supporting files:
Portion of infilper.res file:

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vector	subarea	time	infil	diver&ref	fow	fmult	fr	fd	fw	wpflow
unitless	unitless	yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr
1	1	0.0000E+00	5.8329E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1	1	2.3102E+00	5.8329E+00	4.2099E+00	3.6626E+00	4.0289E-01	4.0289E-01	4.0289E-01	4.0289E-01	4.3429E-01
1	1	4.6744E+00	5.8329E+00	5.6942E+00	4.9540E+00	5.4494E-01	5.4494E-01	5.4494E-01	5.4494E-01	5.8741E-01
1	1	7.0940E+00	5.8329E+00	5.8231E+00	5.0661E+00	5.5727E-01	5.5727E-01	5.5727E-01	5.5727E-01	6.0070E-01
1	1	9.5702E+00	5.8329E+00	5.8321E+00	5.0739E+00	5.5813E-01	5.5813E-01	5.5813E-01	5.5813E-01	6.0163E-01

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- overall test status (PASS/FAIL): **PASS**

Test 2 description:

- objective

The objective of this test is to verify that new intermediate flow multipliers. fr, fd, and fw are correctly propagating through the code.

- assumptions

The current tests are only testing for position and header consistency as the calculations are still being coded at this time. The intermediate flow values of fr, fd, and fw are being finalized in SCR608.

- constraints

- output files to compare or examine: infilper.res

- step by step test procedure to be used

The flow rate factors for rubble, drip shield, and waste package, (fr, fd, and fw respectively) are all hardcoded to values of 1.0. Change the hardcoded flow rate factors of fr, fd, and fw to 0.25, 0.50, and 0.75 respectively in the ebsrel.f file which generates the ebsflo.dat file to test if the factors get propagated through to the infilper.res file.

```
/home/jmench/tpa502j{177}>diff ebsrel.f SCR602/ebsrelModFrFdFw.f
1644c1644,1645
<  835      format( e17.10, '                ! flowfactr: flow factor ' )
---
>  835      format( e17.10, '          ! flowfactr: flow factor, SCR602 ' )
> cjmm+-^--1----+----2----+----3----+----4----+----5----+----6----+----7--!-+----8
1684c1685,1686
<      &     ,sawetnew(1),1.d0,1.d0,1.d0
---
> cjmm test for SCR602    &     ,sawetnew(1),1.d0,1.d0,1.d0
>      &     ,sawetnew(1),0.25d0,0.50d0,0.75d0
1699c1701
<      &       ,sawetnew(it),1.d0,1.d0,1.d0
---
>      &       ,sawetnew(it),0.25d0,0.50d0,0.75d0
/home/jmench/tpa502j{178}>
```

- pass fail criteria

The test passes if the ratio of the values in the infilper.res file reflect the updated values for the test.

Test Results:

- disposition of output and supporting files.

vector unitless	subarea unitless	time yr	infil mm/yr	diver&ref mm/yr	fow mm/yr	fmult mm/yr	fr mm/yr	fd mm/yr	fw mm/yr	wpflow mm/yr
1	1	0.0000E+00	5.8329E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1	1	2.3102E+00	5.8329E+00	4.2099E+00	3.6626E+00	4.0289E-01	1.0072E-01	5.0361E-02	3.7771E-02	4.0715E-02
1	1	4.6744E+00	5.8329E+00	5.6942E+00	4.9540E+00	5.4494E-01	1.3623E-01	6.8117E-02	5.1088E-02	5.5069E-02
1	1	7.0940E+00	5.8329E+00	5.8231E+00	5.0661E+00	5.5727E-01	1.3932E-01	6.9658E-02	5.2244E-02	5.6315E-02
1	1	9.5702E+00	5.8329E+00	5.8321E+00	5.0739E+00	5.5813E-01	1.3953E-01	6.9766E-02	5.2325E-02	5.6403E-02
1	1	1.2104E+01	5.8329E+00	5.8328E+00	5.0746E+00	5.5820E-01	1.3955E-01	6.9775E-02	5.2332E-02	5.6410E-02
1	1	1.4698E+01	5.8329E+00	5.8329E+00	5.0746E+00	5.5821E-01	1.3955E-01	6.9776E-02	5.2332E-02	5.6410E-02

- criterion 1 evidence

Hand calculations show that for any given row, when the fmult column value is non-zero, the following fr value is 25% of the fmult value, the fd is 50% of the fr value, and the fw value is 75% of the fd value. This relationship was verified for the entire file using an excel spreadsheet. The results may be found in unix_infilper_res.xls.

- overall test status (PASS/FAIL): **PASS**

Attachment C
Test Plan for TPA SCR#602

Test Plan Name: Infilper.res test

Tested By: Jose M. Menchaca

Date: March 7, 2006

Host Machine: AMD Opteron PC

Host OS: MS Windows Server 2003 Version 5.2

Baseline Version: TPA 5.0.2g

Test Version: TPA 5.0.2j

Process Level (PL) Tests

PL-1. Name: Test of infilper.res results

Path for run directory: D:\JMenchaca\tpa502j\singleVector (for Test 1)
D:\JMenchaca\tpa502j\SCR602\singleVector (for Test 2)
Note: The D: drive is mapped to "TPA:\public\jmenchaca"

Path for archive of results: R:\pc_tpa502j\singleVector (for Test 1)
R:\pc_tpa502j\SCR602\singleVector (for Test 2)
Note: The R: drive is the designated CD drive for stu2560.

Environment variables: set TPA_TEST=L:\tpa502j
set TPA_DATA=L:\tpa502j
Note: The L: drive is mapped to "ladybug:\public\jmenchaca"

Special input files or modifications to input files required :
For testing the flow rate factors for rubble, drip shield, and waste package, (fr, fd, and fw respectively) change the hardcoded values in the ebsrel.f file to test if they get propagated through to the infilper.res file.

Pertinent Lines in the tpa.inp file:

Special diagnostic code modifications required:

Program modes to be used (append flags, scenario/model switches, etc.):

Utility scripts needed to perform the test:

Utility codes needed in the analysis of the test data:

Test 1 description:

- objective:
The objective of this test is to verify that the data is correctly being written to the infilper.res file, including intermediate flow values, fow, fmult, fr, fd, fw, and wpflow.

- assumptions:
The current tests are only testing for position and header consistency as the calculations are still being coded at this time. The intermediate flow values of fr, fd, and fw are being finalized in SCR608.

- constraints:

- output files to compare or examine: infliper.res

- step by step test procedure to be used:
Execute a single realization run of the standard tpa.inp file. Verify that there are data for each column for the 2010 time steps (201 time steps × 10 subareas = 2010 total time steps).

- pass fail criteria
The pass criteria is achieved if each data column reflects the label header information in the time steps and subarea order as expected.

Test Results:

- disposition of output and supporting files:
Portion of infilper.res file:

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vector	subarea	time	infil	diver&ref	fow	fmult	fr	fd	fw	wpflow
unitless	unitless	yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr
1	1	0.0000E+00	5.8329E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1	1	2.3102E+00	5.8329E+00	4.2099E+00	3.6626E+00	4.0289E-01	4.0289E-01	4.0289E-01	4.0289E-01	4.3429E-01
1	1	4.6744E+00	5.8329E+00	5.6942E+00	4.9540E+00	5.4494E-01	5.4494E-01	5.4494E-01	5.4494E-01	5.8741E-01
1	1	7.0940E+00	5.8329E+00	5.8231E+00	5.0661E+00	5.5727E-01	5.5727E-01	5.5727E-01	5.5727E-01	6.0070E-01
1	1	9.5702E+00	5.8329E+00	5.8321E+00	5.0739E+00	5.5813E-01	5.5813E-01	5.5813E-01	5.5813E-01	6.0163E-01
1	1	1.2104E+01	5.8329E+00	5.8328E+00	5.0746E+00	5.5820E-01	5.5820E-01	5.5820E-01	5.5820E-01	6.0171E-01

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- overall test status (PASS/FAIL): **PASS**

Test 2 description:

- objective

The objective of this test is to verify that new intermediate flow multipliers. fr, fd, and fw are correctly propagating through the code.

- assumptions

The current tests are only testing for position and header consistency as the calculations are still being coded at this time. The intermediate flow values of fr, fd, and fw are being finalized in SCR608.

- constraints

- output files to compare or examine: infilper.res

- step by step test procedure to be used

The flow rate factors for rubble, drip shield, and waste package, (fr, fd, and fw respectively) are all hardcoded to values of 1.0. Change the hardcoded flow rate factors of fr, fd, and fw to 0.25, 0.50, and 0.75 respectively in the ebsrel.f file which generates the ebsflo.dat file to test if the factors get propagated through to the infilper.res file.

```
L:\tpa502j>fc ebsrel.f ebsrelOrig.f
Comparing files ebsrel.f and EBSRELORIG.F
***** ebsrel.f
cc rwj 2-11-06; scr602; temporary values pending new seepage code.
     &     ,sawetnew(1),0.25d0,0.50d0,0.75d0

***** EBSRELORIG.F
cc rwj 2-11-06; scr602; temporary values pending new seepage code.
     &     ,sawetnew(1),1.d0,1.d0,1.d0

*****

***** ebsrel.f
cc rwj 2-11-06; scr602 ; temporary values pending new seepage code.
     &       ,sawetnew(it),0.25d0,0.50d0,0.75d0

***** EBSRELORIG.F
cc rwj 2-11-06; scr602 ; temporary values pending new seepage code.
     &       ,sawetnew(it),1.d0,1.d0,1.d0

*****
```

- pass fail criteria

The test passes if the ratio of the values in the infilper.res file reflect the updated values for the test.

Test Results:

- disposition of output and supporting files.

vector	subarea	time	infil	diver&ref	fow	fmult	fr	fd	fw	wpflow
unitless	unitless	yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr	mm/yr
1	1	0.0000E+00	5.8329E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
1	1	2.3102E+00	5.8329E+00	4.2099E+00	3.6626E+00	4.0289E-01	1.0072E-01	5.0361E-02	3.7771E-02	4.0715E-02
1	1	4.6744E+00	5.8329E+00	5.6942E+00	4.9540E+00	5.4494E-01	1.3623E-01	6.8117E-02	5.1088E-02	5.5069E-02
1	1	7.0940E+00	5.8329E+00	5.8231E+00	5.0661E+00	5.5727E-01	1.3932E-01	6.9658E-02	5.2244E-02	5.6315E-02
1	1	9.5702E+00	5.8329E+00	5.8321E+00	5.0739E+00	5.5813E-01	1.3953E-01	6.9766E-02	5.2325E-02	5.6403E-02
1	1	1.2104E+01	5.8329E+00	5.8328E+00	5.0746E+00	5.5820E-01	1.3955E-01	6.9775E-02	5.2332E-02	5.6410E-02
1	1	1.4698E+01	5.8329E+00	5.8329E+00	5.0746E+00	5.5821E-01	1.3955E-01	6.9776E-02	5.2332E-02	5.6410E-02

- criterion 1 evidence

Hand calculations show that for any given row, when the fmult column value is non-zero, the following fr value is 25% of the fmult value, the fd is 50% of the fr value, and the fw value is 75% of the fd value. This relationship was verified for the entire file using an excel spreadsheet. The results may be found in pc_infilper_res.xls.

- overall test status (PASS/FAIL): **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 603	**2. Software Title and Version:** TPA 5.0.2a	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *exec.f, tpa.inp*

The *wpsfail.res* file format does not allow for explicit listing of the initial waste package failures.

5. Change Requested by: Ron Janetzke Date: 11-7-05	**6. Change Authorized by** (*Software Developer*): Ron Janetzke Date: 11-7-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

The format of the *wpsfail.res* file was changed to include the initial failures. In addition the subarea number for each event is also displayed. This increases the size of the file by about a factor equal to the number of subareas. It was felt that the penalty in size was worth the increase in information supplied. The original code used array **wpsfailedtime**(,,) as the source for the information. This array combines the ejected WPs with the intrusive failure WPs . It also maintains cumulative totals during the subarea loop in order to supply one value for each event in a realization. The new code uses a new array called **releasewpfailedtimer**(,,) that does not contain the ejected WPs in the count. This array provides cumulative storage for a single realization for all subarea instances of the array **releasewpfailedtime**(,), and references to it were changed throughout the *exec.f* file as needed. Each subarea is stored separately and cumulative values are not maintained. The screen print will continue to show volcanic failures as the sum of the intrusive and extrusive failures (up to the limit of WPs in the subarea). Other files that list number of failures are *ebsrel.inp, ebsrel.ech*, and *ebsrel.rlt*.

A cosmetic change was also made to the screen output in order to print the actual path of the system environment variables that are in effect at the time of the run. This was implemented with the aid of a new subroutine called **TranslateEnv**().

The output from the **diff** utility is provided in Attachment A.

8. Implemented by: R. Janetzke	**Date:** 12-7-05

9. Description of Acceptance Tests:

Performed acceptance testing for SCR603 using version 5.0.2e of the tpa code. Performed one process level test and four system level tests. The process level test was used to verify the screen output shows the actual path of the system environment variables. The system level tests were used to verify the correct number of waste packages are being tabulated in wpsfail.res and that these tabulated values reflect the number of waste packages used in the release module.

All process level and system level tests successfully passed.

10. Tested by: G. Adams	**Date:** 1-26-2006

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 603

Status *(ADD, DELETE, MODIFY TO, MODIFY FROM)*	**Module**	**Parameter Name**	**Description** *(Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)*	**Distribution**	**Range**	**Justification** *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	**Source**

ATTACHMENT A

```
2,4c2,4
< c File Name:           exec.f
< c File Date:           11/29/05
< c Release Version:     5.0.2a
---
> c File Name:           %M%
> c File Date:           %G%
> c Release Version:     5.0.2b
272a273
> c             5.0.2b includes SCR 603 include initial failures in
wpsfail.res.
322c323
< c Executive for TPA Version 5.0.2a
---
> c Executive for TPA Version 5.0.2b
580c581,589
<       dimension releasewpfailedtime(2, maxseismointervals+4)
---
> cc rwj 12-5-05; SCR603; convert releasewpfailedtime to releasewpfailedtimer
> cc    releasewpfailedtimer has the same information, but the information is
> cc    retained for all subareas, rather than just the current subarea.
> cc    dimension releasewpfailedtime(2, maxseismointervals+4)
>       double precision
>      &       releasewpfailedtimer(2, maxseismointervals+4,maxnsubarea)
>       double precision field(maxseismointervals+4)
>       logical lprint
>       integer nprint
621a631,634
> c rwj 12-7-05; SCR603
>       integer trimlen
>       external trimlen
>
707a721
>       include 'ieee/part1.i'
735c749
<       print '(10x,a)','exec: Welcome to TPA Version 5.0.2a'
---
>       print '(10x,a)','exec: Welcome to TPA Version 5.0.2b'
1115,1116c1129,1133
<       mes1=' Number of Failed WPs by Type of Disruptive Event'
<       mes2=' Including Time of Event - Values for Each Vector'
---
> cc rwj 12-06-0-5; SCR603
> cc    mes1=' Number of Failed WPs by Type of Disruptive Event'
> cc    mes2=' Including Time of Event - Values for Each Vector'
>       mes1=' Number of Failed WPs for GW by Type of Disruptive Event'
>       mes2=' Including Time of Event and Subarea for Each Vector'
1843,1848c1860,1873
<         write(iunitwpsfail,'(/,6(4x,a,4x))')
<      & ' vector ','  time  ','#corrode','#seismic',
<      & ' #fault ',' #igact '
<         write(iunitwpsfail,'(6(4x,a,4x))')
<      & 'unitless','   yr   ','unitless','unitless',
<      & 'unitless','unitless'
---
> cc rwj scr603; 12-1-05  Add initial failures to wpsfail.res
```

```
> cc      write(iunitwpsfail,'(/,6(4x,a,4x))')
> cc    & ' vector ','  time  ','#corrode','#seismic',
> cc    & ' #fault ',' #igact '
> cc      write(iunitwpsfail,'(6(4x,a,4x))')
> cc    & 'unitless','   yr   ','unitless','unitless',
> cc    & 'unitless','unitless'
> cc
>         write(iunitwpsfail,'(/,2(x,a),6(3x,a,3x))')
>       & ' vector ','subarea ','  time  ','#initial','#corrode',
>       & '#seismic',' #fault ','#ign_act'
>         write(iunitwpsfail,'(2(x,a),6(3x,a,3x))')
>       & 'unitless','unitless','   yr   ','unitless','unitless',
>       & 'unitless','unitless','unitless'
2028a2054,2056
> cc rwj 12-7-05; SCR603
> cc    print '(a,a)',' The specified path for data  = ', dpath
> cc    print '(a,a)',' The specified path for codes = ', path
2030,2031c2058,2066
<       print '(a,a)',' The specified path for data  = ', dpath
<       print '(a,a)',' The specified path for codes = ', path
---
>       call translateEnv( dpath, aline)
>       ilength   = trimlen(aline)
>       print '(a,a)',' The specified path for data  = ', aline(1:ilength)
>
>       call translateEnv( path, aline)
>       ilength   = trimlen(aline)
>       print '(a,a)',' The specified path for codes = ', aline(1:ilength)
> cc End SCR603.
>
4276c4311
<      &                 releasewpfailedtime )
---
>      &                 releasewpfailedtimer(1,1,isa) )
4295,4296c4330,4331
<                   releasewpfailedtime(1,3) = DMAX1( 0.0d0,
<      &               releasewpfailedtime(1,3) - dble(nwpexhumed) )
---
>                   releasewpfailedtimer(1,3,isa) = DMAX1( 0.0d0,
>      &               releasewpfailedtimer(1,3,isa) - dble(nwpexhumed) )
4303,4304c4338,4339
<                  releasewpfailedtime(1,3) = DMAX1( 0.0d0,
<      &              releasewpfailedtime(1,3) - dble(nwpexhumed) )
---
>                  releasewpfailedtimer(1,3,isa) = DMAX1( 0.0d0,
>      &              releasewpfailedtimer(1,3,isa) - dble(nwpexhumed) )
4339c4374,4375
<      &     'INITIAL  ',releasewpfailedtime(1,1),releasewpfailedtime(2,1)
---
>      &     'INITIAL  ',releasewpfailedtimer(1,1,isa),
>      &                 releasewpfailedtimer(2,1,isa)
4341c4377,4378
<      &     'FAULTING ',releasewpfailedtime(1,2),releasewpfailedtime(2,2)
---
>      &     'FAULTING ',releasewpfailedtimer(1,2,isa),
>      &                 releasewpfailedtimer(2,2,isa)
4343c4380,4381
<      &     'VOLCANO  ',releasewpfailedtime(1,3),releasewpfailedtime(2,3)
```

```
---
>       &     'VOLCANO  ',releasewpfailedtimer(1,3,isa),
>       &                 releasewpfailedtimer(2,3,isa)
4345c4383,4384
<       &     'SEISMO 1 ',releasewpfailedtime(1,4),releasewpfailedtime(2,4)
---
>       &     'SEISMO 1 ',releasewpfailedtimer(1,4,isa),
>       &                 releasewpfailedtimer(2,4,isa)
4347c4386,4387
<       &     'SEISMO 2 ',releasewpfailedtime(1,5),releasewpfailedtime(2,5)
---
>       &     'SEISMO 2 ',releasewpfailedtimer(1,5,isa),
>       &                 releasewpfailedtimer(2,5,isa)
4349c4389,4390
<       &     'SEISMO 3 ',releasewpfailedtime(1,6),releasewpfailedtime(2,6)
---
>       &     'SEISMO 3 ',releasewpfailedtimer(1,6,isa),
>       &                 releasewpfailedtimer(2,6,isa)
4351c4392,4393
<       &     'SEISMO 4 ',releasewpfailedtime(1,7),releasewpfailedtime(2,7)
---
>       &     'SEISMO 4 ',releasewpfailedtimer(1,7,isa),
>       &                 releasewpfailedtimer(2,7,isa)
4353c4395,4396
<       &     'CORROSION',releasewpfailedtime(1,8),releasewpfailedtime(2,8)
---
>       &     'CORROSION',releasewpfailedtimer(1,8,isa),
>       &                 releasewpfailedtimer(2,8,isa)
4357c4400
<       &     'EXTRUSIVE', dble(nwpexhumed), releasewpfailedtime(2,3)
---
>       &     'EXTRUSIVE', dble(nwpexhumed), releasewpfailedtimer(2,3,isa)
4360c4403
<       &     'EXTRUSIVE',          0.0d0   , releasewpfailedtime(2,3)
---
>       &     'EXTRUSIVE',          0.0d0   , releasewpfailedtimer(2,3,isa)
4390c4433
<       &          releasewpfailedtime,
---
>       &          releasewpfailedtimer(1,1,isa),
5457,5463c5500,5507
<        do itime = 1, ntim
<          do iwpfail = 1, numdisruptiveevents
<            do iitype = 1, 4
<              if(wpsfailedtime(iitype,iwpfail,2).eq.tim(itime))then
<                write(iunitwpsfail,'(5x,i5,6x,5(1pe13.4,3x))') ir,
<       &          wpsfailedtime(iitype,iwpfail,2),
<       &          (wpsfailedtime(j,iwpfail,1), j = 1,4)
---
> cc rwj scr603; 12-1-05  Add initial failures to wpsfail.res
> c     do itime = 1, ntim
> c       do iwpfail = 1, numdisruptiveevents
> c         do iitype = 1, 4
> c           if(wpsfailedtime(iitype,iwpfail,2).eq.tim(itime))then
> c            write(iunitwpsfail,'(5x,i5,6x,5(1pe13.4,3x))') ir,
> c    &          wpsfailedtime(iitype,iwpfail,2),
> c    &          (wpsfailedtime(j,iwpfail,1), j = 1,4)
5465,5466c5509,5544
```

```
<                 call flush(iunitwpsfail)
<                 goto 937
---
> c               call flush(iunitwpsfail)
> c               goto 937
> c             endif
> c           enddo
> c 937       continue
> c         enddo
> c       enddo
> c
> cc field contents
> cc field(1) = initial
> cc field(2) = faulting
> cc field(3) = igneaous
> cc field(4) = seismic 1
> cc field(5) = seismic 2
> cc field(6) = seismic 3
> cc field(7) = seismic 4
> cc field(8) = corrosion
> c
>         nprint = 0
>         do itime = 1, ntim
>           do iiisa = istartsuba, istopsuba
>             isa = iiisa
> c
>             do ifield = 1,6
>                field(ifield) = 0.0d0
>             end do
> c
>             lprint = .FALSE.
> c
>             do iwpfail = 1, maxseismointervals+4
> cc            If the time of the event is at the TPA time step and the number
> cc            of packages is non-zero, then transfer it to the print array.
>               if(releasewpfailedtimer(2,iwpfail,isa) .eq. tim(itime) .and.
>      &           releasewpfailedtimer(1,iwpfail,isa) .gt. 0.0d0)      then
>                  field(iwpfail) = releasewpfailedtimer(1,iwpfail,isa)
>                  lprint = .TRUE.
5469c5547,5557
<   937       continue
---
> c
> cc          If print flag is set then add all seismic events together.
>             if (lprint) then
>               field(4) = field(4) + field(5) + field(6) + field(7)
>               write(iunitwpsfail,'(x,i5,4x,i5,2x,6(1pe13.5,1x))')
>      &            ir, isa, tim(itime), field(1), field(8),
>      &            field(4), field(2), field(3)
>               nprint = nprint + 1
>               call flush(iunitwpsfail)
>             end if
> c
5471a5560
> cc end SCR603
5473,5480c5562,5579
< cc Loop to write a line of zeroes to the wpsfail.res file
< cc                if there are no disruptive events for this realization.
```

```
<
<         do iwpfail = 1, numdisruptiveevents
<           do iitype = 1, 4
<             if(wpsfailedtime(iitype,iwpfail,2) .ne. -1.D0) goto 938
<           enddo
<         enddo
---
> cc Write a line of zeroes to the wpsfail.res file if there are no
> cc events for this realization.
> cc
> cc rwj 12-06-0-5; SCR603
> cc    do iwpfail = 1, numdisruptiveevents
> cc      do iitype = 1, 4
> cc        if(wpsfailedtime(iitype,iwpfail,2) .ne. -1.D0) goto 938
> cc      enddo
> cc    enddo
> cc
> cc      write(iunitwpsfail,'(5x,i5,6x,5(1pe13.4,3x))') ir,
> cc   &          tim(ntim),
> cc   &          (0.0D0, j = 1,4)
> cc
>       if (nprint .le. 0) then
>          write(iunitwpsfail,'(x,i5,4x,i5,2x,6(1pe13.5,1x))') ir,1,
>      &         tim(ntim), (0.0D0, j = 1,5)
>       end if
5482,5485d5580
<         write(iunitwpsfail,'(5x,i5,6x,5(1pe13.4,3x))') ir,
<      &          tim(ntim),
<      &          (0.0D0, j = 1,4)
<
6856c6951
<  341     format( ' TPA 5.0.2a, Job started: ', a24 )
---
>  341     format( ' TPA 5.0.2b, Job started: ', a24 )
6945c7040
<  341     format( ' TPA 5.0.2a, Job started: ', a24 )
---
>  341     format( ' TPA 5.0.2b, Job started: ', a24 )
9822c9917,9919
<       parameter (kMaxTimeSteps = 5001)
---
> cc rwj
> c     parameter (kMaxTimeSteps = 5001)
>       parameter (kMaxTimeSteps = 501)
10127a10225,10296
> cccccccc
> c=====================================================================
>       subroutine translateEnv( cin, cout)
> c=====================================================================
> c     NAME:     translateEnv
> c
> c     PURPOSE:  Translate system environment variables and explicit
> c               directory path names.
> c
> c     METHOD:
> c               A system command is issued to the host OS to 'echo' the
> c               translation of the path name, and place the resulting
> c               string into file tpasys.tmp.  This file is then opened
```

```
> c                and read, and the contents are displayed on the screen.
> c
> c     INPUT:
> c             cin = character*(*), environment variable or path to translate.
> c
> c     OUTPUT:
> c             cout= character*(*), system translation of environment
> c                   variable or path.
> cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
> c
>       integer iunit
>       save iunit
>
>       integer istatus
>       integer zportsh
>       external zportsh
>
>       integer igetunitnumber
>       external igetunitnumber
>
>       character*(*) cin
>       character*(*) cout
>
>       logical lexist
>       logical lfirst
>
>       save lfirst
>
>       data lfirst /.TRUE./
>
> ccccc
> c     Start here.
> ccccc
>       if (lfirst) then
>          iunit = igetunitnumber('exec    ')
>          lfirst = .FALSE.
>       end if
> c
>       inquire( file='tpasys.tmp', EXIST=lexist)
>       if ( lexist) istatus = zportsh( 'rm tpasys.tmp')
> c
>       call clearchar(len(cout),cout)
>       istatus = zportsh('echo ' // cin // '>tpasys.tmp')
> c
>       if( istatus .ne. 0 ) then
>           print *, ' ***>>> Error in TranslateEnv <<<*** '
>           print *, ' istatus .ne. 0 '
>           print *, ' istatus = sh(echo '// cin //'>tpasys.tmp) '
>           print *, ' istatus = ', istatus
>           STOP
>       endif
> c
>       open (iunit, file='tpasys.tmp', STATUS='OLD')
>       read (iunit,'(a)') cout
>       close(iunit)
>       return
>       end
> ccccccccc
```

```
>       include 'ieee/part2.i'
```

Test Plan and Test Results for TPA SCR # 603

Test Plan Name: WPSFAIL

Tested By: George Adams

Date: January 26, 2006

Host Machine: tpa

Host OS: Windows (tpa),
UNIX (spock, idaho, texas)

Baseline Version: TPA 5.0.2a

Test Version: TPA 5.0.2e

Process Level Tests

The process level test is designed to verify that the screen output shows the actual path of the system environment variables that are in effect at the time of the run.

PL-1 Verify Screen Output of Environment Variables

1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR603\tpa502e
$TPA_TEST and $TPA_DATA = \SCR603\tpa502e
<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR603\testresults\pl1

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR603\tpa502e
$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

4.0 Special Input Files or Modifications to Input Files Required
4.1 Use the default tpa.inp file

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used
6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test
None

8.0 Test Description

8.1 Objective: This test is designed to verify that the screen output shows the actual path of the system environment variables.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: screen capture of test run as well as commands for setting environment variables

8.5 Procedure:

1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: "tpa.exe > pl1.out."

3. Compare the screen output for the actual path for the system environment variables to that displayed from the test run.

8.6 Pass/Fail Criteria: The code runs to completion and the actual path for the system environment variables that is displayed to the screen agrees with the actual path set.

9.0 Test Results

9.1 Output and Supporting Files: All files are archived to a CD labeled, "TPA SCR #603."

9.2 Criterion 1: The actual path for the system environment variables agrees with the screen output.

9.3 Overall Test Status:

This test successfully **PASSED** the criterion above for test PL-1.

As shown below, the screen capture for setting the environment variables matches the information output to the screen when the tpa code executed.

Screen Capture on machine tpa (Windows Server 2003):

```
Microsoft Windows [Version 5.2.3790]
(C) Copyright 1985-2003 Microsoft Corp.

d:\>cd D:\GADAMS\SCR603\tpa502e\test

D:\GADAMS\SCR603\tpa502e\test>
D:\GADAMS\SCR603\tpa502e\test>setup

D:\GADAMS\SCR603\tpa502e\test>set TPA_DATA=D:\GADAMS\SCR603\tpa502e

D:\GADAMS\SCR603\tpa502e\test>set TPA_TEST=D:\GADAMS\SCR603\tpa502e

D:\GADAMS\SCR603\tpa502e\test>
```

Contents of pl1.out showing environment variables for Windows Server 2003:

The specified path for data = D:\GADAMS\SCR603\tpa502e\

The specified path for codes = D:\GADAMS\SCR603\tpa502e\

Screen Capture on machine spock (UNIX):

spock% setenv TPA_DATA $HOME/scr603/tpa502e

spock% setenv TPA_TEST $HOME/scr603/tpa502e

Contents of pl1.out showing environment variables for machine spock (UNIX):

The specified path for data = /home/gadams/scr603/tpa502e/

The specified path for codes = /home/gadams/scr603/tpa502e/

System Level Tests

The system level tests are designed to verify that the number of waste packages tabulated in wpsfail.res reflect the number of waste packages counted in the release module.

SL-1 Verify Results Tabulated

1.0 Path for Run Directory

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results

\SCR603\testresults\sl1

3.0 Environment Variables

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

4.0 Special Input Files or Modifications to Input Files Required

4.1 Set the values in TPA.INP in accordance with the following table:

Parameter	Value
OutputMode(0=None,1=All,2=UserDefined)	1
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
FaultingDisruptiveScenarioFlag(yes=1,no=0)	1
MaximumTime[yr]	100000
NumberOfRealizations	10
OuterWPThickness[m]	2.0e-4

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used

6.1 Input files are modified in accordance with Section 4.0.

7.0 Utility Scripts Needed to Perform the Test

None

8.0 Test Description

8.1 Objective: This test is designed to verify that the number of waste packages tabulated in wpsfail.res reflect the number of waste packages supplied to the release module(EBSREL/RELEASET).

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: ebsrel.ech, faulto.rlt, sl1.out, seismo.rlt, tpa.inp, volcano.rlt, wpsfail.res

8.5 Procedure:

1. At the command prompt from the <<Run Directory>>, type the following: "tpa.exe > sl1.out."

2. Compare the number of failed waste packages tabulated in the output files to verify that wpsfail.res contains the correct number of failed waste packages.

8.6 Pass/Fail Criteria: The code runs to completion and the number of waste packages provided to the release module agrees with the number of waste packages displayed in the wpsfail.res file.

9.0 Test Results

9.1 Output and Supporting Files: All files are archived to a CD labeled, "TPA SCR #603."

9.2 Criterion 1: The number of failed waste packages agree between files ebsrel.ech, wpsfail.res, faulto.rlt, volcano.rlt, seismo.rlt, and the screen output.

9.3 Overall Test Status:

This test successfully **PASSED** the criterion above for test SL-1.

Three different sets of data were compared for which seismic failures occurred along with corrosion failures to verify values were being calculated correctly.

Realization 1
Subarea 6

Failure Types	Type	wpsfail.res		screen output		ebsrel.ech		seismo.rlt				faulto.rlt	
		time	no.	time	no.	time	no.	time	fraction	total - previous	no.	time	fraction
Initial	1	0	3	0	3	0	3						
Faulting	2					28900	0					28900	0.010768
Volcano	3					0	0						
Seismo 1	4	996.39	51	811.3	51	996.39	51	811.317	0.15	340	51		
Seismo 2	5					3465.9	0						
Seismo 3	6					7376.3	0						
Seismo 4	7					55000	0						
Corrosion	8	1562.23	289	1562.2	289	1562.2	289						
Extrusive	3*					0	0						

volcano.rlt	
time	fraction
0	0

Subarea 4

Failure Types	Type	wpsfail.res		screen output		ebsrel.ech		seismo.rlt				faulto.rlt	
		time	no.	time	no.	time	no.	time	fraction	total - previous	no.	time	fraction
Initial	1	0	17	0	17	0	17						
Faulting	2					0	0					0	0
Volcano	3	1313.84	73	1313.8	73	1313.8	73						
Seismo 1	4	996.39	266	730.9	266	996.39	266	730.863	0.15	1776	266		
Seismo 2	5					3465.9	0						
Seismo 3	6					7376.3	0						
Seismo 4	7					55000	0						
Corrosion	8	1809.62	1437	1809.6	1437	1809.6	1437						
Extrusive	3*					1313.8	0						

volcano.rlt			
time	fraction	total - previous	no.
1313.8	0.048522	1510	73

Realization 4
Subarea 2

Failure Types	Type	wpsfail.res		screen output		ebsrel.ech		seismo.rlt				faulto.rlt	
		time	no.	time	no.	time	no.	time	fraction	total - previous	no.	time	fraction
Initial	1	0	7	0	7	0	7						
Faulting	2					0	0					0	0.00E+00
Volcano	3					0	0						
Seismo 1	4	996.39	1055	693.3	158	996.39	1055	693.345	0.15	1055	158		
				730.9	897			730.863	1	897	897		
Seismo 2	5					3465.9	0						
Seismo 3	6					7376.3	0						
Seismo 4	7					55000	0						
Corrosion	8					1640.9	0						
Extrusive	3*					0	0						

volcano.rlt	
time	fraction
0	0

Test was repeated on UNIX machine spock and the wpsfail.res files were compared to verify they accounted for the same number of waste package failures. The following is a screen print of the differences between the PC test and the UNIX test wpsfail.res files:

As shown below, the only difference between the PC and UNIX version of wpsfail.res is the date time stamp:

```
3c3
<  TPA 5.0.2e, Job started: Fri Jan 20 17:58:30 2006
---
>  TPA 5.0.2e, Job started: Mon Jan 23 14:33:03 2006
```

SL-2 Verify Results when the Code is Restarted

1.0 Path for Run Directory

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results

\SCR603\testresults\sl2

3.0 Environment Variables

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

4.0 Special Input Files or Modifications to Input Files Required

4.1 Set the values in TPA.INP in accordance with the following table:

Parameter	**Value**
OutputMode(0=None,1=All,2=UserDefined)	1
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
FaultingDisruptiveScenarioFlag(yes=1,no=0)	1
MaximumTime[yr]	100000
NumberOfRealizations	10
OuterWPThickness[m]	2.0e-4
GenerateRestartFiles(yes=1,no=0)	1

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used

6.1 Input files are modified in accordance with Section 4.0.

7.0 Utility Scripts Needed to Perform the Test

None

8.0 Test Description

8.1 Objective: This test is designed to verify that the same results are obtained from test SL-1 when the tpa code is restarted.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: wpsfail.res

8.5 Procedure:

1. At the command prompt from the <<Run Directory>>, type the following: "tpa.exe"

2. After the first realization, stop the code and restart it.

3. Compare the number of failed waste packages in file wpsfail.res with those generated previously in test SL-1.

8.6 Pass/Fail Criteria: The code runs to completion and generates the same number of failed waste packages in file wpsfail.res after restarting the code as was generated previously in test SL-1.

9.0 Test Results

9.1 Output and Supporting Files: All files are archived to a CD labeled, "TPA SCR #603."

9.2 Criterion 1: The number of failed waste packages agree in file wpsfail.res between this test and test SL-1.

9.3 Overall Test Status:

This test successfully **PASSED** the criterion above for test SL-2.

The tpa code was stopped during realization 4 and then restarted.

The wpsfail.res files were compared using the UNIX diff command. There were no differences except for the date time stamp.

Test executed on Windows machine tpa:

The tpa code was stopped during realization 4 and then restarted.

Diff command showing the only difference is the date time stamp.

```
3c3
< TPA 5.0.2e, Job started: Fri Jan 20 17:58:30 2006^M
---
> TPA 5.0.2e, Job started: Mon Jan 23 10:05:53 2006^M
```

Test executed on UNIX machine idaho:

The tpa code was stopped during realization 2 and then restarted.

Diff command showing the only difference is the date time stamp.

```
3c3
<  TPA 5.0.2e, Job started: Mon Jan 23 14:33:03 2006
---
>  TPA 5.0.2e, Job started: Mon Jan 23 16:49:17 2006
```

SL-3 Verify Failures for Corrosion at Longer Times

1.0 Path for Run Directory

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results

\SCR603\testresults\sl2

3.0 Environment Variables

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

4.0 Special Input Files or Modifications to Input Files Required

4.1 Set the values in TPA.INP in accordance with the following table:

Parameter	**Value**
OutputMode(0=None,1=All,2=UserDefined)	1
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
FaultingDisruptiveScenarioFlag(yes=1,no=0)	1
MaximumTime[yr]	100000
NumberOfRealizations	10

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used

6.1 Input files are modified in accordance with Section 4.0.

7.0 Utility Scripts Needed to Perform the Test

None

8.0 Test Description

8.1 Objective: This test is designed to verify that the corrosion failures are removed from the wpsfail.res results obtained from test SL-1.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: ebsrel.ech, faulto.rlt, sl-3.out, seismo.rlt, tpa.inp, volcano.rlt, wpsfail.res

8.5 Procedure:

1. At the command prompt from the <<Run Directory>>, type the following: "tpa.exe > sl-3.out"

2. Compare the number of failed waste packages in file wpsfail.res with those generated previously in test SL-1.

8.6 Pass/Fail Criteria: The code runs to completion and removes corrosion failed waste packages from wpsfail.res in subareas where corrosion failures no longer occur.

9.0 Test Results

9.1 Output and Supporting Files: All files are archived to a CD labeled, "TPA SCR #603."

9.2 Criterion 1: The number of failed waste packages agree in file wpsfail.res between this test and test SL-1 except corrosion failed waste packages are removed in those subareas where corrosion failures no longer occurred.

9.3 Overall Test Status:

This test successfully **PASSED** the criterion above for test SL-3.

The below results compare to those from test SL-1; however, the corrosion failures have been removed.

Realization 1
Subarea 6

Failure Types	Type	wpsfail.res		screen output		ebsrel.ech		seismo.rlt			
		time	no.	time	no.	time	no.	time	fraction	total - previous	no.
Initial	1	0	3	0	3	0	3				
Faulting	2	28900	3	28900	3	28900	3				
Volcano	3					0	0				
Seismo 1	4	996.39	51	811.3	51	996.39	51	811.317	0.15	340	51
Seismo 2	5					3465.9	0				
Seismo 3	6					7376.3	0				
Seismo 4	7					55000	0				
Corrosion	8					100000	0				
Extrusive	3*					0	0				

faulto.rlt				volcano.rlt	
time	fraction	total - previous	no.	time	fraction
28900	0.010768	289	3.111952		
				0	0

Subarea 4

Failure Types	Type	wpsfail.res		screen output		ebsrel.ech		seismo.rlt				faulto.rlt	
		time	no.	time	no.	time	no.	time	fraction	total - previous	no.	time	fraction
Initial	1	0	17	0	17	0	17						
Faulting	2					0	0					0	0
Volcano	3	1313.84	73	1313.8	73	1313.8	73						
Seismo 1	4	996.39	266	730.9	266	996.39	266	811.317	0.15	1776	266		
Seismo 2	5					3465.9	0						
Seismo 3	6					7376.3	0						
Seismo 4	7					55000	0						
Corrosion	8					100000	0						
Extrusive	3*					1313.8	0						

volcano.rlt			
time	fraction	total - previous	no.
1313.8	0.048522	1510	73

Realization 4
Subarea 2

Failure Types	Type	wpsfail.res		screen output		ebsrel.ech		seismo.rlt				faulto.rlt	
		time	no.	time	no.	time	no.	time	fraction	total - previous	no.	time	fraction
Initial	1	0	7	0	7	0	7						
Faulting	2					0	0					0	0
Volcano	3					0	0						
Seismo 1	4	996.39	1055	693.3	158	996.39	1055	693.345	0.15	1055	158		
				730.9	897			730.863	1	897	897		
Seismo 2	5					3465.9	0						
Seismo 3	6					7376.3	0						
Seismo 4	7					55000	0						
Corrosion	8					100000	0						
Extrusive	3*					0	0						

volcano.rlt	
time	fraction
0	0

Test was repeated on UNIX machine spock and the wpsfail.res files were compared to verify they accounted for the same number of waste package failures. The following is a screen print of the differences between the PC test and the UNIX test wpsfail.res files:

As shown below, the only difference between the PC and UNIX version of wpsfail.res is the date time stamp:

```
3c3
<  TPA 5.0.2e, Job started: Mon Jan 23 12:57:57 2006
---
>  TPA 5.0.2e, Job started: Tue Jan 24 08:08:36 2006
```

SL-4 Test Simultaneous Failures

1.0 Path for Run Directory

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results

\SCR603\testresults\sl4

3.0 Environment Variables

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

$TPA_TEST and $TPA_DATA = \SCR603\tpa502e

4.0 Special Input Files or Modifications to Input Files Required

4.1 Set the values in TPA.INP in accordance with the following table:

Parameter	**Value**
OutputMode(0=None,1=All,2=UserDefined)	1
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
FaultingDisruptiveScenarioFlag(yes=1,no=0)	1
MaximumTime[yr]	1.0e5
StartAtSubarea	3
StopAtSubarea	3
OuterWPThickness[m]	0.0002
CriticalRelativeHumidityHumidAirCorrosion	0.073
CriticalRelativeHumidityAqueousCorrosion	0.073
ContactAngle[degrees]	normal: 44.9, 45.0
SeismicHazardCurveforSEISMO	hazardcurve: 6; 4.0, 1000; 4.1, 2000; 4.2, 10000; 4.3, 100000; 5.0, 1000000; 6.0, 10000000
BulkingFactorRockTypeOneSubarea_3[]	uniform: 1.19, 1.191
BulkingFactorRockTypeTwoSubarea_3[]	uniform: 1.19, 1.191
DripShieldBucklingLoadSubarea_3[kg/m]	uniform: 25000.0, 25005.0
TimeOfNextVolcanicEventinRegionOfInterest[yr]	constant: 474.2 (add uniform: test 0.1, 0.2 before)
SubareaOfVolcanicEvent[]	iuniform: 3,4
TimeOfNextFaultingEventinRegionOfInterest[yr]	constant: 474.2 (add uniform: Test2Test2: 0.1, 0.3)

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used

6.1 Input files are modified in accordance with Section 4.0.

7.0 Utility Scripts Needed to Perform the Test

None

8.0 Test Description

8.1 Objective: This test is designed to verify that waste package failures at the same time step are counted correctly.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: ebsrel.ech, faulto.rlt, sl4.out, seismo.rlt, tpa.inp, volcano.rlt, wpsfail.res

8.5 Procedure:

1. At the command prompt from the <<Run Directory>>, type the following: "tpa.exe > sl4.out."

2. Compare the number of failed waste packages tabulated in the output files to verify that wpsfail.res contains the correct number of failed waste packages.

8.6 Pass/Fail Criteria: The code runs to completion and the number of waste packages provided to the release module agrees with the number of waste packages displayed in the wpsfail.res file.

9.0 Test Results

9.1 Output and Supporting Files: All files are archived to a CD labeled, "TPA SCR #603."

9.2 Criterion 1: The number of failed waste packages agree between files ebsrel.ech, wpsfail.res, faulto.rlt, volcano.rlt, seismo.rlt, and the screen output. For the second seismic failure and corrosion failure at the same time step, corrosion failure will be counted instead of seismic failure.

9.3 Overall Test Status:

This test successfully **PASSED** the criterion above for test SL-4.

The following tables show that the waste packages are being counted correctly for simultaneous failures. In this case, seismic failures do not appear in wpsfail.res or the screen output because the seismic failures occur at the same time as the corrosion failures, and, in this case, corrosion failures will be counted instead. For the same time, corrosion failures will be the waste packages remaining after initial, faulting, and volcanic failures have occurred as shown below.

Realization 1
Subarea 3

Failure Types	Type	wpsfail.res		screen output		ebsrel.ech		seismo.rlt			
		time	no.	time	no.	time	no.	time	fraction	total - previous	no.
Initial	1	0	7	0	7	0	7				
Faulting	2	474.163	1	474.2	1	474.16	1				
Volcano	3					474.16	0				
Seismo 1	4					996.39	0	474.163	1	0	0
Seismo 2	5					3465.9	0				
Seismo 3	6					7376.3	0				
Seismo 4	7					55000	0				
Corrosion	8	474.163	2895	474.2	2895	474.16	2895				
Extrusive	3*			474.2	2	474.16	2				

faulto.rlt				volcano.rlt			
time	fraction	total - previous	no.	time	fraction	total - previous	no.
474.16	3.19E-04	2888	1				
				474.16	8.23E-04	2888	2

Test was repeated on UNIX machine texas and the wpsfail.res files were compared to verify they accounted for the same number of waste package failures. The following is a screen print of the differences between the PC test and the UNIX test wpsfail.res files:

As shown below, the only difference between the PC and UNIX version of wpsfail.res is the date time stamp:

```
3c3
<  TPA 5.0.2e, Job started: Thu Jan 26 13:28:39 2006
---
>  TPA 5.0.2e, Job started: Thu Jan 26 13:02:20 2006
```

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 604	**2. Software Title and Version:** TPA 5.0.2c	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *tpa.inp, nfenv.f, condxyzt.f, driftcmt.i, cond3dxyzt.h, tpa.inp, tpanames.dbs*

The current TPA code uses a single parameter, '**TimeOfRepositoryClosure[yr]**' to assign a single time for the end of repository maintenance, forced ventilation and repository closure. This does not reflect the current planned activities of the YM repository, which is outlined as 50 yr of forced ventilation followed by another 50 yr before closure. There could be natural ventilation during the 50 yr after termination of forced ventilation, but the potential heat loss owing to natural ventilation has not been defined.

The TPA parameter '**TimeOfRepositoryClosure[yr]**' will be renamed to more accurately describe this parameter as the end of maintenance and forced ventilation. In addition two new parameters will be introduced; A user defined parameter which reflects the final closure time of the YM repository, and a parameter which describes the heat removal by natural ventilation for the interim period between the end of forced ventilation and repository closure.

5. Change Requested by:	**6. Change Authorized by** (*Software Developer*):
J. Mancillas Date:11-1-05	Ron Janetzke Date:11-4-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Modified files to use a passive ventilation period in addition to an active ventilation period. This required the use of factors for ventilation heat loss during both active and passive periods. Thermal calculation algorithms were modified to use the active and passive heat loss factors, and the mountain scale conduction model routine was modified to consider these two preclosure ventilation periods.

Consider changing the NumberOfWeightsForGaussLegendreIntegration[] to 100. See attached (Attachment A) test results for the case of a passive ventilation period of 50 years with the same factor for ventilation heat loss between active and passive ventilation.

8. Implemented by:	**Date:**
G. Adams	12-19-2005

9. Description of Acceptance Tests:

See attachments B and C for Unix and Window platforms

10. Tested by:	**Date:**
James Mancillas	1-25-2006

CNWRA Form TOP-5 (05/2000)

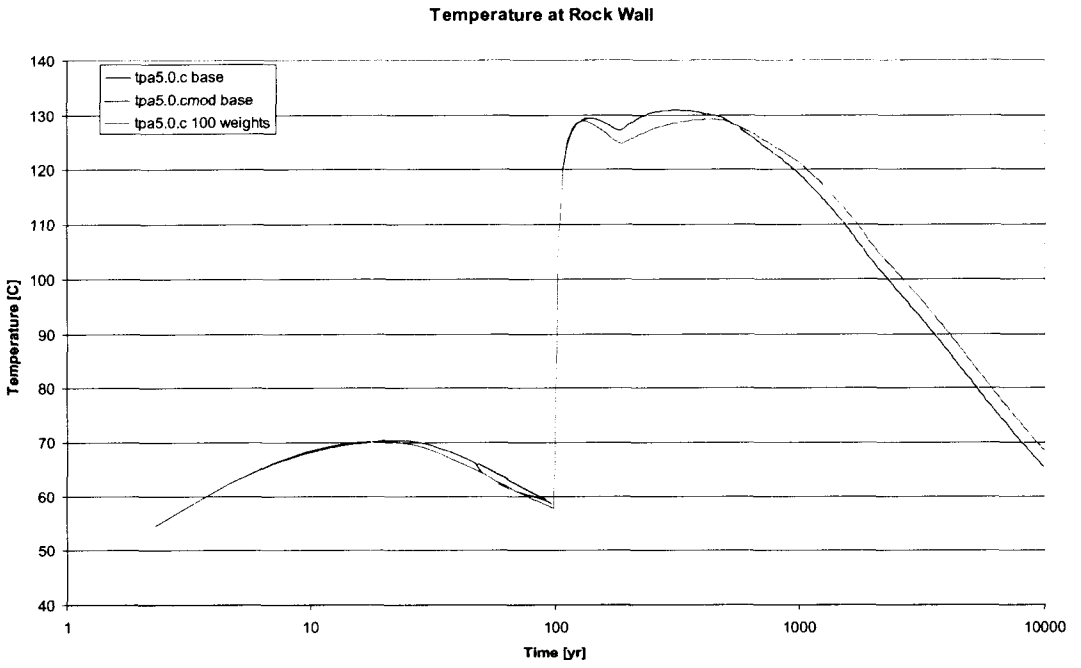
UPDATE REQUIREMENTS for TPA.INP

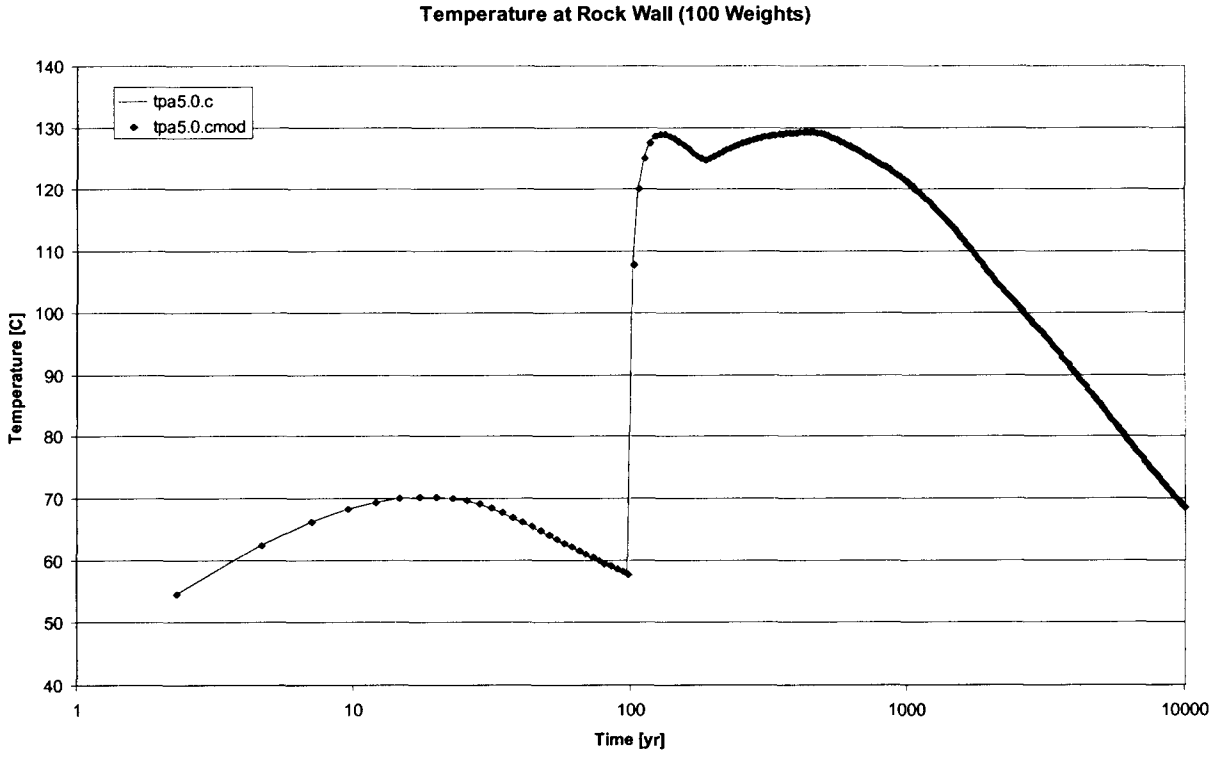
SCR 604

Status ***(ADD, DELETE, MODIFY TO, MODIFY FROM)***	**Module**	**Parameter Name**	**Description** ***(Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)***	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
Add	nfenv	TimeActiveVentilationEnds[yr]	The year in which active ventilation ends and passive ventilation may begin.	Constant	50.0	Parameter taken from current DOE design concept. Harrington (2005) presentation to NWTRB.	
Modify to	nfenv	FactorForActiveVentilationHeatLosses[]	Do not change	Do not change	Do not change	Just renaming parameter.	

Modify from	nfenv	FactorForVentilationHeatLosses[]	N/A	N/A	N/A	N/A	
Add	nfenv	FactorForPassiveVentilationHeatLosses[]	Heat loss factor for passive ventilation	Constant	0.0	Set to zero because the potential heat loss owing to natural ventilation has not been defined.	
Modify to	nfenv	NumberOfWeightsForGaussLegendreIntegration[]	Do not change	Do not change	100	Smaller numerical error in integration	

ATTACHMENT A





Attachment B

Test Plan for TPA SCR604

Test Plan Name: Active and Passive Ventilation Periods

Tested By: James Mancillas **Date:** 25 January 2006

Host Machine (UNIX): spock **Host OS**: SunOS 5.9

Baseline Version: TPA 5.0.2c **Test Version**: TPA 5.0.2f

System Level (SL) Tests

SL-1. Name: Examination of source code modifications

Path for run directory: None

Path for archive of results:
Basecase: Unix /SCR604/ tpa502c
Testcase: Unix /SCR604/ tpa502f
(Archived to CD [titled : TPA SCR604 Testing])

Environment variables: None

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description:

- **objective** Compare the differences between the basecase and testcase TPA codes, which affect the inclusion of a passive ventilation period into the TPA code.

- **assumptions** None other than those made by TPA

- **constraints** None

- **output files to compare or examine** None

- **step by step test procedure to be used**

1) examine the differences in the modified source code files; *tpa.inp, nfenv.f, cond3dxyzt.h, condxyzt.f, driftcmn.i*
2)examine the modified files for proper logic and consistent variable naming and usage.

- **pass fail criteria** The modifications made to the TPA source code should be logical and function to incorporate the inclusion of a passive ventilation period in to the TPA code.

Test Results:

- **criterion 1**
The following text depicts to differences between the basecase and testcase *tpa.inp* files which are a result of SCR604.

```
*****************************************************************************
2c2
<  Input file tpa.inp as supplied with TPA Version 5.0.2c Code.
---
>  Input file tpa.inp as supplied with TPA Version 5.0.2f Code.
237c237
< 0
---
> 1
1043a1044,1051
> **
> ** GADAMS PA-SCR-604 12-13-2005: Renamed to indicate
> ** active ventilation heat loss and added parameter
> ** for passive ventilation heat loss
> **constant
> **FactorForVentilationHeatlosses[]
> **0.83
> **
1045c1053
< FactorForVentilationHeatlosses[]
---
> FactorForActiveVentilationHeatLosses[]
1047a1056,1061
> constant
> FactorForPassiveVentilationHeatLosses[]
> 0.83
> **
> ** GADAMS PA-SCR-604 12-13-2005: End of change
> **
1062a1077,1087
> ** GADAMS PA-SCR-604 12-13-2005: Added TimeActiveVentilationEnds[yr]
> constant
> TimeActiveVentilationEnds[yr]
> 50.0
> **
> ** GADAMS PA-SCR-604 12-13-2005: End of change
> ** The TPA run time is sensitive to the number of weights used.
> ** A crude approximation is an increase of 1 weight will increase the run time by
10%.
> ** An increase of 80 weights will give about a 3C degree change toward a more
accurate
> ** post-closure temperature.
> **
*****************************************************************************
```

These differences provide evidence of the proper the inclusion of a passive ventilation period and an associated heat loss factor (HLF).

The following text depicts the differences between the basecase and testcase *nfenv.f* module.

```
*****************************************************************************
3c3
< c File Date:           10/06/05
---
> c File Date:           01/20/06
367a368,374
> c     GADAMS PA-SCR-604 12-13-2005: Added time for end of active
> c     ventilation
>       double precision timeofventend
>       integer i_timeofventend
>       save i_timeofventend
> c     GADAMS PA-SCR-604 12-13-2005: End of change
>
398a406,410
>
> c     GADAMS SCR604 12-13-2005: Modified for active and passive
> c     ventilation
> c      common / nfenv17 / iconde_n, icondbf1, icondbf2, icondds,
> c     &                   ihloss_fact
400c412,413
<      &                   ihloss_fact
---
>      &                   ihlossact_fact, ihlosspas_fact
> c     GADAMS SCR604 12-13-2005: End of change
637a651,652
> c       GADAMS PA-SCR-604 12-13-2005: Added time for active
> c       ventilation to end
638a654,658
>         name = 'TimeActiveVentilationEnds[yr]'
>         i_timeofventend = ispquery(name)
> c       GADAMS PA-SCR-604 12-13-2005: End of change
>
>         call clearchar(60, name)
717a738,739
> c       GADAMS PA-SCR-604 12-13-2005: Modified to include
> c       active and passive ventilation periods.
719,720c741,750
<         name = 'FactorForVentilationHeatlosses[]'
<         ihloss_fact = ispquery( name )
---
> c        name = 'FactorForVentilationHeatlosses[]'
>         name = 'FactorForActiveVentilationHeatLosses[]'
> c        ihloss_fact = ispquery( name )
>         ihlossact_fact = ispquery( name )
>
>         call clearchar( 60, name )
>         name = 'FactorForPassiveVentilationHeatLosses[]'
>         ihlosspas_fact = ispquery( name )
> c       GADAMS PA-SCR-604 12-13-2005: End of change
>
1093a1124,1139
>
> c     GADAMS PA-SCR-604 12-13-2005: Added time for active ventilation
> c     to end
>       timeofventend = valuesp(i_timeofventend)
>
> c     Need to ensure that the time for end of ventilation is
> c     less than or equal to the time of repository closure
>       if(timeofventend .gt. timeofclosure) then
>         print *, ' ***>>> Error in NFENV <<<*** '
>         print *, ' Ventilation end time cannot exceed '
>         print *, '   time of closure:'
>         print *, 'Time for end of ventilation: ', timeofventend
```

```
>         print *, 'Time of closure: ', timeofclosure
>         STOP
>       endif
> c     GADAMS PA-SCR-604 12-13-2005: End of change
1178c1224,1230
<       hloss_fact = valuesp( ihloss_fact )
---
>
> c     GADAMS PA-SCR-604 12-13-2005: Modified to include active and
> c     passive heat loss
> c      hloss_fact = valuesp( ihloss_fact )
>       hlossact_fact = valuesp( ihlossact_fact )
>       hlosspas_fact = valuesp( ihlosspas_fact )
> c     GADAMS PA-SCr-604 12-13-2005: End of change
1273a1326,1332
>
> c         GADAMS PA-SCR-604 12-13-2005: Modified to include active
> c         and passive ventilation
> c          call cond3dxyzt(  aL, aB, aH,
> c     &          rho, cp, cond, amld,
> c     &          x, y, z, tend, timeofclosure, hloss_fact,
> c     &          npoints, tbump )
1276,1277c1335,1337
<      &          x, y, z, tend, timeofclosure, hloss_fact,
<      &          npoints, tbump )
---
>      &          x, y, z, tend, timeofclosure, timeofventend,
>      &          hlossact_fact, hlosspas_fact, npoints, tbump )
> c         GADAMS PA-SCR-604 12-13-2005: End of change
1423c1483,1489
<         D_HLossFact = hloss_fact
---
>
> c       GADAMS PA-SCR-604 12-13-2005: Modified to include active
> c       and passive ventilation
>         D_HLossActiveFact = hlossact_fact
>         D_HLossPassiveFact = hlosspas_fact
> c       GADAMS PA-SCR-604 12-13-2005: End of change
>
1589c1655,1664
<              call calcTempsLinear(tim(it), timeofclosure,
---
>
> c            GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
> c            period
> c             call calcTempsLinear(tim(it), timeofclosure,
> c     &         tempwp(it), tempdsiA(it), tempdsiB(it),
> c     &         tempdsoA(it), tempdsoB(it),
> c     &         tempbfoA(it), tempbfoB(it),
> c     &         temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
>               call calcTempsLinear(tim(it), timeofclosure,
>      &         timeofventend,
1593a1669,1670
> c            GADAMS PA-SCR-604 12-13-2005: End of change
>
1602a1680,1686
>
> c            GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
> c            period
> c             call calcTempsIterative(tim(it), timeofclosure,
> c     &         temprep(it), tempbfoA(it),
> c     &         tempdsoA(it), tempdsiA(it),
> c     &         tempwp(it), qwp, qwp_dA, qwp_i)
1603a1688
```

```
>      &         timeofventend,
1606a1692
> c            GADAMS PA-SCR-604 12-13-2005: End of change
4919,4921d5004
<
<
<
5237c5320,5327
<       subroutine calcTempsLinear(time, timeClosure,
---
>
> c     GADAMS PA-SCR-604 12-13-2005: Added time for end of active
> c     ventilation
> c      subroutine calcTempsLinear(time, timeClosure,
> c     &  tempWP, tempDSIA, tempDSIB, tempDSOA, tempDSOB, tempBFOA,
> c     &  tempBFOB, tempRep,
> c     &  qwp, qwpInvert, qwpRWA, qwpRWB)
>       subroutine calcTempsLinear(time, timeClosure, timeActVentEnd,
5240a5331,5332
> c     GADAMS PA-SCR-604 12-13-2005: End of change
>
5272a5365,5367
> c     GADAMS PA-SCR-604 12-13-2005: Added time of active ventilation end
>       double precision timeActVentEnd
>
5384c5479,5486
<           qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
---
> c         GADAMS PA-SCR-604 12-13-2005: Added passive ventilation.
>           if(time .lt. timeActVentEnd) then
> c          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
>           qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossActiveFact)
>           else
>           qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossPassiveFact)
>           endif
> c         GADAMS PA-SCR-604 12-13-2005: End of change
5644a5747,5755
>
> c         GADAMS PA-SCR-604 12-13-2005: Added passive ventilation.
>           if(time .lt. timeActVentEnd) then
> c          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
>           qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossActiveFact)
>           else
>           qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossPassiveFact)
>           endif
> c         GADAMS PA-SCR-604 12-13-2005: End of change
5646,5648d5756
< c         Calculate the heat flux during the ventilation period
<           qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
<
6124,6125c6232,6240
<       subroutine calcTempsIterative(time, timeClosure, tempRW, tempBF,
<      &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
---
>
> c     GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
> c      subroutine calcTempsIterative(time, timeClosure, tempRW, tempBF,
> c     &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
>       subroutine calcTempsIterative(time, timeClosure,
>      &  timeActVentEnd, tempRW, tempBF,
>      &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
> c     GADAMS PA-SCR-604 12-13-2005: End of change
>
6162a6278,6281
```

```
> c     GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
>       double precision timeActVentEnd
> c     GADAMS PA-SCR-604 12-13-2005: End of change
>
6211c6330,6340
<         qwpTotal = qpermtu(time) * D_WPPayload * (1.0d0 - D_HLossFact)
---
> c       GADAMS PA-SCR-604 12-13-2005: Added passive ventilation.
>         if(time .lt. timeActVentEnd) then
> c        qwpTotal = qpermtu(time) * D_WPPayload * (1.0d0 - D_HLossFact)
>          qwpTotal = qpermtu(time) * D_WPPayload *
>      &     (1.d0-D_HLossActiveFact)
>         else
>          qwpTotal = qpermtu(time) * D_WPPayload *
>      &     (1.d0-D_HLossPassiveFact)
>         endif
> c       GADAMS PA-SCR-604 12-13-2005: End of change
>
6234d6362
<
6544d6671
<
*****************************************************************************
```

These differences provide evidence for the proper inclusion of a passive ventilation period, with its own unique HLF. These changes include logical arguments which are self-consistent and functional.

The following text depicts the differences between the basecase and testcase files *condxyzt.f*.

```
*****************************************************************************
3c3
< c File Date:          07/23/05
---
> c File Date:          01/20/06
77a78,82
>
> c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation
> c      subroutine cond3dxyzt(  aLin, aBin, aHin,
> c     &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, closetimein,
> c     &  hloss_factin, npoints, tempbump )
79,80c84,87
<      &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, closetimein,
<      &  hloss_factin, npoints, tempbump )
---
>      &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, closetimein,
>      &  endventin, hlossact_factin, hlosspas_factin, npoints, tempbump )
> c     GADAMS PA-SCR-604 12-16-2005: End of change
>
120,121c127,133
< c           closetimein = double precision, ventilation end time.
< c           hloss_factin =
---
> c           closetimein = double precision, time of closure
> c           endventin = double precision, end of active ventilation time
> c           hlossact_factin = double precision, factor for active
> c                 ventilation heat loss
> c           hlosspas_factin = double presision, factor for passive
> c                 ventilation heat loss
> c
193c205,211
< c     GADAMS PA-SCR-553 2-4-2005: End of change
---
> c     GADAMS PA-SCR-553 2-4-2005: End of change
>
```

```
> c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation time
>       double precision endvent
>       double precision hlossact_fact
>       double precision hlosspas_fact
> c     GADAMS PA-SCR-604 12-16-2005: End of change
197c215,219
<       double precision hloss_fact
---
>
> c     GADAMS PA-SCR-604 12-16-2005: Renamed when passive ventilation
> c     period was added
> c      double precision hloss_fact
>
200a223,229
>
> c     GADAMS PA-SCR-604 12-16-2005: Added tempbum3 because three
> c     periods may be available for analysis when passive ventilation
> c     is included
>       double precision tempbump3
> c     GADAMS PA-SCR-604 12-16-2005: End of change
>
209a239,244
> c
> c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation
> c     period
> c      common / tempgl1 / aL, aB, aH, x, y, z,
> c     & aml, rho, cp, cond, tend, alpha, closetime,
> c     & hloss_fact
212c247,248
<      & hloss_fact
---
>      & endvent, hlossact_fact, hlosspas_fact
> c     GADAMS PA-SCR-604 12-16-2005: End of change
246a283
>
254c291,296
<       hloss_fact = hloss_factin
---
> c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
> c      hloss_fact = hloss_factin
>       endvent = endventin
>       hlossact_fact = hlossact_factin
>       hlosspas_fact = hlosspas_factin
> c     GADAMS PA-SCR-604 12-16-2005: End of change
258c300,306
<       if (tend.le.closetime) then
---
>
> c     GADAMS PA-SCR-604 12-16-2005: Modified condition from .le. to .lt.
> c     for consistency with other conditional checks for active and
> c     passive ventilation
> c      if (tend.le.closetime) then
>       if (tend .lt. closetime) then
>
261,262c309,320
<          call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
<          tempbump = tempbump1
---
> c        GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
>          if(tend .lt. endvent) then
> c          call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
>            call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
>            tempbump = tempbump1
>          else
```

```
>            call xgauleg(tempgl, 0.0d0, endvent, npoints, tempbump1)
>            call xgauleg(tempgl, endvent, tend, npoints, tempbump2)
>            tempbump = tempbump1 + tempbump2
>          endif
> c        GADAMS PA-SCR-604 12-16-2005: End of change
>
267c325,327
<         call xgauleg(tempgl, 0.0d0, closetime, npoints, tempbump1)
---
>
> c       GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
> c        call xgauleg(tempgl, 0.0d0, closetime, npoints, tempbump1)
269c329,334
<         call xgauleg(tempgl, closetime, tend, npoints, tempbump2)
---
> c        call xgauleg(tempgl, closetime, tend, npoints, tempbump2)
>         call xgauleg(tempgl, 0.0d0, endvent, npoints, tempbump1)
>         call xgauleg(tempgl, endvent, closetime, npoints, tempbump2)
>         call xgauleg(tempgl, closetime, tend, npoints, tempbump3)
> c       GADAMS PA-SCR-604 12-16-2005: End of change
>
272c337,341
<         tempbump = tempbump1 + tempbump2
---
> c       GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
> c        tempbump = tempbump1 + tempbump2
>         tempbump = tempbump1 + tempbump2 + tempbump3
> c       GADAMS PA-SCR-604 12-16-2005: End of change
>
343c412,418
< c     GADAMS PA-SCR-553 2-4-2005: End of change
---
> c     GADAMS PA-SCR-553 2-4-2005: End of change
>
> c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation time
>       double precision endvent
>       double precision hlossact_fact
>       double precision hlosspas_fact
> c     GADAMS PA-SCR-604 12-16-2005: End of change
347c422,425
<       double precision hloss_fact
---
>
> c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
> c      double precision hloss_fact
>
359c437,443
<       common / tempgl1 / aL, aB, aH, x, y, z,
---
>
> c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation
> c     period
> c      common / tempgl1 / aL, aB, aH, x, y, z,
> c     & aml, rho, cp, cond, tend, alpha, closetime,
> c     & hloss_fact
>       common / tempgl1 / aL, aB, aH, x, y, z,
361c445,447
<      & hloss_fact
---
>      & endvent, hlossact_fact, hlosspas_fact
> c     GADAMS PA-SCR-604 12-16-2005: End of change
>
382c468,476
<          qpp = qpermtu( t ) * (1.d0 - hloss_fact) * aml / 4047.0d0
```

```
---
> c       GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
> c         qpp = qpermtu( t ) * (1.d0 - hloss_fact) * aml / 4047.0d0
>         if (t .lt. endvent) then
>           qpp = qpermtu( t ) * (1.d0 - hlossact_fact) * aml / 4047.0d0
>         else
>           qpp = qpermtu( t ) * (1.d0 - hlosspas_fact) * aml / 4047.0d0
>         endif
> c       GADAMS PA-SCR-604 12-16-2005: End of change
>
```
****

These differences provide further evidence for the proper implementation of a passive ventilation period and associated HLF. The logical argument changes are functional and self-consistent.

The following text depicts the differences between the basecase and testcase files *cond3dxyzt.h.*

****

```
22c22,30
<        double precision hloss_factin
---
> c      GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
>        double precision endventin
>
> c      GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
> c       double precision hloss_factin
>        double precision hlossact_factin
>        double precision hlosspas_factin
> c      GADAMS PA-SCR-604 12-16-2005: End of change
>
```
****

The differences between these *cond3dxyzt.h* files supports the inclusion of the new parameters and the renaming of parameters used by the testcase to implement a passive ventilation period.

The following text depicts the differences between the basecase and testcase files *driftcmn.i.*

****

```
6c6,12
<     double precision D_HLossFact
---
>
> c    GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
> c     double precision D_HLossFact
>     double precision D_HLossActiveFact
>     double precision D_HLossPassiveFact
> c    GADAMS PA-SCR-604 12-13-2005: End of change
>
21a28,35
>
> c    GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
> c     common /nfenv_thermal1/ D_SBolt, D_ViewFactor, D_WPPayload,
> c    & D_HLossFact, D_FracInv, D_FracWedge,
> c    & D_WPSpace, D_WPDia, D_DSDiaI, D_DSThick, D_DriftDiaFloor,
> c    & D_CondFloor, D_CondRW, D_CondConv, D_CondBF, D_EmissWP,
> c    & D_EmissRW, D_EmissDS, D_EmissBF
>
```

```
23c37
<     & D_HLossFact, D_FracInv, D_FracWedge,
---
>     & D_HLossActiveFact, D_HLossPassiveFact, D_FracInv, D_FracWedge,
26c40,41
<     & D_EmissRW, D_EmissDS, D_EmissBF
---
>     & D_EmissRW, D_EmissDS, D_EmissBF
> c    GADAMS PA-SCR-604 12-13-2005: End of change
```

****

The differences between these *driftcmn.i* files supports the inclusion of the new parameters and the renaming of common parameters used by the testcase to implement a passive ventilation period.

- overall test status: PASS

SL-2. Name: Examine Thermal Profile of Repository Wall

Path for run directory:

Basecase: [spock]:/home/jmancillas/SCR604/tpa502c/run1, run2
Testcase: [spock]:/home/jmancillas/SCR604/tpa502f/ run1, run2

Path for archive of results:

Basecase: Unix/SCR604/tpa502c/run1, run2
Testcase: Unix/SCR604/tpa502f/run1, run2
(Archived to CD [titled : TPA SCR604 Testing])

Environment variables:

Basecase: TPA_TEST=/home/jmancillas/SCR604/tpa502c
TPA_DATA=/home/jmancillas/SCR604/tpa502c

Testcase: TPA_TEST=/home/jmancillas/SCR604/tpa502f
TPA_DATA=/home/jmancillas/SCR604/tpa502f

Special input files or modifications to input files required : *tpa.inp*

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Append All

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: MS Excel (2002 SP3)

Test description: SCR604 has increased the functionality of the TPA code by introducing a passive ventilation period. Through this change the TPA simulation has the ability to evaluate two unique periods prior to pre-closure: A period of active ventilation, and a period of passive ventilation. Each of these ventilation periods has its own heat removal capacity. This test will examine the behavior of the TPA code with two ventilation periods, and evaluate for proper behavior. Included in this test is an examination of the effect of the number of Gauss-Legendre weights.

- **objective** Verify the proper implementation of SCR604, with respect to the generation of wall temperature profiles which agree between the basecase and testcase.

- **assumptions** None other than those made within the TPA code

- **constraints** None

- **output files to compare or examine** *nfenv.rlt*

- step by step test procedure to be used

1) Compare repository wall temperature profiles for subarea 1 with the following values in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.83
# of Gauss-Legendre weights	20	20
End of active ventilation	50	50

2) Compare repository wall temperature profiles for subarea 1 with the following conditions:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.83
# of Gauss-Legendre weights	100	100
End of active ventilation	50	50

- pass fail criteria A comparison of temperature profiles for the repository walls should show similar trends with temperatures differing by less than 2 degrees.

Test Results:

- criterion 1 The TPA code was run for both the basecase and testcase. The temperature profiles of the repository walls for subarea one were plotted from the data collected in the append file *nfenv.rlt*.

Figure 1 shows the repository temperature profile for subarea 1 using 20 Gauss-Legendre (GL) weights. The maximum temperature difference is 1.49 degrees Celsius occurring 58 years into the simulation. Near this time there is a minor difference in the behaviors of the basecase and testcase temperature profiles. It is suspected that this is a result of the numeric integration method and not a result of an improper implementation of the passive ventilation period. A second simulation with the number of GL weighs increased to 100 is shown in figure 2. While using 100 GL weights, the temperature profiles between the basecase and testcase show nearly identical behaviors and have a maximum temperature which gradually builds to a difference of 1.00 degree Celsius at 181 years.

The plots of these behaviors shown in figures 1 and 2 are provided as evidence that the passive ventilation period has been properly implemented. And that the minor differences are a result of the numerical integration method.

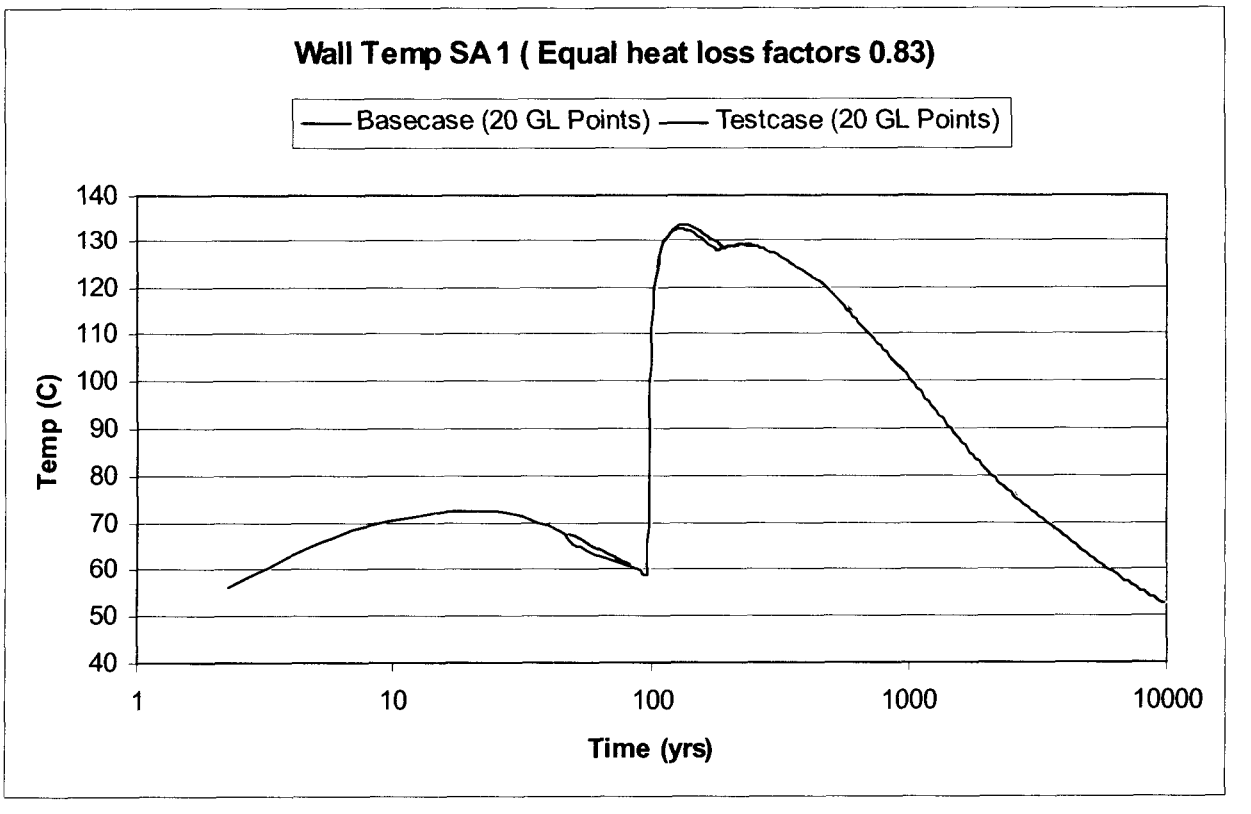


Figure 1 Repository wall temperature profile, 20 GL weights, with end of active ventilation at 50 years.

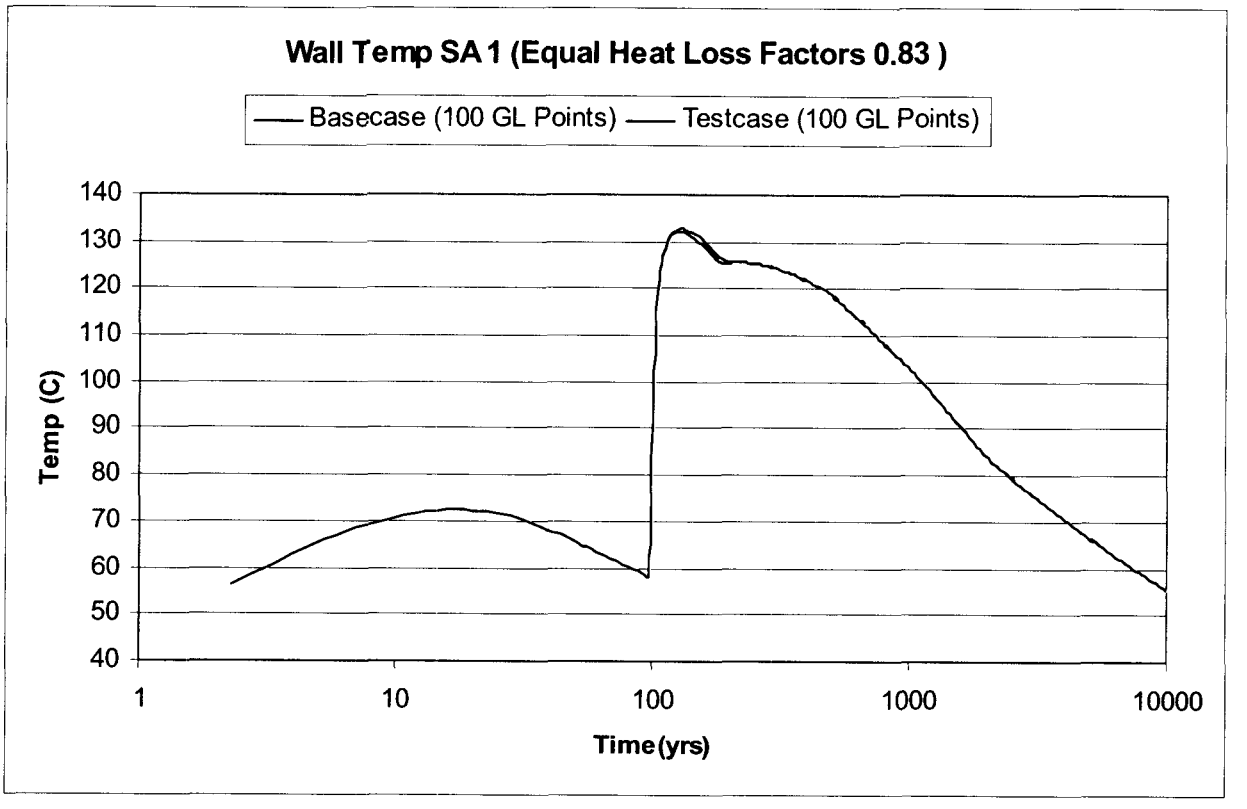


Figure 2 Repository wall temperature profile, 100 GL weights, with end of active ventilation at 50 years.

- overall test status : PASS

Notes:

The issue of integration approximation using 20 weights versus 100 weights should probably be addressed, because of the increased computational time required when using 100 weights.
The MS Excel worksheet used to generate this plot, named *nfenve_c_20_unix*, is included on the archive of this SCR.

SL-3. Name: Examine Thermal Profile of Repository Wall with Differing Passive and Active Heat Losses

Path for run directory:

Basecase: [spock]:/home/jmancillas/SCR604/tpa502c/run1
Testcase: [spock]:/home/jmancillas/SCR604/tpa502f/ run3

Path for archive of results:

Basecase: Unix/SCR604/tpa502c/run1
Testcase: Unix/SCR604/tpa502f/run3
(Archived to CD [titled : TPA SCR604 Testing])

Environment variables:

Basecase: TPA_TEST=/home/jmancillas/SCR604/tpa502c
TPA_DATA=/home/jmancillas/SCR604/tpa502c

Testcase: TPA_TEST=/home/jmancillas/SCR604/tpa502f
TPA_DATA=/home/jmancillas/SCR604/tpa502f

Special input files or modifications to input files required : *tpa.inp*

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Append All

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: MS Excel (2002 SP3)

Test description: SCR604 has increased the functionality of the TPA code by introducing a passive ventilation period. Through this change the TPA simulation has the ability to evaluate two unique periods prior to pre-closure: A period of active ventilation, and a period of passive ventilation. Each of these ventilation periods has its own heat removal capacity. This test will examine the behavior of the TPA code with differing heat loss factors for the passive ventilation period

- **objective** Verify the proper implementation of SCR604, with respect to allowing differing heat loss factors (HLF) for the active and passive ventilation periods.

- **assumptions** None other than those made within the TPA code

- **constraints** None

- **output files to compare or examine** *nfenv.rlt*

- **step by step test procedure to be used**

  1) compare repository wall temperature profiles for subarea 1 with the following values in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.50
# of Gauss-Legendre weights	20	20
End of active ventilation	50	50

- **pass fail criteria** The temperature profile of the testcase should show a sharp rise in temperature, relative to the basecase, at the end of active ventilation.

Test Results: The temperature profile of the testcase should show a sharp increase in wall temperature because of the reduction in the passive ventilation heat loss factor.

- **criterion 1** Figure 3. Shows the differences between the basecase and testcase. The temperature profiles of the repository walls for subarea one were plotted from the data collected in the append file *nfenv.rlt*. temperature profiles. These results exhibit the behavior expected with a decreased passive heat loss factor and is used as evidence that

SCR604 has been properly implemented. The sharp increase in temperature at time equals 50yr, shown in figure 3, is used as evidence of the proper implementation of SCR604.

- overall test status : PASS

Note
The MS Excel worksheet used to generate these comparison plots, named *nfenve_c_unix*, is included on the archive of this SCR. There is a slight integration error at the transition point from active to passive ventilation.

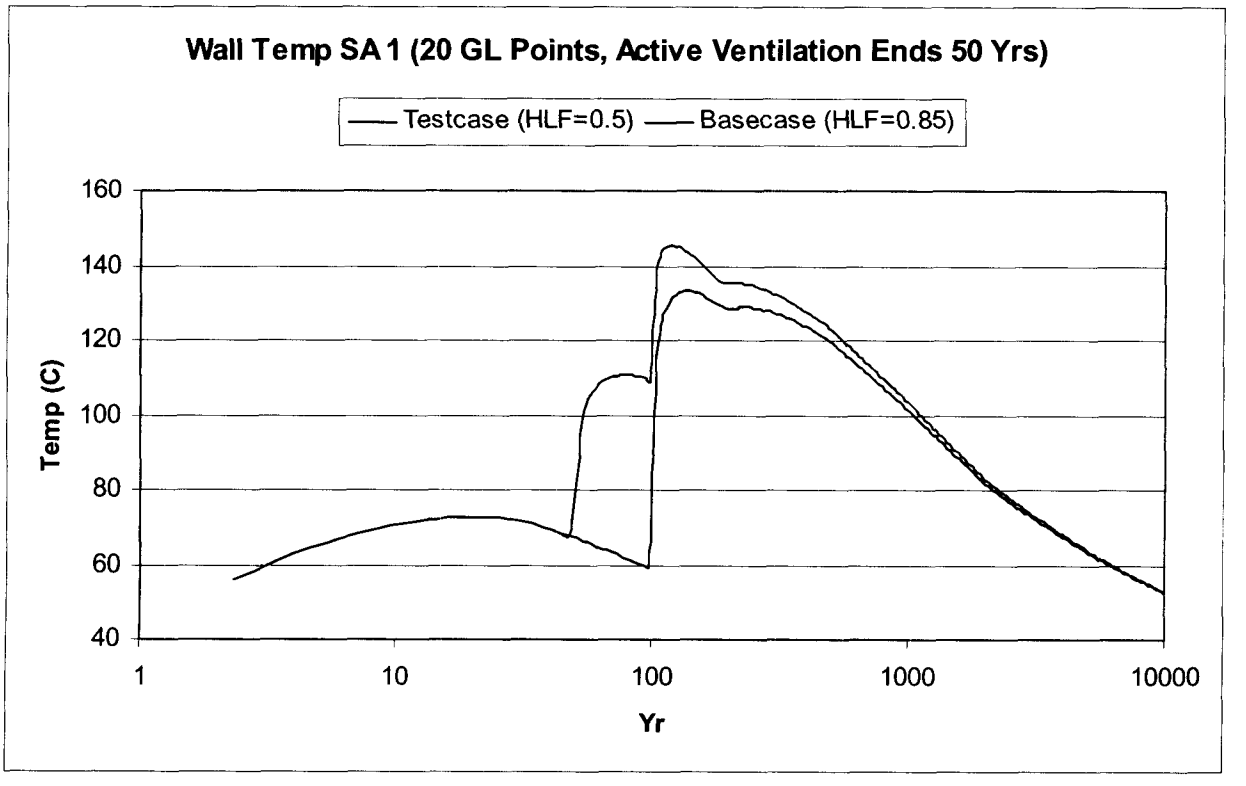


Figure 3. Repository wall temperature as a function of time. The testcase has a reduced passive ventilation h which results is a sharp increase in temperature at the end of active ventilation

SL-4. Name: Examine Thermal Profile of Repository Wall with Differing Passive and Active Heat Losses and Differing End Times for Active Ventilation

Path for run directory:

Basecase: [spock]:/home/jmancillas/SCR604/tpa502c/run1
Testcase: [spock]:/home/jmancillas/SCR604/tpa502f/ run4, run5

Path for archive of results:

Basecase: Unix/SCR604/tpa502c/run1
Testcase: Unix/SCR604/tpa502f/run4 ,run5
(Archived to CD [titled : TPA SCR604 Testing])

Environment variables:

Basecase: TPA_TEST=/home/jmancillas/SCR604/tpa502c
TPA_DATA=/home/jmancillas/SCR604/tpa502c

Testcase: TPA_TEST=/home/jmancillas/SCR604/tpa502f
TPA_DATA=/home/jmancillas/SCR604/tpa502f

Special input files or modifications to input files required : *tpa.inp*

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Append All

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: MS Excel (2002 SP3)

Test description: SCR604 has increased the functionality of the TPA code by introducing a passive ventilation period. Through this change the TPA simulation has the ability to evaluate two unique periods prior to pre-closure: A period of active ventilation, and a period of passive ventilation. Each of these ventilation periods has its own heat removal capacity. This test will examine the behavior of the TPA code with differing heat loss factors for the passive ventilation period and with differing start periods for the passive ventilation.

- **objective** Verify the proper implementation of SCR604, with respect to allowing variable times for the end of the active ventilation period.

- **assumptions** None other than those made within the TPA code

- **constraints** None

- **output files to compare or examine** *nfenv.rlt*

- **step by step test procedure to be used**

1) compare repository wall temperature profiles for subarea 1 with the following values

in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.50
# of Gauss-Legendre weights	20	20
End of active ventilation	50	25

2) compare repository wall temperature profiles for subarea 1 with the following values in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.50
# of Gauss-Legendre weights	20	20
End of active ventilation	50	0

3)compare repository wall temperature profiles for subarea 1 with the following values in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.50
# of Gauss-Legendre weights	20	20
End of active ventilation	50	100

- **pass fail criteria** The temperature profile of the testcase should show a sharp rise in temperature, relative to the basecase, at the end of active ventilation.

Test Results: The temperature profile of the testcase should show a sharp increase in wall temperatures at the end of active ventilation. The temperature profiles of the repository walls for subarea one were plotted from the data collected in the append file *nfenv.rlt*. The following two plots (figures 4 and 5) have differing time for the end of active ventilation 25 years and 0 years.

- **criterion 1** There should be a sharp increase in wall temperature a 25 years when active ventilation ends at 25 years. This behavior is shown in figure 4 and is used as evidence that SCR604 is properly implemented.

- **criterion 2** In this instance the end of active ventilation is set to time equal to zero. This should

result in large initial temperature prior to closure. This behavior is shown in figure 5 and is used as evidence that SCR604 is properly implemented.

-criterion 3 In this comparison the end of active ventilation is set to 100 years, which is the same time as the repository closure. This should result in a wall temperature profile for the testcase which is the same as the basecase. This behavior is shown in figure 6 and is used as further evidence that SCR604 is properly inplemented.

- overall test status: PASS

Note:
The MS Excel worksheet used to generate this plot, named *nfenve_c_unix*, is included on the archive of this SCR.. Slight integration errors are visible at the transition points from active to passive ventilation periods, but these are within acceptable limits.

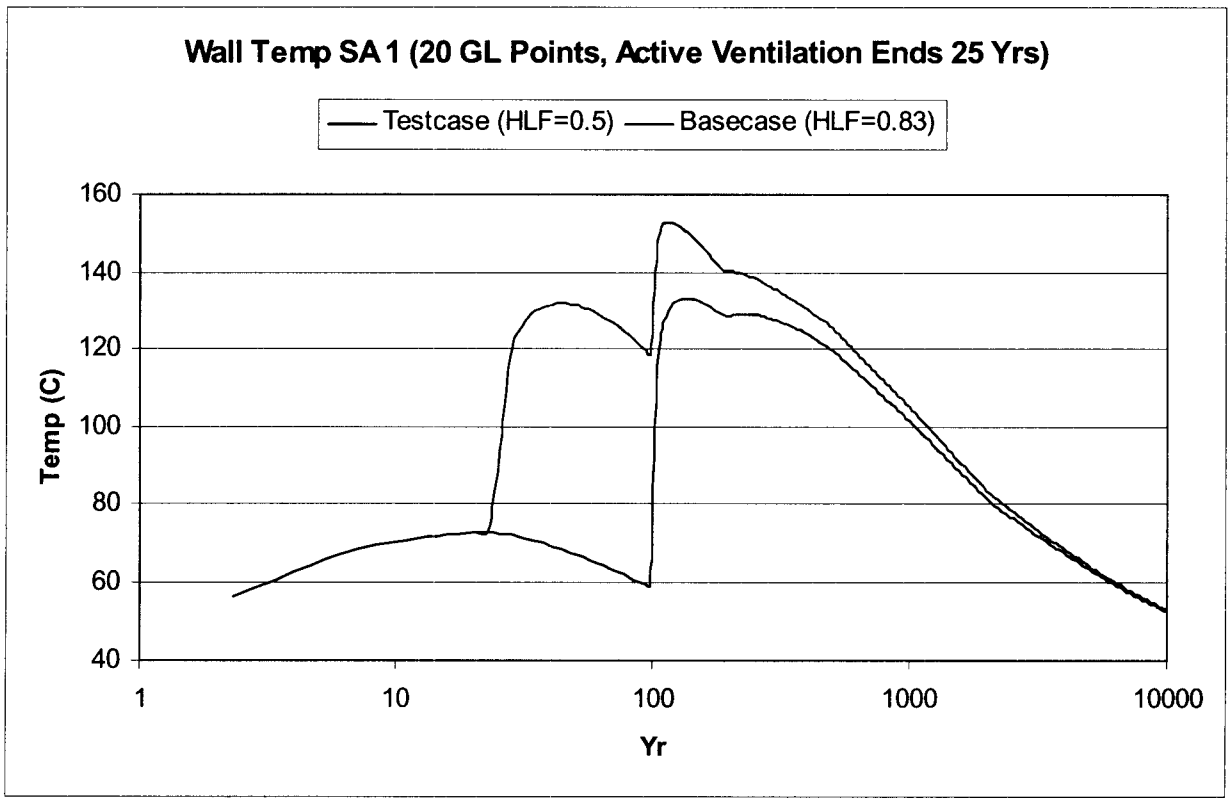


Figure 4 Repository wall temperature profile with differing HLFs and a end of active ventilation at 25 year.

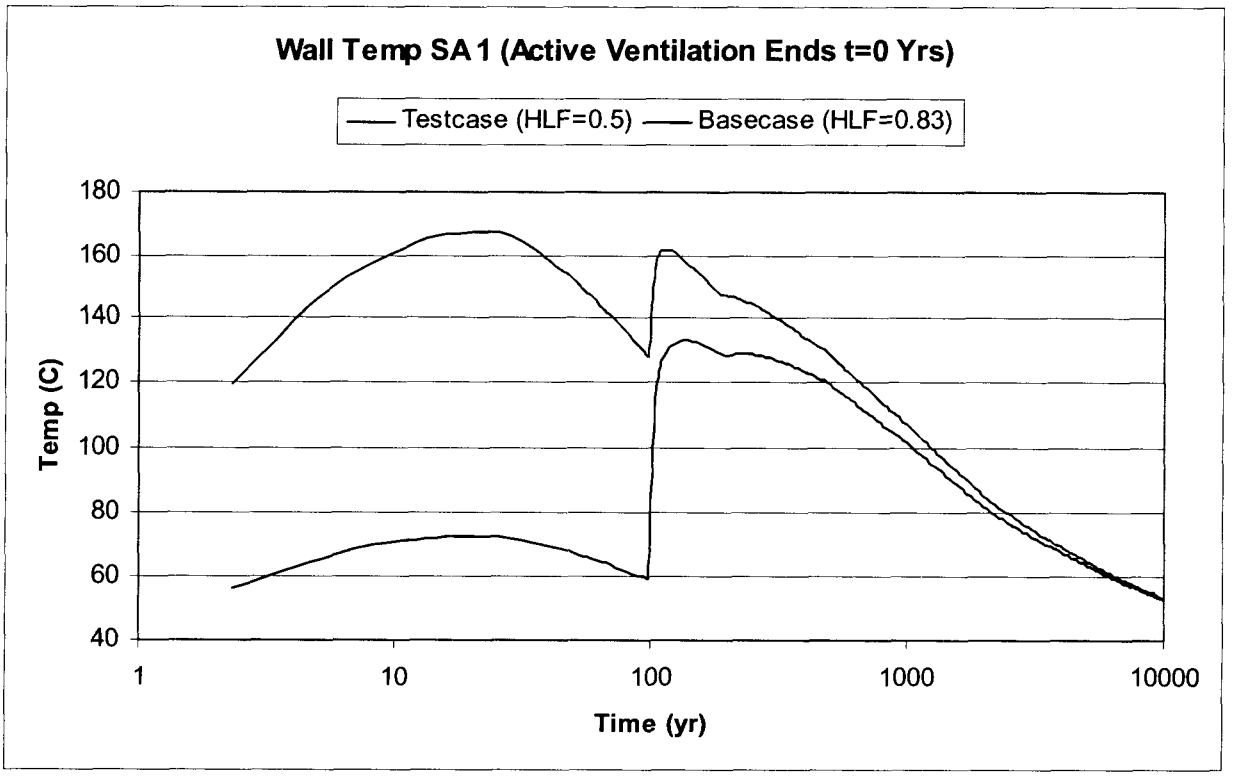


Figure 5 Repository wall temperature profile with differing HLFs and an end of active ventilation at time equ

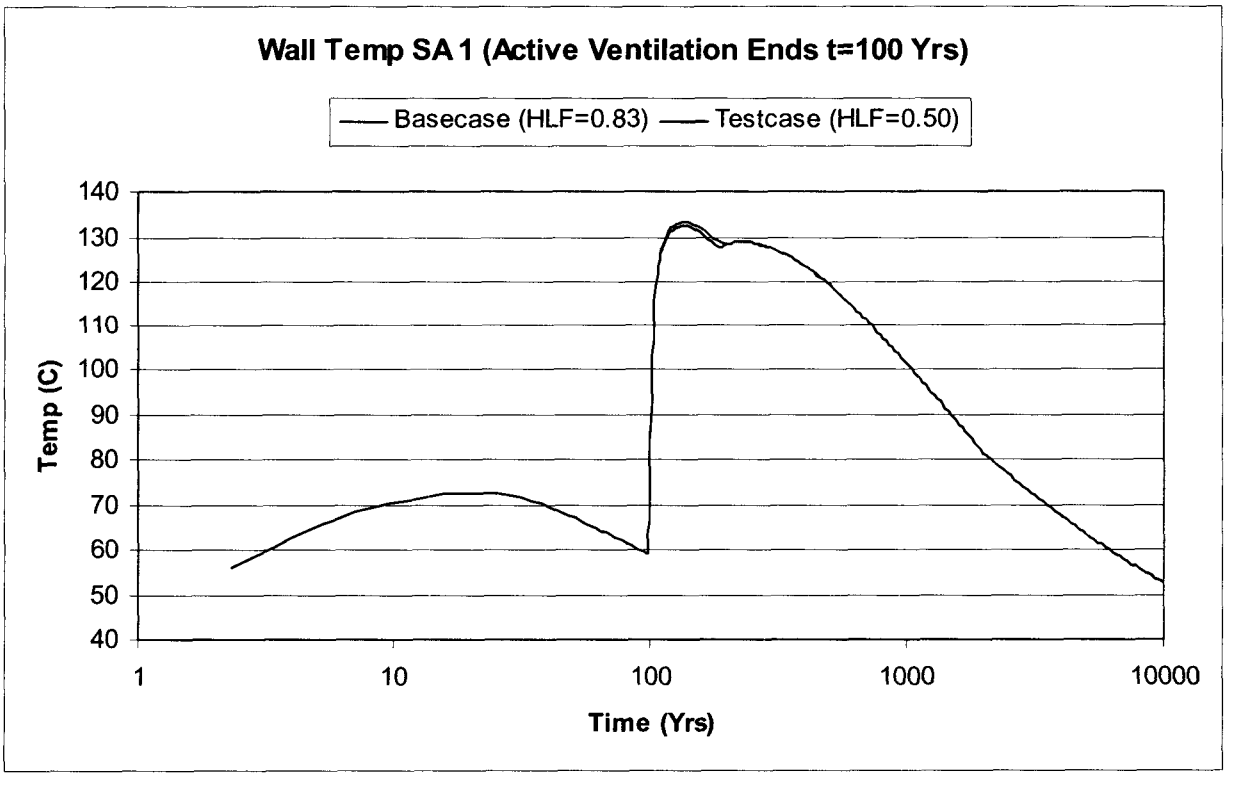


Figure 6 Repository wall temperature profile, with differing HLFs and an end of active ventilation set to one hundred years (same as closure time for both the testcase and basecase).

Attachment C

Test Plan for TPA SCR604

Test Plan Name: Active and Passive Ventilation Periods

Tested By: James Mancillas

Date: 25 January 2006

Host Machine : tpa

Host OS: Windows MS Server 2003 (SP1)

Baseline Version: TPA 5.0.2c

Test Version: TPA 5.0.2f

System Level (SL) Tests

SL-1. Name: Examination of source code modifications

Path for run directory: None

Path for archive of results:
Basecase: Windows /SCR604/ tpa502c
Testcase: Windows /SCR604/ tpa502f
(Archived to CD [titled : TPA SCR604 Testing])

Environment variables: None

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description:

- **objective** Compare the differences between the basecase and testcase TPA codes, which affect the inclusion of a passive ventilation period into the TPA code.

- **assumptions** None other than those made by TPA

- **constraints** None

- **output files to compare or examine** None

- **step by step test procedure to be used**
1) examine the differences in the modified source code files; *tpa.inp, nfenv.f, cond3dxyzt.h, condxyzt.f, driftcmn.i*
2)examine the modified files for proper logic and consistent variable naming and usage.

- **pass fail criteria** The modifications made to the TPA source code should be logical and function to incorporate the inclusion of a passive ventilation period in to the TPA code.

Test Results:

- criterion 1
The following text depicts to differences between the basecase and testcase *tpa.inp* files which are a result of SCR604.

```
*******************************************************************************
Comparing files TPA502F\tpa.inp and TPA502C\TPA.INP
***** TPA502F\tpa.inp
title
 Input file tpa.inp as supplied with TPA Version 5.0.2f Code.
 Base case.
***** TPA502C\TPA.INP
title
 Input file tpa.inp as supplied with TPA Version 5.0.2c Code.
 Base case.
*****

***** TPA502F\tpa.inp
**
**
** GADAMS PA-SCR-604 12-13-2005: Renamed to indicate
** active ventilation heat loss and added parameter
** for passive ventilation heat loss
**constant
**FactorForVentilationHeatlosses[]
**0.83
**
constant
FactorForActiveVentilationHeatLosses[]
0.83
***** TPA502C\TPA.INP
**
constant
FactorForVentilationHeatlosses[]
0.83
*****

***** TPA502F\tpa.inp
**
constant
FactorForPassiveVentilationHeatLosses[]
0.83
**
** GADAMS PA-SCR-604 12-13-2005: End of change
**
** GADAMS PA-SCR-553 2-6-2005: Removed time of backfill emplaced
```

```
***** TPA502C\TPA.INP
**
** GADAMS PA-SCR-553 2-6-2005: Removed time of backfill emplaced
*****

***** TPA502F\tpa.inp
**
** GADAMS PA-SCR-604 12-13-2005: Added TimeActiveVentilationEnds[yr]
constant
TimeActiveVentilationEnds[yr]
50.0
**
** GADAMS PA-SCR-604 12-13-2005: End of change
** The TPA run time is sensitive to the number of weights used.
** A crude approximation is an increase of 1 weight will increase the run time by 10%.
** An increase of 80 weights will give about a 3C degree change toward a more accurate
** post-closure temperature.
**
** GADAMS PA-SCR-553 2-6-2005: End of change
***** TPA502C\TPA.INP
**
** GADAMS PA-SCR-553 2-6-2005: End of change
*****
*******************************************************************************
```

These differences provide evidence of the proper the inclusion of a passive ventilation period and an associated heat loss factor (HLF).

The following text depicts the differences between the basecase and testcase *nfenv.f* module.

```
*******************************************************************************
Comparing files TPA502F\nfenv.f and TPA502C\NFENV.F
***** TPA502F\nfenv.f
c File Name:           nfenv.f
c File Date:           01/20/06
c Release Version:     5.0
***** TPA502C\NFENV.F
c File Name:           nfenv.f
c File Date:           10/06/05
c Release Version:     5.0
*****

***** TPA502F\nfenv.f

c     GADAMS PA-SCR-604 12-13-2005: Added time for end of active
c     ventilation
      double precision timeofventend
      integer i_timeofventend
      save i_timeofventend
c     GADAMS PA-SCR-604 12-13-2005: End of change

c   Common declarations
***** TPA502C\NFENV.F

c   Common declarations
*****

***** TPA502F\nfenv.f
c      common / nfenv17 / iconde_n, icondbf, icondds, ihloss_fact

c     GADAMS SCR604 12-13-2005: Modified for active and passive
c     ventilation
c      common / nfenv17 / iconde_n, icondbf1, icondbf2, icondds,
c     &                   ihloss_fact
```

```
      common / nfenv17 / iconde_n, icondbf1, icondbf2, icondds,
     &                   ihlossact_fact, ihlosspas_fact
c     GADAMS SCR604 12-13-2005: End of change
c     GADAMS SCR562 4-18-2005: End of change
***** TPA502C\NFENV.F
c      common / nfenv17 / iconde_n, icondbf, icondds, ihloss_fact
      common / nfenv17 / iconde_n, icondbf1, icondbf2, icondds,
     &                   ihloss_fact
c     GADAMS SCR562 4-18-2005: End of change
*****

***** TPA502F\nfenv.f

c       GADAMS PA-SCR-604 12-13-2005: Added time for active
c       ventilation to end
        call clearchar(60, name)
        name = 'TimeActiveVentilationEnds[yr]'
        i_timeofventend = ispquery(name)
c       GADAMS PA-SCR-604 12-13-2005: End of change

***** TPA502C\NFENV.F

        call clearchar(60, name)
        name = 'BackfillParticleDiameter[m]'
        i_thdi = ispquery(name)

*****

***** TPA502F\nfenv.f
        call clearchar(60, name)
        name = 'BackfillParticleDiameter[m]'
        i_thdi = ispquery(name)

***** TPA502C\NFENV.F
        call clearchar(60, name)
        name = 'BackfillPorosity[]'
        i_thphi = ispquery(name)

*****

***** TPA502F\nfenv.f
        call clearchar(60, name)
        name = 'BackfillPorosity[]'
        i_thphi = ispquery(name)

***** TPA502C\NFENV.F
        call clearchar(60, name)
        name = 'ThermalConductivityOfAir[W/(m-C)]'
        i_thkair = ispquery(name)

*****

***** TPA502F\nfenv.f
        call clearchar(60, name)
        name = 'ThermalConductivityOfAir[W/(m-C)]'
        i_thkair = ispquery(name)

        call clearchar(60, name)
c BLW - SCR552 5/13/05 changed name
***** TPA502C\NFENV.F
        call clearchar(60, name)
c BLW - SCR552 5/13/05 changed name
*****
```

```
***** TPA502F\nfenv.f

c       GADAMS PA-SCR-604 12-13-2005: Modified to include
c       active and passive ventilation periods.
        call clearchar( 60, name )
c        name = 'FactorForVentilationHeatlosses[]'
        name = 'FactorForActiveVentilationHeatLosses[]'
c        ihloss_fact = ispquery( name )
        ihlossact_fact = ispquery( name )

        call clearchar( 60, name )
        name = 'FactorForPassiveVentilationHeatLosses[]'
        ihlosspas_fact = ispquery( name )
c       GADAMS PA-SCR-604 12-13-2005: End of change


***** TPA502C\NFENV.F

        call clearchar( 60, name )
        name = 'FactorForVentilationHeatlosses[]'
        ihloss_fact = ispquery( name )

*****

***** TPA502F\nfenv.f
      timeofclosure = valuesp(i_timeofclosure)

c     GADAMS PA-SCR-604 12-13-2005: Added time for active ventilation
c     to end
      timeofventend = valuesp(i_timeofventend)

c     Need to ensure that the time for end of ventilation is
c     less than or equal to the time of repository closure
      if(timeofventend .gt. timeofclosure) then
        print *, ' ***>>> Error in NFENV <<<*** '
        print *, ' Ventilation end time cannot exceed '
        print *, '   time of closure:'
        print *, 'Time for end of ventilation: ', timeofventend
        print *, 'Time of closure: ', timeofclosure
        STOP
      endif
c     GADAMS PA-SCR-604 12-13-2005: End of change

***** TPA502C\NFENV.F
      timeofclosure = valuesp(i_timeofclosure)

*****

***** TPA502F\nfenv.f
      aB = driftdia/2.0d0

c     GADAMS PA-SCR-604 12-13-2005: Modified to include active and
c     passive heat loss
c      hloss_fact = valuesp( ihloss_fact )
      hlossact_fact = valuesp( ihlossact_fact )
      hlosspas_fact = valuesp( ihlosspas_fact )
c     GADAMS PA-SCr-604 12-13-2005: End of change
      npoints = ivaluesp ( inpoints )
***** TPA502C\NFENV.F
      aB = driftdia/2.0d0
      hloss_fact = valuesp( ihloss_fact )
      npoints = ivaluesp ( inpoints )
*****
```

```
***** TPA502F\nfenv.f
c     &          npoints, tbump )

c         GADAMS PA-SCR-604 12-13-2005: Modified to include active
c         and passive ventilation
c          call cond3dxyzt(  aL, aB, aH,
c     &          rho, cp, cond, amld,
c     &          x, y, z, tend, timeofclosure, hloss_fact,
c     &          npoints, tbump )
          call cond3dxyzt(  aL, aB, aH,
***** TPA502C\NFENV.F
c     &          npoints, tbump )
          call cond3dxyzt(  aL, aB, aH,
*****

***** TPA502F\nfenv.f
     &          rho, cp, cond, amld,
     &          x, y, z, tend, timeofclosure, timeofventend,
     &          hlossact_fact, hlosspas_fact, npoints, tbump )
c         GADAMS PA-SCR-604 12-13-2005: End of change
c         GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\NFENV.F
     &          rho, cp, cond, amld,
     &          x, y, z, tend, timeofclosure, hloss_fact,
     &          npoints, tbump )
c         GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\nfenv.f
        D_WPPayload = wppayload

c       GADAMS PA-SCR-604 12-13-2005: Modified to include active
c       and passive ventilation
        D_HLossActiveFact = hlossact_fact
        D_HLossPassiveFact = hlosspas_fact
c       GADAMS PA-SCR-604 12-13-2005: End of change

        D_FracInv = frac_inv
***** TPA502C\NFENV.F
        D_WPPayload = wppayload
        D_HLossFact = hloss_fact
        D_FracInv = frac_inv
*****

***** TPA502F\nfenv.f
c     &          temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)

c            GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
c            period
c             call calcTempsLinear(tim(it), timeofclosure,
c     &          tempwp(it), tempdsiA(it), tempdsiB(it),
c     &          tempdsoA(it), tempdsoB(it),
c     &          tempbfoA(it), tempbfoB(it),
c     &          temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
              call calcTempsLinear(tim(it), timeofclosure,
     &         timeofventend,
     &         tempwp(it), tempdsiA(it), tempdsiB(it),
***** TPA502C\NFENV.F
c     &          temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
            call calcTempsLinear(tim(it), timeofclosure,
     &         tempwp(it), tempdsiA(it), tempdsiB(it),
*****

***** TPA502F\nfenv.f
```

```
     &          temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
c            GADAMS PA-SCR-604 12-13-2005: End of change

c            GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\NFENV.F
     &          temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
c            GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\nfenv.f
c     &          tempwp(it), qwp, qwp_dA, qwp_i)

c            GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
c            period
c             call calcTempsIterative(tim(it), timeofclosure,
c     &          temprep(it), tempbfoA(it),
c     &          tempdsoA(it), tempdsiA(it),
c     &          tempwp(it), qwp, qwp_dA, qwp_i)
             call calcTempsIterative(tim(it), timeofclosure,
     &          timeofventend,
     &          temprep(it), tempbfoA(it),
***** TPA502C\NFENV.F
c     &          tempwp(it), qwp, qwp_dA, qwp_i)
             call calcTempsIterative(tim(it), timeofclosure,
     &          temprep(it), tempbfoA(it),
*****

***** TPA502F\nfenv.f
     &          tempwp(it), qwp, qwp_dA, qwp_i)
c            GADAMS PA-SCR-604 12-13-2005: End of change
c            GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\NFENV.F
     &          tempwp(it), qwp, qwp_dA, qwp_i)
c            GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\nfenv.f

c ZW SCR478 05-25-04 Updated sub assignConcentrations to assignConcentrationsFl
***** TPA502C\NFENV.F



c ZW SCR478 05-25-04 Updated sub assignConcentrations to assignConcentrationsFl
*****

***** TPA502F\nfenv.f
c     &  qwp, qwpInvert, qwpRWA, qwpRWB)

c     GADAMS PA-SCR-604 12-13-2005: Added time for end of active
c     ventilation
c      subroutine calcTempsLinear(time, timeClosure,
c     &  tempWP, tempDSIA, tempDSIB, tempDSOA, tempDSOB, tempBFOA,
c     &  tempBFOB, tempRep,
c     &  qwp, qwpInvert, qwpRWA, qwpRWB)
      subroutine calcTempsLinear(time, timeClosure, timeActVentEnd,
     &  tempWP, tempDSIA, tempDSIB, tempDSOA, tempDSOB, tempBFOA,
***** TPA502C\NFENV.F
c     &  qwp, qwpInvert, qwpRWA, qwpRWB)
      subroutine calcTempsLinear(time, timeClosure,
     &  tempWP, tempDSIA, tempDSIB, tempDSOA, tempDSOB, tempBFOA,
*****
```

```
***** TPA502F\nfenv.f
     &  qwp, qwpInvert, qwpRWA, qwpRWB)
c     GADAMS PA-SCR-604 12-13-2005: End of change

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\NFENV.F
     &  qwp, qwpInvert, qwpRWA, qwpRWB)
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\nfenv.f

c     GADAMS PA-SCR-604 12-13-2005: Added time of active ventilation end
      double precision timeActVentEnd

      double precision tempWP
***** TPA502C\NFENV.F

      double precision tempWP
*****

***** TPA502F\nfenv.f
c         Calculate the heat flux during the ventilation period
c         GADAMS PA-SCR-604 12-13-2005: Added passive ventilation.
          if(time .lt. timeActVentEnd) then
c          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossActiveFact)
          else
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossPassiveFact)
          endif
c         GADAMS PA-SCR-604 12-13-2005: End of change

***** TPA502C\NFENV.F
c         Calculate the heat flux during the ventilation period
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)

*****

***** TPA502F\nfenv.f
          iCase_B = 1

c         GADAMS PA-SCR-604 12-13-2005: Added passive ventilation.
          if(time .lt. timeActVentEnd) then
c          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossActiveFact)
          else
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossPassiveFact)
          endif
c         GADAMS PA-SCR-604 12-13-2005: End of change

***** TPA502C\NFENV.F
          iCase_B = 1

c         Calculate the heat flux during the ventilation period
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)

*****

***** TPA502F\nfenv.f
c     &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)

c     GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
c      subroutine calcTempsIterative(time, timeClosure, tempRW, tempBF,
c     &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
```

```
      subroutine calcTempsIterative(time, timeClosure,
     &  timeActVentEnd, tempRW, tempBF,
     &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
c     GADAMS PA-SCR-604 12-13-2005: End of change

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\NFENV.F
c     &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
      subroutine calcTempsIterative(time, timeClosure, tempRW, tempBF,
     &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\nfenv.f

c     GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
      double precision timeActVentEnd
c     GADAMS PA-SCR-604 12-13-2005: End of change

      double precision tempRW
***** TPA502C\NFENV.F

      double precision tempRW
*****

***** TPA502F\nfenv.f

c       GADAMS PA-SCR-604 12-13-2005: Added passive ventilation.
        if(time .lt. timeActVentEnd) then
c        qwpTotal = qpermtu(time) * D_WPPayload * (1.0d0 - D_HLossFact)
         qwpTotal = qpermtu(time) * D_WPPayload *
     &      (1.d0-D_HLossActiveFact)
        else
         qwpTotal = qpermtu(time) * D_WPPayload *
     &      (1.d0-D_HLossPassiveFact)
        endif
c       GADAMS PA-SCR-604 12-13-2005: End of change

        B_Early = .true.
***** TPA502C\NFENV.F

        qwpTotal = qpermtu(time) * D_WPPayload * (1.0d0 - D_HLossFact)
        B_Early = .true.
*****

***** TPA502F\nfenv.f

      do i = 1, nb1
***** TPA502C\NFENV.F


      do i = 1, nb1
*****

***** TPA502F\nfenv.f

c          print *, 'nb2: ', nb2
***** TPA502C\NFENV.F


c          print *, 'nb2: ', nb2
*****3c3
*******************************************************************************
```

These differences provide evidence for the proper inclusion of a passive ventilation period, with its own

unique HLF. These changes include logical arguments which are self-consistent and functional.

The following text depicts the differences between the basecase and testcase files *condxyzt.f*.

```
*******************************************************************************
Comparing files TPA502F\condxyzt.f and TPA502C\CONDXYZT.F
***** TPA502F\condxyzt.f
c File Name:           condxyzt.f
c File Date:           01/20/06
c Release Version:     5.0
***** TPA502C\CONDXYZT.F
c File Name:           condxyzt.f
c File Date:           07/23/05
c Release Version:     5.0
*****

***** TPA502F\condxyzt.f
c     &  hloss_factin, npoints, tempbump )

c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation
c      subroutine cond3dxyzt(  aLin, aBin, aHin,
c     &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, closetimein,
c     &  hloss_factin, npoints, tempbump )
      subroutine cond3dxyzt(  aLin, aBin, aHin,
     &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, closetimein,
     &  endventin, hlossact_factin, hlosspas_factin, npoints, tempbump )
c     GADAMS PA-SCR-604 12-16-2005: End of change

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\CONDXYZT.F
c     &  hloss_factin, npoints, tempbump )
      subroutine cond3dxyzt(  aLin, aBin, aHin,
     &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, closetimein,
     &  hloss_factin, npoints, tempbump )
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\condxyzt.f
c                  in units of [yr]
c           closetimein = double precision, time of closure
c           endventin = double precision, end of active ventilation time
c           hlossact_factin = double precision, factor for active
c                 ventilation heat loss
c           hlosspas_factin = double presision, factor for passive
c                 ventilation heat loss
c
c           npoints =
***** TPA502C\CONDXYZT.F
c                  in units of [yr]
c           closetimein = double precision, ventilation end time.
c           hloss_factin =
c           npoints =
*****

***** TPA502F\condxyzt.f
      double precision closetime
c     GADAMS PA-SCR-553 2-4-2005: End of change

c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation time
      double precision endvent
      double precision hlossact_fact
      double precision hlosspas_fact
c     GADAMS PA-SCR-604 12-16-2005: End of change
```

```
***** TPA502C\CONDXYZT.F
      double precision closetime
c     GADAMS PA-SCR-553 2-4-2005: End of change

*****

***** TPA502F\condxyzt.f
      double precision cp

c     GADAMS PA-SCR-604 12-16-2005: Renamed when passive ventilation
c     period was added
c      double precision hloss_fact

      double precision rho
***** TPA502C\CONDXYZT.F
      double precision cp
      double precision hloss_fact
      double precision rho
*****

***** TPA502F\condxyzt.f
      double precision tempbump2

c     GADAMS PA-SCR-604 12-16-2005: Added tempbum3 because three
c     periods may be available for analysis when passive ventilation
c     is included
      double precision tempbump3
c     GADAMS PA-SCR-604 12-16-2005: End of change

      double precision tend
***** TPA502C\CONDXYZT.F
      double precision tempbump2
      double precision tend
*****

***** TPA502F\condxyzt.f
c     & hloss_fact
c
c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation
c     period
c      common / tempgl1 / aL, aB, aH, x, y, z,
c     & aml, rho, cp, cond, tend, alpha, closetime,
c     & hloss_fact
      common / tempgl1 / aL, aB, aH, x, y, z,
***** TPA502C\CONDXYZT.F
c     & hloss_fact
      common / tempgl1 / aL, aB, aH, x, y, z,
*****

***** TPA502F\condxyzt.f
     & aml, rho, cp, cond, tend, alpha, closetime,
     & endvent, hlossact_fact, hlosspas_fact
c     GADAMS PA-SCR-604 12-16-2005: End of change
c     GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\CONDXYZT.F
     & aml, rho, cp, cond, tend, alpha, closetime,
     & hloss_fact
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\condxyzt.f
      z = zin

      tend = timin
```

```
***** TPA502C\CONDXYZT.F
      z = zin
      tend = timin
*****

***** TPA502F\condxyzt.f

c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
c      hloss_fact = hloss_factin
      endvent = endventin
      hlossact_fact = hlossact_factin
      hlosspas_fact = hlosspas_factin
c     GADAMS PA-SCR-604 12-16-2005: End of change

***** TPA502C\CONDXYZT.F

      hloss_fact = hloss_factin

*****

***** TPA502F\condxyzt.f
c      if (tend.le.bftime) then

c     GADAMS PA-SCR-604 12-16-2005: Modified condition from .le. to .lt.
c     for consistency with other conditional checks for active and
c     passive ventilation
c      if (tend.le.closetime) then
      if (tend .lt. closetime) then

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\CONDXYZT.F
c      if (tend.le.bftime) then
      if (tend.le.closetime) then
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\condxyzt.f

c        GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
         if(tend .lt. endvent) then
c          call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
           call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
           tempbump = tempbump1
         else
           call xgauleg(tempgl, 0.0d0, endvent, npoints, tempbump1)
           call xgauleg(tempgl, endvent, tend, npoints, tempbump2)
           tempbump = tempbump1 + tempbump2
         endif
c        GADAMS PA-SCR-604 12-16-2005: End of change

      else
***** TPA502C\CONDXYZT.F

         call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
         tempbump = tempbump1
      else
*****

***** TPA502F\condxyzt.f
c        call xgauleg(tempgl, 0.0d0, bftime, npoints, tempbump1)

c       GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
c        call xgauleg(tempgl, 0.0d0, closetime, npoints, tempbump1)
c        call xgauleg(tempgl, bftime, tend, npoints, tempbump2)
```

```
c        call xgauleg(tempgl, closetime, tend, npoints, tempbump2)
        call xgauleg(tempgl, 0.0d0, endvent, npoints, tempbump1)
        call xgauleg(tempgl, endvent, closetime, npoints, tempbump2)
        call xgauleg(tempgl, closetime, tend, npoints, tempbump3)
c       GADAMS PA-SCR-604 12-16-2005: End of change

c       GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\CONDXYZT.F
c        call xgauleg(tempgl, 0.0d0, bftime, npoints, tempbump1)
        call xgauleg(tempgl, 0.0d0, closetime, npoints, tempbump1)
c        call xgauleg(tempgl, bftime, tend, npoints, tempbump2)
        call xgauleg(tempgl, closetime, tend, npoints, tempbump2)
c       GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\condxyzt.f

c       GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
c        tempbump = tempbump1 + tempbump2
        tempbump = tempbump1 + tempbump2 + tempbump3
c       GADAMS PA-SCR-604 12-16-2005: End of change

      endif
***** TPA502C\CONDXYZT.F

        tempbump = tempbump1 + tempbump2
      endif
*****

***** TPA502F\condxyzt.f
      double precision closetime
c     GADAMS PA-SCR-553 2-4-2005: End of change

c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation time
      double precision endvent
      double precision hlossact_fact
      double precision hlosspas_fact
c     GADAMS PA-SCR-604 12-16-2005: End of change

***** TPA502C\CONDXYZT.F
      double precision closetime
c     GADAMS PA-SCR-553 2-4-2005: End of change

*****

***** TPA502F\condxyzt.f
      double precision cp

c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
c      double precision hloss_fact

      double precision qpp
***** TPA502C\CONDXYZT.F
      double precision cp
      double precision hloss_fact
      double precision qpp
*****

***** TPA502F\condxyzt.f
c     & hloss_fact

c     GADAMS PA-SCR-604 12-16-2005: Added passive ventilation
c     period
c      common / tempgl1 / aL, aB, aH, x, y, z,
```

```
c      & aml, rho, cp, cond, tend, alpha, closetime,
c      & hloss_fact
       common / tempgl1 / aL, aB, aH, x, y, z,
      & aml, rho, cp, cond, tend, alpha, closetime,
      & endvent, hlossact_fact, hlosspas_fact
c      GADAMS PA-SCR-604 12-16-2005: End of change

c      GADAMS PA-SCR-553 2-4-2005: End of change
***** TPA502C\CONDXYZT.F
c      & hloss_fact
       common / tempgl1 / aL, aB, aH, x, y, z,
      & aml, rho, cp, cond, tend, alpha, closetime,
      & hloss_fact
c      GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** TPA502F\condxyzt.f

c        GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
c          qpp = qpermtu( t ) * (1.d0 - hloss_fact) * aml / 4047.0d0
         if (t .lt. endvent) then
           qpp = qpermtu( t ) * (1.d0 - hlossact_fact) * aml / 4047.0d0
         else
           qpp = qpermtu( t ) * (1.d0 - hlosspas_fact) * aml / 4047.0d0
         endif
c        GADAMS PA-SCR-604 12-16-2005: End of change

       else
***** TPA502C\CONDXYZT.F

          qpp = qpermtu( t ) * (1.d0 - hloss_fact) * aml / 4047.0d0
       else
*****
```

****

These differences provide further evidence for the proper implementation of a passive ventilation period and associated HLF. The logical argument changes are functional and self-consistent.

The following text depicts the differences between the basecase and testcase files *cond3dxyzt.h.*

****

```
Comparing files TPA502F\cond3dxyzt.h and TPA502C\COND3DXYZT.H
***** TPA502F\cond3dxyzt.h

c       GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
        double precision endventin

***** TPA502C\COND3DXYZT.H

        double precision hloss_factin
        double precision npoints
        double precision tempbump


*****

***** TPA502F\cond3dxyzt.h
c       GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
c        double precision hloss_factin
        double precision hlossact_factin
        double precision hlosspas_factin
c       GADAMS PA-SCR-604 12-16-2005: End of change
```

```
      double precision npoints
      double precision tempbump


***** TPA502C\COND3DXYZT.H
*****

22c22,30
<        double precision hloss_factin
---
> c      GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
>        double precision endventin
>
> c      GADAMS PA-SCR-604 12-16-2005: Added passive ventilation period
> c       double precision hloss_factin
>        double precision hlossact_factin
>        double precision hlosspas_factin
> c      GADAMS PA-SCR-604 12-16-2005: End of change
>
*******************************************************************************
```

The differences between these *cond3dxyzt.h* files supports the inclusion of the new parameters and the renaming of parameters used by the testcase to implement a passive ventilation period.

The following text depicts the differences between the basecase and testcase files *driftcmn.i*.

```
*******************************************************************************
Comparing files TPA502F\driftcmn.i and TPA502C\DRIFTCMN.I
***** TPA502F\driftcmn.i
      double precision D_WPPayload

c     GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
c      double precision D_HLossFact
      double precision D_HLossActiveFact
      double precision D_HLossPassiveFact
c     GADAMS PA-SCR-604 12-13-2005: End of change

      double precision D_FracInv
***** TPA502C\DRIFTCMN.I
      double precision D_WPPayload
      double precision D_HLossFact
      double precision D_FracInv
*****

***** TPA502F\driftcmn.i
      double precision D_EmissBF

c     GADAMS PA-SCR-604 12-13-2005: Added passive ventilation
c      common /nfenv_thermal1/ D_SBolt, D_ViewFactor, D_WPPayload,
c     &  D_HLossFact, D_FracInv, D_FracWedge,
c     &  D_WPSpace, D_WPDia, D_DSDiaI, D_DSThick, D_DriftDiaFloor,
c     &  D_CondFloor, D_CondRW, D_CondConv, D_CondBF, D_EmissWP,
c     &  D_EmissRW, D_EmissDS, D_EmissBF

      common /nfenv_thermal1/ D_SBolt, D_ViewFactor, D_WPPayload,
     &  D_HLossActiveFact, D_HLossPassiveFact, D_FracInv, D_FracWedge,
     &  D_WPSpace, D_WPDia, D_DSDiaI, D_DSThick, D_DriftDiaFloor,
***** TPA502C\DRIFTCMN.I
      double precision D_EmissBF
      common /nfenv_thermal1/ D_SBolt, D_ViewFactor, D_WPPayload,
     &  D_HLossFact, D_FracInv, D_FracWedge,
     &  D_WPSpace, D_WPDia, D_DSDiaI, D_DSThick, D_DriftDiaFloor,
*****
```

```
***** TPA502F\driftcmn.i
     &  D_CondFloor, D_CondRW, D_CondConv, D_CondBF, D_EmissWP,
     &  D_EmissRW, D_EmissDS, D_EmissBF
c     GADAMS PA-SCR-604 12-13-2005: End of change

***** TPA502C\DRIFTCMN.I
     &  D_CondFloor, D_CondRW, D_CondConv, D_CondBF, D_EmissWP,
     &  D_EmissRW, D_EmissDS, D_EmissBF

*****
```

****

The differences between these *driftcmn.i* files supports the inclusion of the new parameters and the renaming of common parameters used by the testcase to implement a passive ventilation period.

- overall test status: PASS

SL-2. Name: Examine Thermal Profile of Repository Wall

Path for run directory:

Basecase: [tpa]D:\Mancillas\SCR604\tpa502c\run1, run2
Testcase: [tpa]D:\Mancillas\SCR604\tpa502f\ run1, run2

Path for archive of results:

Basecase: Windows\SCR604\tpa502c\run1, run2
Testcase: Windows\SCR604\tpa502f\run1, run2
(Archived to CD [titled : TPA SCR604 Testing])

Environment variables:

Basecase: TPA_TEST=D:\Mancillas\SCR604\tpa502c
TPA_DATA=D:\Mancillas\SCR604\tpa502c

Testcase: TPA_TEST=D:\Mancillas\SCR604\tpa502f
TPA_DATA=D:\ancillas\SCR604\tpa502f

Special input files or modifications to input files required : *tpa.inp*

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Append All

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: MS Excel (2002 SP3)

Test description: SCR604 has increased the functionality of the TPA code by introducing a passive ventilation period. Through this change the TPA simulation has the ability to evaluate two unique periods prior to pre-closure: A period of active ventilation, and a period of passive ventilation. Each of these ventilation periods has its own heat removal capacity. This test will examine the behavior of the TPA code with two ventilation periods, and evaluate for proper behavior. Included in this test is an examination of the effect of the number of Gauss-Legendre weights.

- **objective** Verify the proper implementation of SCR604, with respect to the generation of wall temperature profiles, which agree between the basecase and testcase.

- **assumptions** None other than those made within the TPA code

- **constraints** None

- **output files to compare or examine** *nfenv.rlt*

- step by step test procedure to be used

1) compare repository wall temperature profiles for subarea 1 with the following values in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.83
# of Gauss-Legendre weights	20	20
End of active ventilation	50	50

2) compare repository wall temperature profiles for subarea 1 with the following conditions:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.83
# of Gauss-Legendre weights	100	100
End of active ventilation	50	50

- pass fail criteria A comparison of temperature profiles for the repository walls should show similar trends with temperatures differing by less than 2 degrees.

Test Results:

- criterion 1 The TPA code was run for both the basecase and testcase. The temperature profiles of the repository walls for subarea one were plotted from the data collected in the append file *nfenv.rlt*.

Figure 1 shows the repository temperature profile for subarea 1 using 20 Gauss-Legendre (GL) weights. The maximum temperature difference is 1.49 degrees Celsius occurring 58 years into the simulation. Near this time there is a minor difference in the behaviors of the basecase and testcase temperature profiles. It is suspected that this is a result of the numeric integration method and not a result of an improper implementation of the passive ventilation period. A second simulation with the number of GL weighs increased to 100 is shown in figure 2. While using 100 GL weights, the temperature profiles between the basecase and testcase show nearly identical behaviors and have a maximum temperature which gradually builds to a difference of 1.00 degree Celsius at 181 years.

The plots of these behaviors shown in figures 1 and 2 are provided as evidence that the passive ventilation period has been properly implemented. And that the minor differences are a result of the numerical integration method.

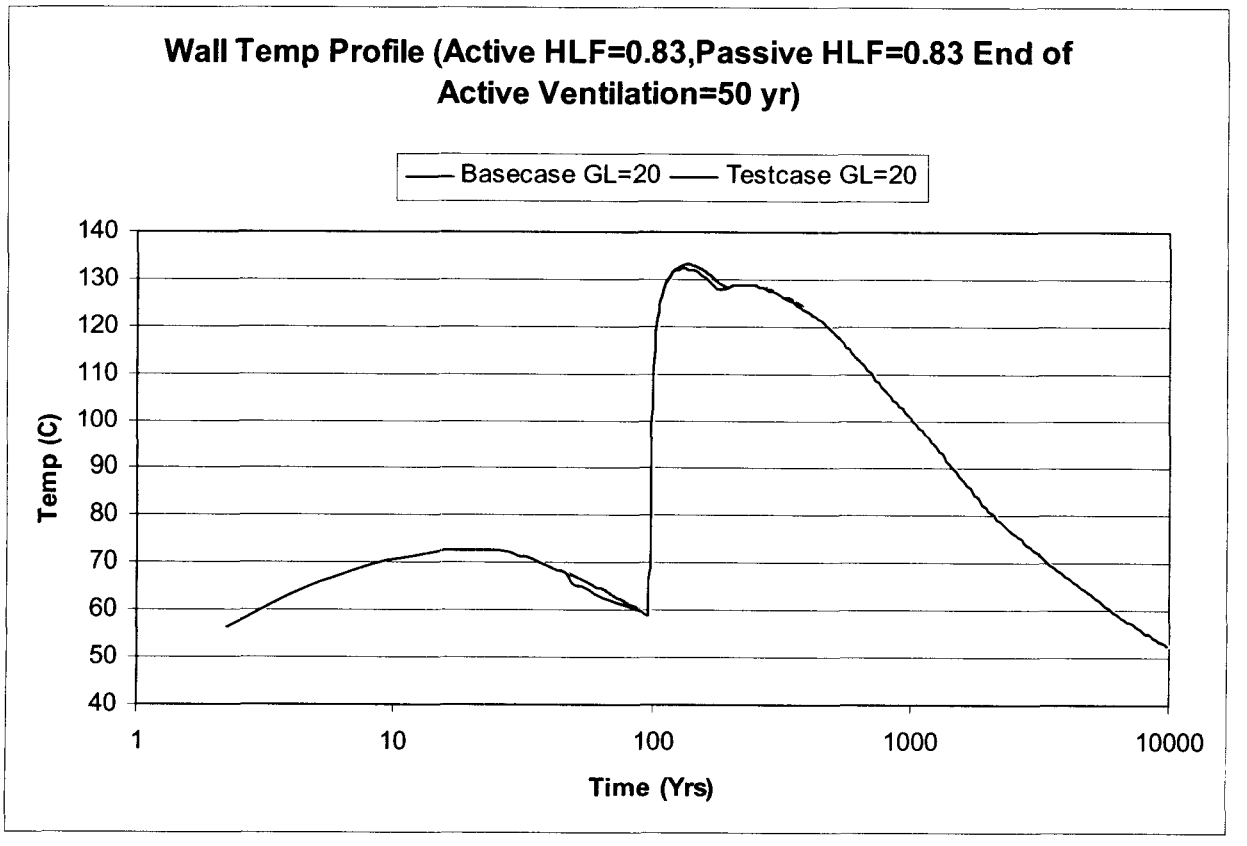


Figure 1 Repository Temperature profile for subarea 1

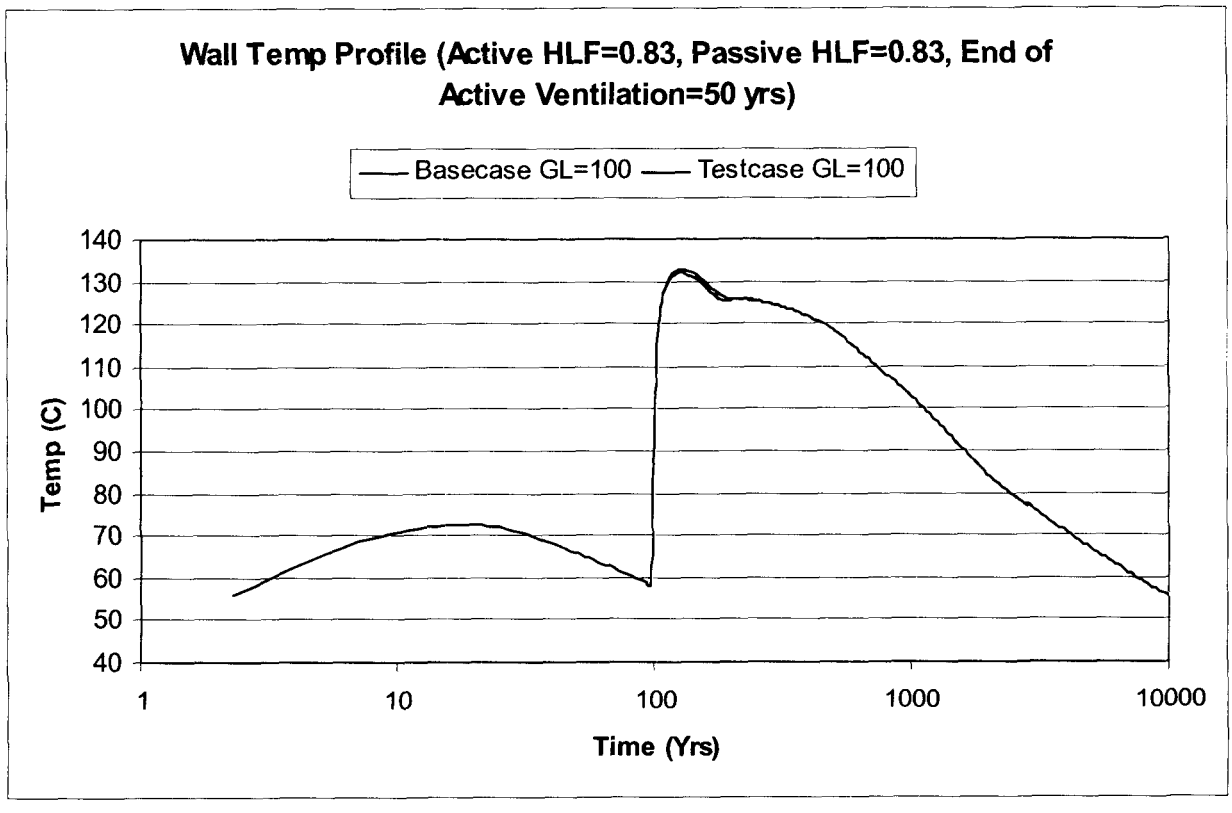


Figure 2 Repository temperature profile for subarea 1, using 100 GL weights.

- overall test status : PASS

Notes:

The issue of integration approximation using 20 weights versus 100 weights should probably be addressed, because of the increased computational time required when using 100 weights.
The MS Excel worksheet used to generate this plot, named *nfenve_win*, is included on the archive of this SCR.

SL-3. Name: Examine Thermal Profile of Repository Wall with Differing Passive and Active Heat Losses

Path for run directory:

Basecase: [tpa]D:\Mancillas\SCR604\tpa502c\run1
Testcase: [tpa]D:\Mancillas\SCR604\tpa502f\ run3

Path for archive of results:

Basecase: Windows\SCR604\tpa502c\run1
Testcase: Windows\SCR604\tpa502f\run3
(Archived to CD [titled : TPA SCR604 Testing])

Environment variables:

Basecase: TPA_TEST=D:\Mancillas\SCR604\tpa502c
TPA_DATA=D:\Mancillas\SCR604\tpa502c

Testcase: TPA_TEST=D:\Mancillas\SCR604\tpa502f
TPA_DATA=D:\ancillas\SCR604\tpa502f

Special input files or modifications to input files required : *tpa.inp*

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Append All

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: MS Excel (2002 SP3)

Test description: SCR604 has increased the functionality of the TPA code by introducing a passive ventilation period. Through this change the TPA simulation has the ability to evaluate two unique periods prior to pre-closure: A period of active ventilation, and a period of passive ventilation. Each of these ventilation periods has its own heat removal capacity. This test will examine the behavior of the TPA code with differing heat loss factors for the passive ventilation period

- **objective** Verify the proper implementation of SCR604, with respect to differing heat loss factors (HLF).

- **assumptions** None other than those made within the TPA code

- **constraints** None

- **output files to compare or examine** *nfenv.rlt*

- **step by step test procedure to be used**

  1) compare repository wall temperature profiles for subarea 1 with the following values in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.50
# of Gauss-Legendre weights	20	20
End of active ventilation	50	50

- **pass fail criteria** The temperature profile of the testcase should show a sharp rise in temperature, relative to the basecase, at the end of active ventilation.

Test Results: The temperature profile of the testcase should show a sharp increase in wall temperature because of the reduction in the passive ventilation heat loss factor.

- **criterion 1** Figure 3. Shows the differences between the basecase and testcase temperature profiles. The temperature profiles of the repository walls for subarea one were plotted from the data collected in the append file *nfenv.rlt*. These results exhibit the behavior expected with a decreased passive heat loss factor and is used as evidence that SCR604 has been properly implemented.

The sharp increase in temperature at time equals 50yr, shown in figure 3, is used as evidence of the proper implementation of SCR604.

- **overall test status** : **PASS**

Note
The MS Excel worksheet used to generate these comparison plots, named *nfenve_win*, is included on the archive of this SCR.

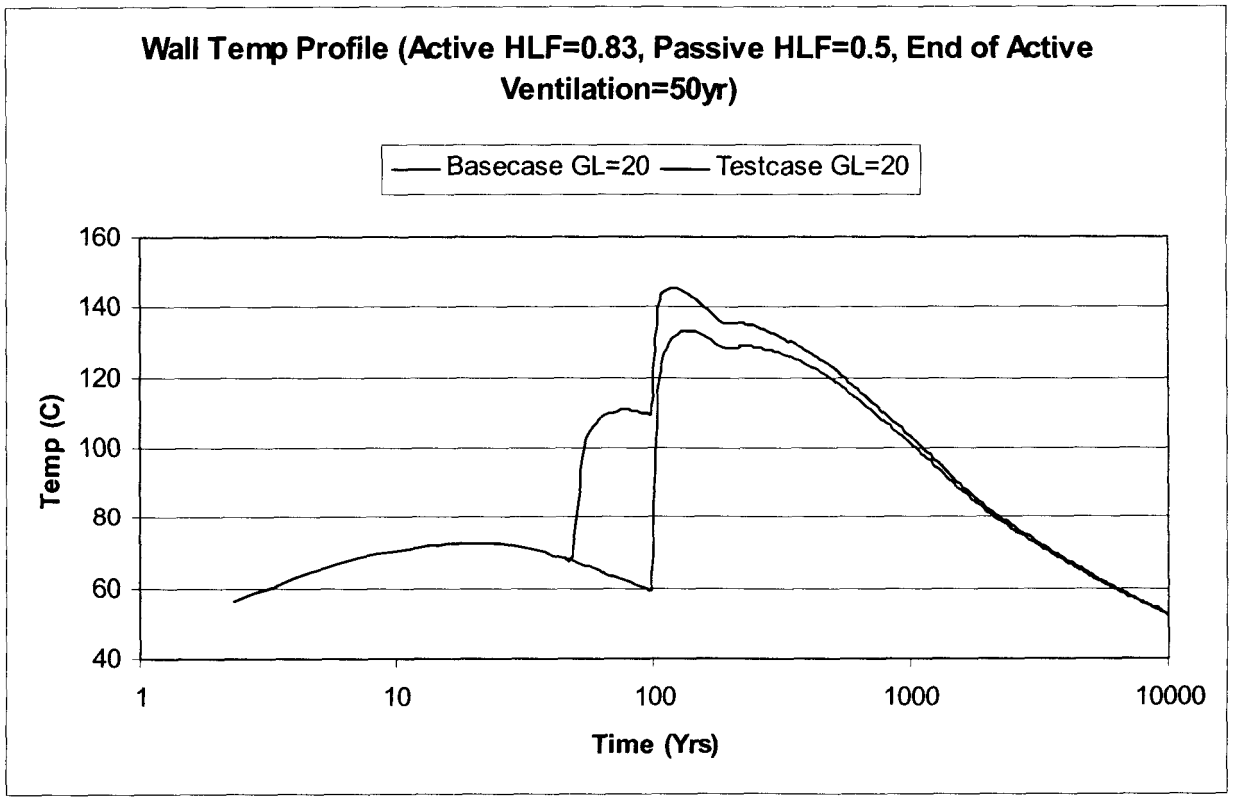


Figure 3 Repository wall temperature for subarea 1.

SL-4. Name: Examine Thermal Profile of Repository Wall with Differing Passive and Active Heat Losses and Differing End Times for Active Ventilation

Path for run directory:

Basecase: [tpa]D:\Mancillas\SCR604\tpa502c\run1
Testcase: [tpa]D:\Mancillas\SCR604\tpa502f\ run4, run5

Path for archive of results:

Basecase: Windows\SCR604\tpa502c\run1
Testcase: Windows\SCR604\tpa502f\run4, run5
(Archived to CD [titled : TPA SCR604Testing])

Environment variables:

Basecase: TPA_TEST=D:\Mancillas\SCR604\tpa502c
TPA_DATA=D:\Mancillas\SCR604\tpa502c

Testcase: TPA_TEST=D:\Mancillas\SCR604\tpa502f
TPA_DATA=D:\ancillas\SCR604\tpa502f

Special input files or modifications to input files required : *tpa.inp*

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Append All

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: MS Excel (2002 SP3)

Test description: SCR604 has increased the functionality of the TPA code by introducing a passive ventilation period. Through this change the TPA simulation has the ability to evaluate two unique periods prior to pre-closure: A period of active ventilation, and a period of passive ventilation. Each of these ventilation periods has its own heat removal capacity. This test will examine the behavior of the TPA code with differing heat loss factors for the passive ventilation period and with differing start periods for the passive ventilation.

- **objective** Verify the proper implementation of SCR60, with respect to adjustable time for ventilation periods.

- **assumptions** None other than those made within the TPA code

- **constraints** None

- **output files to compare or examine** *nfenv.rlt*

- **step by step test procedure to be used**

1) compare repository wall temperature profiles for subarea 1 with the following values

in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.50
# of Gauss-Legendre weights	20	20
End of active ventilation	50	25

2) compare repository wall temperature profiles for subarea 1 with the following values in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.50
# of Gauss-Legendre weights	20	20
End of active ventilation	50	0

3) compare repository wall temperature profiles for subarea 1 with the following values in the *tpa.inp* file:

	Basecase	Testcase
Active Heat loss Factor	0.83	0.83
Passive Heat Loss Factor	0.83	0.50
# of Gauss-Legendre weights	20	20
End of active ventilation	50	100

- **pass fail criteria** The temperature profile of the testcase should show a sharp rise in temperature, relative to the basecase, at the end of active ventilation.

Test Results: The temperature profile of the testcase should show a sharp increase in wall temperatures at the end of active ventilation. The following two plots (figures 4 and 5) have differing time for the end of active ventilation 25 years and 0 years.

- **criterion 1** There should be a sharp increase in wall temperature a 25 years when active ventilation ends at 25 years. This behavior is shown in figure 4 and is used as evidence that SCR604 is properly implemented.

- **criterion 2** In this instance the end of active ventilation is set to time equal to zero. This should result in large initial temperature prior to closure. This behavior is shown in figure 5 and is used

as evidence that SCR604 is properly implemented.

- **criterion 3** In this comparison the testcase end of active ventilation was set to time equals 100 years, which is the same as the closure time. This should result in a temperature profile which is the same as basecase profile. This behavior is shown to occur in figure 6 and is used as further evidence that SCR604 has been properly implemented.

- **overall test status: PASS**

Note:
The MS Excel worksheet used to generate this plot, named *nfenve_win*, is included on the archive of this SCR. Slight integration errors are visible at the transition from differing ventilation periods, but these are within acceptable limits.

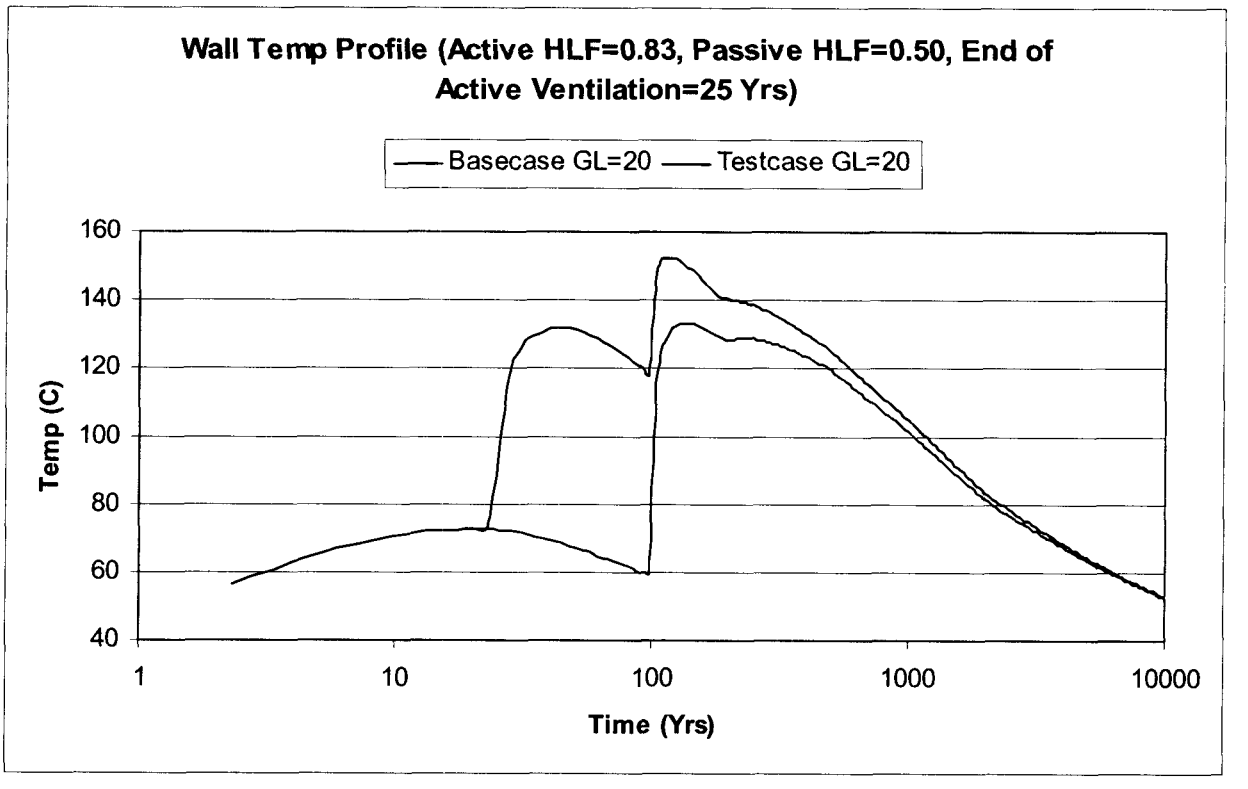


Figure 4 Repository wall temperature for subarea 1: end of active ventilation 25 years.

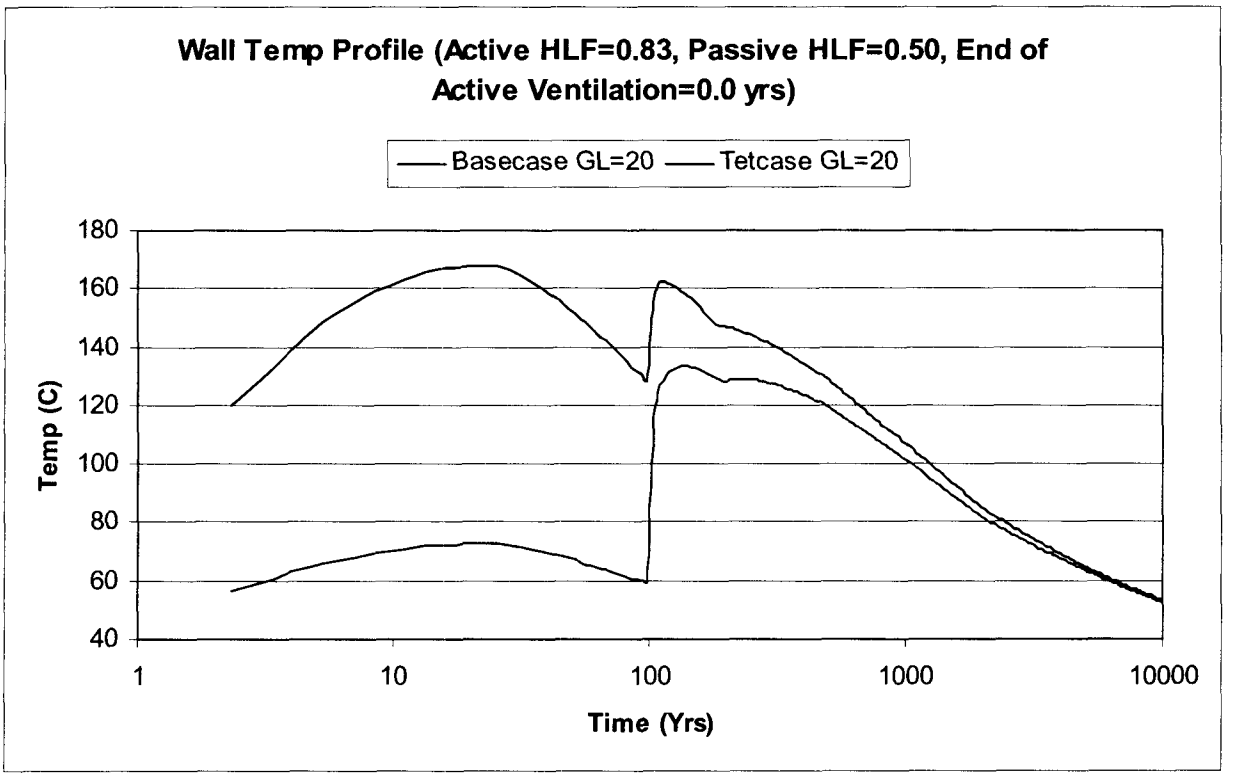


Figure 5 Repository wall temperature for subarea 1: end of active ventilation 0 years.

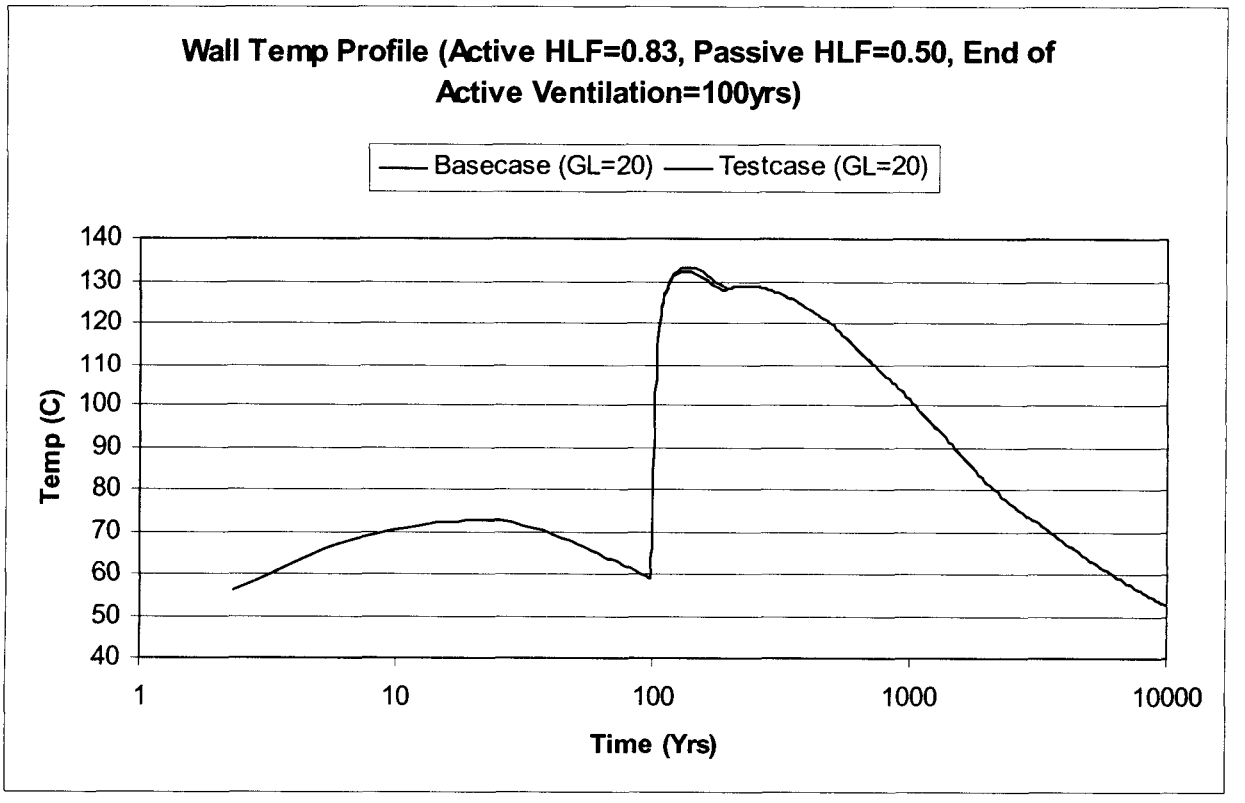


Figure 6 Repository wall temperature for subarea 1: end of active ventilation 100 years.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 605	**2. Software Title and Version:** TPA 5.0.2f	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *nfenv.f, exec.f, seismo2.f, drythick.dat, ebsrel.f*

1) The dryout zone thickness as a function of time is defined in the file *drythick.dat*. Currently, there is no distinction between the open drift and degraded drift scenarios. Additional data will be added to the file *drythick.dat* to account for two different scenarios. The appropriate data will be read depending on the time for full degradation of the drift.

2) The *ebsrel.inp* file is overwritten when both the spent fuel and glass waste forms are analyzed.

5. Change Requested by: O. Pensado Date: 11/3/2005	**6. Change Authorized by** (*Software Developer*): Ron Janetzke Date: 11-4-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

1) Updated *drythick.dat* to contain dryout zone thicknesses for both the degraded and non-degraded cases. Also included the time for the end of the thermal pulse in *drythick.dat*. For a degradation time less than the time for the end of the thermal pulse, the degraded drift dryout values are used; otherwise, the non-degraded drift dryout values are used.

2) Updated *ebsrel.f* to copy *ebsrel.inp* to *ebsrelsf.inp* before running the glass waste form.

3) The time of degradation that is used to compare with the time for the end of the thermal pulse in *drythick.dat* is the time of first full drift degradation (either rock type 1 drifts or rock type 2 drifts).

8. Implemented by: G. Adams	**Date:** 2-10-2006

9. Description of Acceptance Tests:

Test description has been included on Attachments A and B

10. Tested by: J Mancillas	**Date:** 4-4-2006

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 605

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
No changes							

ATTACHMENT A

Test Plan for TPA SCR605 (UNIX)

Test Plan Name: TestPlan SCR605

Tested By: James Mancillas

Date: 4-4-2006

Host Machine: Spock

Host OS: SunOS 5.9 (unix)

Baseline Version: TPA5.0.2f

Test Version: TPA 5.0.2g

Process Level (PL) Tests

PL-1.Name: Evaluate source code changes, and basic execution of code

Path for run directory:
Basecase: [Spock]:/home/jmancillas/TPA/SCR605/tpa502f
Testcase: [Spock]:/home/jmancillas/TPA/SCR605/tpa502g

Path for archive of results:
Basecase and Testcase : SCR605/diff_files

Archived to CD titled :SCR605 Testing

Environment variables:
Basecase: TPA_DATA=[spock]:/home/jmancillas/TPA/SCR605/tpa502f
TPA_TEST =[spock]:/home/jmancillas/TPA/SCR605/tpa502f

Testcase : TPA_DATA=[spock]:/home/jmancillas/TPA/SCR605/tpa502g
TPA_TEST =[spock]:/home/jmancillas/TPA/SCR605/tpa502g

Special input files or modifications to input files required : None

Special diagnostic code modifications required : itpa flag turn on in nfenv.f file

Program modes to be used (append flags, scenario/model switches, etc.): Default

Utility scripts needed to perform the test: none

Utility codes needed in the analysis of the test data: none

Test description: examine differences between the source code in the basecase and testcase TPA versions. Execute basecase and testcase version of the TPA code and evaluate for basic execution with basecase tpa.inp input.

- objective

Identify changes in the TPA code, ensure that the changes are consistent with the requested changes specified in SCR605. Ensure that the testcase TPA code executes with typical input parameters.

- assumptions

None other than those made within the TPA code.

- constraints

None

- output files to compare or examine

Differences in the files *exec.f, nfenv.f, seismo2.f ,ebsrel.f* and the input data file *drythick.dat*

- step by step test procedure to be used

1) perform a difference examination using the unix diff command and record the differences to **_diff* files.
2) execute the basecase and testcase and capture the screen outputs and examine the differences for any outstanding or unexpected differences.

- pass fail criteria

1) The differences between the testcase and basecase TPA source codes should be identified within the code by an SCR number. Those changes should be logical and consistent with the requested SCR605 changes.
2) The differences between the basecase and testcase screen captures should have release rate which are consistent with the impact of the SCR changes.

Test Results:

1) the following text depicts the differences between the basecase and testcase files :

differences in the files *exec.f*:
/SCR605/diff_files/*exec_diff*

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
3,4c3,4
< c File Date:          01/20/06
< c Release Version:    5.0.2f
---
> c File Date:          02/08/06
> c Release Version:    5.0.2g
277a278
> c            5.0.2g includes SCR 605 accomodate degraded drift info in
drythick.dat.
327c328
< c Executive for TPA Version 5.0.2f
---
> c Executive for TPA Version 5.0.2g
```

```
456c457,464
< c     GADAMS PA-SCr-480 7-14-2004: End of change
---
> c     GADAMS PA-SCr-480 7-14-2004: End of change
>
> c     GADAMS SCR605 2-2-2006: Added drift failure parameters
>       integer drift_flag_one
>       double precision drift_time_one
>       integer drift_flag_two
>       double precision drift_time_two
> c     GADAMS SCR605 2-2-2006: End of change
752c760
<       print '(10x,a)','exec: Welcome to TPA Version 5.0.2f'
---
>       print '(10x,a)','exec: Welcome to TPA Version 5.0.2g'
3112a3121,3127
> c       GADAMS SCR605 2-2-2006: Added drift failure parameters
> c        call eqvdia( ntim, tim(1),
> c     &    numberofseismicevents, timeofseismicevents(1),
> c     &    typeofseismicevents(1), nsa, isa,
> c     &    equivdriftdiaAsubarea(1, isa), equivdriftdiaBsubarea(1, isa),
> c     &    equivbfdiaAsubarea(1, isa), equivbfdiaBsubarea(1, isa),
> c     &    driftheightsubarea(1, isa))
3118c3133,3135
<      &    driftheightsubarea(1, isa))
---
>      &    driftheightsubarea(1, isa), drift_flag_one, drift_time_one,
>      &    drift_flag_two, drift_time_two)
> c       GADAMS SCR605 2-2-2006: End of change
3166a3184,3196
>
> c           GADAMS SCR605 2-2-2006: Added drift failure parameters
>             WRITE(iunitresultseqvdia, FMT = '(/, A, I2,/,
>      &            A, 1pe12.5,/A, I2,/A, 1pe12.5)')
>      &        'Rock Type One Drift Failure (yes=1, no=0): ',
>      &         drift_flag_one,
>      &        'Rock Type One Failure Time:                ',
  >      &         drift_flag_one,
>      &        'Rock Type One Failure Time:                ',
>      &         drift_time_one,
>      &        'Rock Type Two Drift Failure (yes=1, no=0): ',
>      &         drift_flag_two,
>      &        'Rock Type Two Failure Time:                ',
>      &         drift_time_two
> c           GADAMS SCR605 2-2-2006: End of change
3263a3294,3302
>
> c         GADAMS SCR605 2-3-2006: Added drift degradation parameters
> c          call nfenvFl( isa, ntim, tim(1), qm3peryrperwpinsa(1),
> c     &     temprep(1), tempbfoA(1), tempbfoB(1), tempdsoA(1),
> c     &     tempdsoB(1), tempdsiA(1), tempdsiB(1), tempwp(1),
> c     &     relhumwp(1), flds(1), qm3peryrperwpinsamisswp(1),
> c     &     qm3peryrperwpinsahitwp(1), equivdriftdiaAsubarea(1, isa),
> c     &     equivdriftdiaBsubarea(1, isa), equivbfdiaAsubarea(1, isa),
> c     &     equivbfdiaBsubarea(1, isa))
3270c3309,3311
<      &     equivbfdiaBsubarea(1, isa))
---
>      &     equivbfdiaBsubarea(1, isa), drift_flag_one,
>      &     drift_time_one, drift_flag_two, drift_time_two)
> c         GADAMS SCR605 2-3-2006: End of change
6957c6998
<  341     format( ' TPA 5.0.2f, Job started: ', a24 )
```

```
---
>  341      format( ' TPA 5.0.2g, Job started: ', a24 )
7046c7087
<  341      format( ' TPA 5.0.2f, Job started: ', a24 )
---
>  341      format( ' TPA 5.0.2g, Job started: ', a24 )
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

These changes are presented as evidence that the *exec.f* file has been modified to allow the TPA code to respond to drift failure conditions as described in SCR605 in issues 1 and 3.

The following text depicts the differences in *nfenv.f* in the basecase and testcase TPA codes SCR605/diff_files/*nfenv_diff*

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
< c File Date:           01/20/06
---
> c File Date:           02/08/06
142a143,149
> c     GADAMS SCR605 2-2-2006: Added drift degradation parameters
> c      subroutine nfenvFl( isa, ntim, tim, qm3peryrperwpinsa, temprep,
> c     &                    tempbfoA, tempbfoB, tempdsoA, tempdsoB,
> c     &                    tempdsiA, tempdsiB, tempwp, relhumwp, flds,
> c     &                    qm3peryrperwpinsamisswp,
> c     &                    qm3peryrperwpinsahitwp, eqDriftDiaA,
> c     &                    eqDriftDiaB, eqBFDiaA, eqBFDiaB  )
148c155,158
<      &                   eqDriftDiaB, eqBFDiaA, eqBFDiaB  )
---
>      &                   eqDriftDiaB, eqBFDiaA, eqBFDiaB,
>      &                   flagDegrade1, timeDegrade1, flagDegrade2,
>      &                   timeDegrade2)
> c     GADAMS SCR605 2-2-2006: End of change
250a261,267
>
> c     GADAMS SCR605 2-2-2006: Added drift degradation parameters
>       integer flagDegrade1
>       double precision timeDegrade1
>       integer flagDegrade2
>       double precision timeDegrade2
> c     GADAMS SCR605 2-2-2006: End of change
1894,1895c1911,1915
<         call reflux3 (itpa, isa, ntim, tim(1),
<      &                wpcellwidth, wpspacedrift,
---
>
> c       GADAMS SCR605 2-2-2006: Added drift degradation
> c       parameters
> c        call reflux3 (itpa, isa, ntim, tim(1),
> c     &                wpcellwidth, wpspacedrift,
1897a1918,1924
> c     &                rf3porosity, rf3sat_init, rf3sat_resid,
> c     &                fracndrm, fracndto, fracndtorm,
> c     &                densboil, enthalphase, tempgradboil, cond,
> c     &                qm3peryrperwpinsa(1),
> c     &                qm3peryrperwpinsahitwp(1) )
>         call reflux3 (itpa, isa, ntim, tim(1),
>      &                wpcellwidth, wpspacedrift,
1902c1929,1931
<      &                qm3peryrperwpinsahitwp(1) )
```

```
---
>      &                qm3peryrperwpinsahitwp(1),
>      &                flagDegrade1, timeDegrade1)
> c       GADAMS SCR605 2-2-2006: End of change
3647a3677,3684
> c     GADAMS SCR605 2-2-2006: Added degradation and non-degradation
> c     values to drythick.dat
> c      subroutine reflux3 (itpa, isa, ntim, tim,
> c     &                    cellwidth, celllength,
> c     &                    xmprs_tsw, satinit, residSat,
> c     &                    shed1fact, qfact, shed2fact,
> c     &                    rholiq, h, delt, xkrock,
> c     &                    qm3peryrinsa, qm3peryrinsaatrep)
3653c3690,3693
<      &                   qm3peryrinsa, qm3peryrinsaatrep)
---
>      &                   qm3peryrinsa, qm3peryrinsaatrep,
>      &                   flagDegrade, timeDegrade)
> c     GADAMS SCR605 2-2-2006: End of change
>
3776a3817,3821
>
> c      GADAMS SCR605 2-3-2006: Added drift degradation parameters
>        integer flagDegrade
>        double precision timeDegrade
> c      GADAMS SCR605 2-3-2006: End of change
3823a3869,3874
>
> c     GADAMS SCR605 2-2-2006: Added degradation and non-degradation
> c     values to drythick.dat
> c       call interpolate (newtim, ntim, tim, qm3peryrinsa,
> c     &       xmperyrinsa, nreflux, xinterp_tim,
> c     &       xinterp_xmperyrinsa, xinterp_thick, isa )
3826,3827c3877,3880
<      &       xinterp_xmperyrinsa, xinterp_thick, isa )
<
---
>      &       xinterp_xmperyrinsa, xinterp_thick, isa,
>      &       flagDegrade, timeDegrade )
> c     GADAMS SCR605 2-2-2006: End of change
>
3870a3926,3930
> c      GADAMS SCR605 2-2-2006: Included degradation and non-degradation
> c      values in drythick.dat
> c       subroutine interpolate (newtim, ntim, tim, qm3peryrinsa,
> c     & xmperyrinsa, nreflux, xinterp_tim, xinterp_xmperyrinsa,
> c     & xinterp_thick, isa )
3873c3933,3934
<      & xinterp_thick, isa )
>      & xinterp_thick, isa, flagDegrade, timeDegrade)
> c      GAAMS SCR605 2-2-2006: End of change
3894a3956,3960
>
> c      GADAMS SCR605 2-2-2006: Added drift degradation parameters
>        integer flagDegrade
>        double precision timeDegrade
> c      GADAMS SCR605 2-2-2006: End of change
3910,3911c3976,3982
<        call thickness_reader (nreflux, xinterp_tim, xinterp_thick )
<
---
> c      GADAMS SCR605 2-2-2006: Included degradation and non-degradation
> c      parameters in drythick.dat
> c       call thickness_reader (nreflux, xinterp_tim, xinterp_thick )
```

```
>        call thickness_reader (nreflux, xinterp_tim, xinterp_thick,
>      &   flagDegrade, timeDegrade)
> c      GADAMS SCR605 2-2-2006: End of change
>
3915a3987,3990
> c     GADAMS SCR605 2-2-2006: Added logic to retrieve dryout values
> c                             with or without degradation
> c       subroutine thickness_reader (nreflux,
> c     &                              xinterp_tim, xinterp_thick )
3917c3992,3993
<      &                             xinterp_tim, xinterp_thick )
---
>      &                             xinterp_tim, xinterp_thick,
>      &                             flagDegrade, timeDegrade )
3935a4012,4018
>
> c      GADAMS SCR605 2-2-2006: Added drift failure parameters
>        CHARACTER * 1 init_char
>        double precision timeDegrade
>        integer flagDegrade
> c      GADAMS SCR605 2-2-2006: End of change
>
3951,3952c4034,4101
<        read (ithicklun, fmt='(i4)') nthick
<        do i = 1,  nthick
---
>
> c      GADAMS SCR605 2-2-2006: Included both degradation and
> c      non-degradation dryout zone data
> c      Read data file until the time for end of the thermal
> c      pulse is obtained
>        READ(ithicklun, FMT = '(A1)') init_char
>        DO WHILE(init_char .EQ. ':')
>          READ(ithicklun, FMT = '(A1)') init_char
>        ENDDO
>        BACKSPACE(ithicklun)
>
> c      Read the time for end of the thermal pulse
>        READ(ithicklun, *) timePulseEnd
>
> c      If the drift reached full degradation and the time
> c      to reach full degradation was within the time
> c      for the thermal pulse...
>        IF(timeDegrade .LT. timePulseEnd .AND.
>      &   flagDegrade .EQ. 1)THEN
> c        Use the degraded drift data
>
> c        Skip comments
>          READ(ithicklun, FMT = '(A1)') init_char
>          DO WHILE(init_char .EQ. ':')
>            READ(ithicklun, FMT = '(A1)') init_char
>          ENDDO
>          BACKSPACE(ithicklun)
>
> c        Retrieve data
>          read(ithicklun, fmt = '(i4)') nthick
>          DO i=1, nthick
>            read(ithicklun, *) itimestepdum, thickness_tim(i),
>      &       thickness(i)
>          ENDDO
>        ELSE
> c        Use the non-degraded drift data
> c        Skip over the degraded drift data
>
```

```
> c         Skip comments
>           READ(ithicklun, FMT = '(A1)') init_char
>           DO WHILE(init_char .EQ. ':')
>             READ(ithicklun, FMT = '(A1)') init_char
>           ENDDO
>           BACKSPACE(ithicklun)
>
> c         Skip degraded drift data
>           read(ithicklun, fmt = '(i4)') nthick
>           DO i=1, nthick
>             read(ithicklun, *)
>           ENDDO
>
> c         Skip comments
>           READ(ithicklun, FMT = '(A1)') init_char
>           DO WHILE(init_char .EQ. ':')
>             READ(ithicklun, FMT = '(A1)') init_char
>           ENDDO
>           BACKSPACE(ithicklun)
>
> c         Retrieve data
>           read(ithicklun, fmt = '(i4)') nthick
>           DO i=1, nthick
>             read(ithicklun, *) itimestepdum, thickness_tim(i),
>       &       thickness(i)
>           ENDDO
>         ENDIF
>
> c        read (ithicklun, fmt='(i4)') nthick
> c        do i = 1,  nthick
3955,3957c4104,4108
<           read (ithicklun, *)
<       &                    itimestepdum, thickness_tim(i), thickness(i)
<         enddo
---
> c          read (ithicklun, *)
> c      &                    itimestepdum, thickness_tim(i), thickness(i)
> c        enddo
> c       GADAMS SCR605 2-2-2006: End of change
>
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

These differences depict the inclusion in *nfenv.f* code the ability to select from two possible data sets, depending on the degradation time of the repository drift. These changes are provided as evidence that TPA code has been modified to incorporate the changes described by SCR605 in issues 1 and 3.

The following text excerpts depict the differences between the basecase and testcase file *seismo2.f*
SCR605/diff_files/*seismo2_diff*

```
Ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
< C File Date:           02/25/05
---
> C File Date:           02/08/06
65a66,72
>
> c      GADAMS SCR605 2-2-2006: Added drift failure information
> c       subroutine eqvdia(numTime, time,
> c      &                    numSeismicEvents,timeSeismicEvents,
> c      &                    typeSeismicEvents, numSubareas, iSubarea,
> c      &                    eqDriftDiaA, eqDriftDiaB, eqBFDiaA,
> c      &                    eqBFDiaB, driftHeight)
```

```
70c77,80
<      &                   eqBFDiaB, driftHeight)
---
>      &                   eqBFDiaB, driftHeight, driftFailFlagRockOne,
>      &                   driftFailTimeRockOne, driftFailFlagRockTwo,
>      &                   driftFailTimeRockTwo)
> c     GADAMS SCR605 2-2-2006: End of change
75c85,86
< c               the backfill
---
> c               the backfill.  Provides drift failure information to
> c               executive
91a103,106
> c             integer, driftFailFlagRockOne
> c             double precision, driftFailTimeRockOne
> c             integer, driftFailFlagRockTwo
> c             double precision, driftFailTimeRockTwo
112a128,134
> c     GADAMS SCR605 2-2-2006: Added drift failure information
>       integer driftFailFlagRockOne
>       double precision driftFailTimeRockOne
>       integer driftFailFlagRockTwo
>       double precision driftFailTimeRockTwo
> c     GADAMS SCR605 2-2-2006: End of change
>
249a272,276
> c     GADAMS SCR605 2-2-2006: Added drift failure parameters
> c      call calculateDriftBFParameters(numTime, time,
> c     &                   numSeismicEvents,timeSeismicEvents,
> c     &                   typeSeismicEvents, numSubareas, iSubarea,
> c     &                   driftHeight, area_fallen)
253c280,283
<      &                   driftHeight, area_fallen)
---
>      &                   driftHeight, area_fallen,
>      &                   driftFailFlagRockOne, driftFailTimeRockOne,
>      &                   driftFailFlagRockTwo, driftFailTimeRockTwo)
> c     GADAMS SCR605 2-2-2006: End of change
272a303,307
> c     GADAMS SCR605 2-2-2006: Added drift failure parameters
> c      subroutine calculateDriftBFParameters(numTime, time,
> c     &  numSeismicEvents, timeSeismicEvents, typeSeismicEvents,
> c     &  numSubareas, iSubarea,
> c     &  driftHeight, areaFallen)
276c311,313
<      &  driftHeight, areaFallen)
---
>      &  driftHeight, areaFallen, driftFlagOne, driftTimeOne,
>      &  driftFlagTwo, driftTimeTwo)
> c     GADAMS SCR605 2-2-2006: End of change
295a333,336
> c             integer, driftFlagOne
> c             double precision, driftTimeOne
> c             integer, driftFlagTwo
> c             double precision, driftTimeTwo
313a355,361
> c     GADAMS SCR605 2-2-2006: Added drift failure parameters
>       integer driftFlagOne
>       double precision driftTimeOne
>       integer driftFlagTwo
>       double precision driftTimeTwo
> c     GADAMS SCR605 2-2-2006: End of change
>
414d461
```

```
<
415a463,470
> c     GADAMS SCR605 2-2-2006: Added drift failure parameters
> c     Initialize return values
>       driftFlagOne = 0
>       driftTimeOne = 0.0D0
>       driftFlagTwo = 0
>       driftTimeTwo = 0.0D0
> c     GADAMS SCR605 2-2-2006: End of change
>
420d474
<
701c755,773
<      &        i_value_seismicity_flag)
---
>      &        i_value_seismicity_flag)
>
> c             GADAMS SCR605 2-2-2006: Added drift failure parameters
> c             Set the drift failure parameters
>               IF(((index3 / 2) * 2) .EQ. index3) THEN
>                 IF(drift_failure_flag(index3).AND.
>                 IF(drift_failure_flag(index3).AND.
>      &                     driftFlagTwo .NE. 1) THEN
>                   driftFlagTwo = 1
>                   driftTimeTwo = timeSeismicEvents(index2)
>                 ENDIF
>               ELSE
>                 IF(drift_failure_flag(index3).AND.
>      &                     driftFlagOne .NE. 1) THEN
>                   driftFlagOne = 1
>                   driftTimeOne = timeSeismicEvents(index2)
>                 ENDIF
>               ENDIF
> c             GADAMS SCR605 2-2-2006: End of change
>
742a815,832
>
> c           GADAMS SCR605 2-2-2006: Added drift failure parameters
> c           Set the drift failure parameters
>             IF(((index3 / 2) * 2) .EQ. index3) THEN
>               IF(drift_failure_flag(index3).AND.
>      &                    driftFlagTwo .NE. 1) THEN
>                 driftFlagTwo = 1
>                 driftTimeTwo = time(index1)
>               ENDIF
>             ELSE
>               IF(drift_failure_flag(index3).AND.
>      &                    driftFlagOne .NE. 1) THEN
>                 driftFlagOne = 1
>                 driftTimeOne = time(index1)
>               ENDIF
>             ENDIF
> c           GADAMS SCR605 2-2-2006: End of change
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

These differences depict changes in *seismo2.f* code which allow seismo2.f to return drift failure flags and times to the *exec.f* to support the selection two possible data sets, depending on the degradation time of the repository drift. These changes are provided as evidence that TPA code has been modified to incorporate the changes described by SCR605 issues 1 and 3.

The follow text depicts the differences between the basecase and testcase *ebsrel.f* files SCR605/diff_files/*ebsrel_diff*

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
< c File Date:           07/15/05
---
> c File Date:           02/08/06
1394a1395,1414
>
> c     GADAMS SCR605 2-3-2006: Save ebsrel.inp for spent fuel
> c     wasteform
> c     Save ebsrel.inp for the spent fuel wasteform;
> c     otherwise, it will get overwritten when the glass
> c     model is run
>       if (iwasteform .eq. 1) then
>         call clearchar(80,command)
>         command = 'cp ebsrel.inp ebsrelsf.inp'
>         istatus=zportsh(command)
>         if( istatus .ne. 0 ) then
>           print *, ' ***>>> Error in ebsrel <<<*** '
>           print *, ' istatus .ne. 0 '
>           print *, ' istatus = sh( ', command, ' )'
>           print *, ' istatus = ', istatus
>           STOP
>         endif
>       end if
> c     GADAMS SCR605 2-3-2006: End of change
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The preceding text shows that the *ebsrel.f* has been modified to save *ebsrel.inp* data for the spent fuel waste form before calculating the glass form model has been run. This is evidence that issue 2 of SCR605 has been properly addressed.

The following text are *drythick.dat* files for the basecase and test case

Base case (TPA502f *drythick.dat)*
SCR605/tpa502f/data/*drythick.dat*

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
 17
 1       0.00       0.00
 2       20.00      0.00
 3       50.00      0.00
 4       55.00      2.68
 5       67.00      4.04
 6       74.00      4.92
 7       86.00      4.82
 8       102.00     5.62
 9       123.00     7.25
 10      148.00     6.75
 11      232.00     7.89
 12      456.00     9.31
 13      690.00     7.00
 14      1000.00    6.00
 15      2290.00    4.00
 16      3790.00    1.00
 17      4300.00    0.00


Input data file for the reflux3 model (nfenv.f).
The numbers were derived from METRA runs for the drift degradation case
(C.Manepally et al., 2004 - CNWRA report 2004-05) applicable only to case with Drift
Degradation..
It contains:
```

```
number of data lines in the file line number,  year,  dry-out zone thickness (m)...
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

Test case (TPA502g *drythick.dat*)
SCR605/tpa502g/data/*drythick.dat*

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
: Title - drythick.dat
: Date - February 2, 2006
: Input data file for the relux3 model (nfenv.f)
: (Manepally, C., A. Sun, r. Fedors, and D. Farrell.
: "Drift-Scale Thermohydrological Process Modeling--
:  In-Drift Heat Transfer and Drift Degradation."
: CNWRA 2004-5. San Antonio, TX: CNWRA. 2004.)
:
: This file is structured to have the first data value
: as the time for the end of the thermal pulse. Then,
: it includes the block of data for the degraded case,
: and finally, the block of data for the non-degraded
: case.  The code requires the data in this order.
:
: Time for the end of the thermal pulse.  This value
: is used to determine if the degraded scenario dryout
: zone thicknesses should be used or if the non-degraded
: zone thicknesses should instead be used.
 4000.0
:
: Data applicable to the case with drift degradation.
: Data derived from METRA runs for the drift degradation case.
: (Manepally, et. al., 2004 - Table 3.1)
: Entry No.  Time(yr)   Dryout Thickness (m)
 17
 1       0.00       0.00
 2       20.00      0.00
 3       50.00      0.00
 4       55.00      2.68
 5       67.00      4.04
 6       74.00      4.92
 7       86.00      4.82
 8       102.00     5.62
 9       123.00     7.25
 10      148.00     6.75
 11      232.00     7.89
 12      456.00     9.31
 13      690.00     7.00
 14      1000.00    6.00
 15      2290.00    4.00
 16      3790.00    1.00
 17      4300.00    0.00
: Data applicable to the case without drift degradation.
: (Manepally, et. al., 2004 - Table 2-2 Boiling Point - 96.3 C)
: Entry No.  Time(yr)   Dryout Thickness (m)
:
22
 1       0.00       0.00
 2       20.00      0.00
 3       50.00      0.00
 4       60.00      1.60
 5       70.00      3.16
 6       80.00      3.38
 7       100.00     3.47
 8       200.00     6.97
```

```
 9        300.00      8.06
 10       500.00      8.17
 11       700.00      8.13
 12       800.00      8.87
 13       900.00      9.46
 14       1000.00     11.75
 15       1300.00     5.87
 16       1400.00     3.51
 17       1500.00     2.24
 18       1600.00     1.58
 19       1700.00     0.95
 20       1800.00     0.54
 21       1900.00     0.00
 22       2000.00     0.00
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The test case *drythick.dat* file includes two dry out thickness data sets: one for a degraded drift and a second for a non-degraded drift. This is provided as evidence that issues 1 and 3 of SCR605 have been addressed.

notes: No unexpected changes to the testcase code (TPA502g) were observed and those changes that were made appeared logical.

- overall test status: **PASS**

SL-1.Name: Test if the proper drythick.dat data set is being properly chosen and used when the drift degrades before the end of the thermal pulse.

Path for run directory:

Testcase: [Spock]:/home/jmancillas/TPA/SCR605/tpa502g/rung1

Path for archive of results:

Testcase: SCR605/tpa502g/rung1

Archived to CD titled :SCR605 Testing

Environment variables:

Testcase : TPA_DATA=[spock]:/home/jmancillas/TPA/SCR605/tpa502g
TPA_TEST =[spock]:/home/jmancillas/TPA/SCR605/tpa502g

Special input files or modifications to input files required : itpa flag in nfenv.f is turned on

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Baseline

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data:

Test description: To determine if the proper *drythick.dat* data is being used by the TPA code, I will compare the *drythick.dat* data against the output data file *reflux3.out*. When the Degradation time is less than the end of the Thermal pulse the first data set in *drythick.dat* should be used and this should be the data contained in the *reflux3.out* data file..

- **objective** Identify if the proper *drythick.dat* data set is used when drift degradation occurs prior to the end of the thermal pulse

- **assumptions** None other than those made within the TPA code

- **constraints** Drift degradation time as determined by the data file *eqvdia.rlt* should be less than the time for the end of the thermal pulse. The time for the end of the thermal pulse is also contained in file *drythick.dat*

- **output files to compare or examine** Compare the *drythick.dat* data with the *reflux3.out* data

- **step by step test procedure to be used**

1) set itpa flag on to output *reflux3.out* file
2) execute one realization for one subarea
3) examine the drift degradation time in *eqvdia.rlt*
4) evaluate wether the appropriate data set from *drythick.dat* was used

- pass fail criteria

1) if driftdegradation time is less than the time for the end of the thermal pulse, the reflux3.out file should contain dryout thicknesses derived from the first data set in drythick.dat (degradation occurs prior to end of thermal pulse)

Test Results: The earliest failure time for the drift degradation is 606.8 yrs. This is less than the time for the end of the thermal pulse as defined in *drythick.dat* as 4000.00 yrs.

/SCR605/rung1/eqvdia.rlt

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
 Input file tpa.inp as supplied with TPA Version 5.0.2g Code.
  Base case.
  TPA 5.0.2g, Job started: Mon Mar 27 10:42:58 2006
  EQVDIA Results

  with the output mode specified in "tpa.inp"


REALIZATION    1


Equivalent diameters due to degradation of the drift

Equivalent Diameters, Subarea Analysis: Subarea   1

Rock Type One Drift Failure (yes=1, no=0):  1
Rock Type One Failure Time:                 7.11887E+02
Rock Type Two Drift Failure (yes=1, no=0):  1
Rock Type Two Failure Time:                 6.06805E+02
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

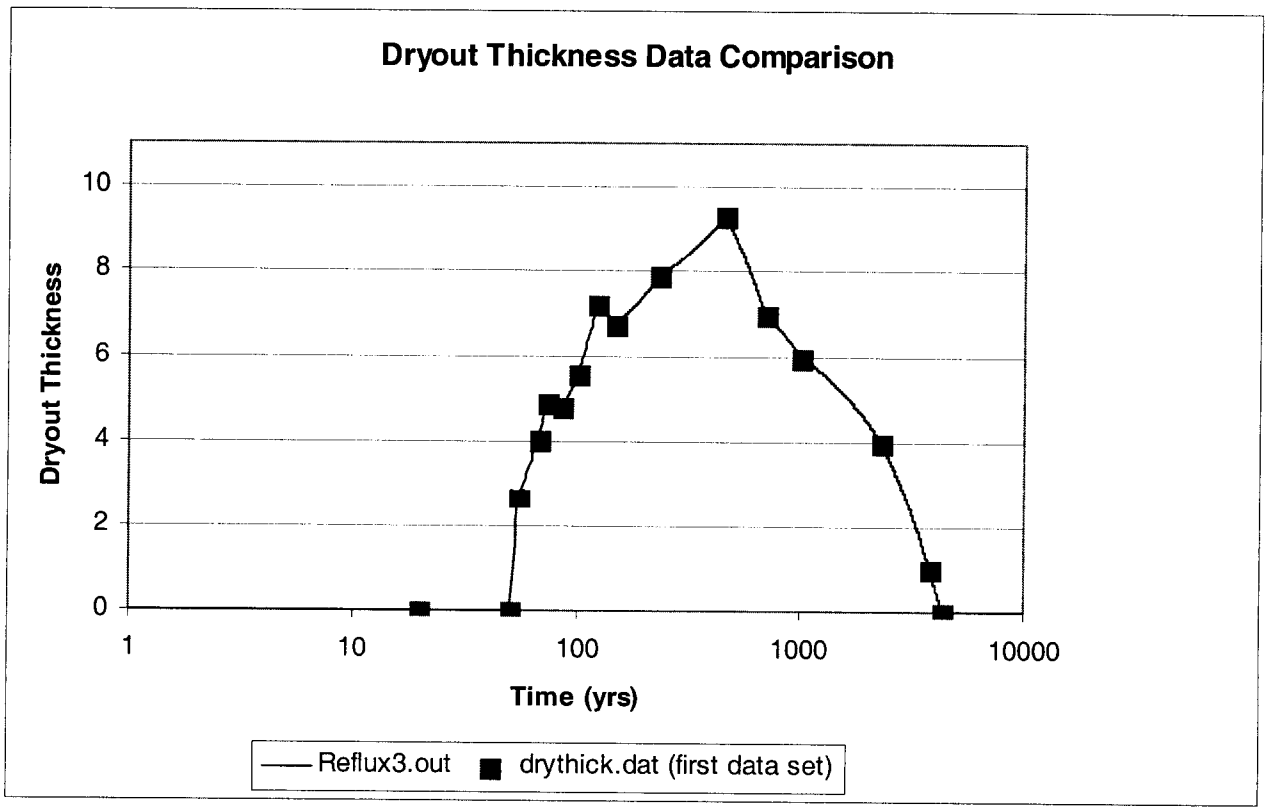
/SCR605/rung1/drythick.dat

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
: Time for the end of the thermal pulse.  This value
: is used to determine if the degraded scenario dryout
: zone thicknesses should be used or if the non-degraded
: zone thicknesses should instead be used.
 4000.0
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The following plot is a plot of the data contained in
/SCR605/rung1/drythick.dat

/SCR605/rung1/reflux3.out

This graph shows that when the degradation time is less than the time for the end of the thermal pulse, the proper data set in *drythick.dat* is chosen. This is provided as evidence that SCR605 has been properly implemented.



- overall test status: PASS

SL-2.Name: Test if the proper drythick.dat data set is being properly chosen and used when the drift degrades after the end of the thermal pulse

Path for run directory:

Testcase: [Spock]:/home/jmancillas/TPA/SCR605/tpa502g/rung2

Path for archive of results:

Testcase: SCR605/tpa502g/rung2

Archived to CD titled :SCR605 Testing

Environment variables:

Testcase : TPA_DATA=[spock]:/home/jmancillas/TPA/SCR605/tpa502g
TPA_TEST =[spock]:/home/jmancillas/TPA/SCR605/tpa502g

Special input files or modifications to input files required : itpa flag in nfenv.f is turned on

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Seismic and Drift Degradation scenarios are turned off

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data:

Test description: To determine if the proper *drythick.dat* data is being used by the TPA code, I will compare the *drythick.dat* data against the output data file *reflux3.out*. When the Degradation time is greater than the end of the Thermal pulse the second data set in *drythick.dat* should be used and this should be the data contained in the *reflux3.out* data file..

- **objective** Identify if the proper *drythick.dat* data set is used when drift degradation does not occur or degradation occurs after the end of the thermal pulse

- **assumptions** None other than those made within the TPA code

- **constraints** Drift degradation time as determined by the data file *eqvdia.rlt* should be greater than the time for the end of the thermal pulse. The time for the end of the thermal pulse is contained in file *drythick.dat*

- **output files to compare or examine** Compare the *drythick.dat* data with the *reflux3.out* data

- step by step test procedure to be used

1) set itpa flag on to output *reflux3.out* file
2) execute one realization for one subarea with degradation and seismic flags turned off
3) examine the drift degradation time in *eqvdia.rlt*
4) evaluate wether the appropriate data set from *drythick.dat* was used

- pass fail criteria

1) if driftdegradation time is greater than the time for the end of the thermal pulse, the reflux3.out file should contain dryout thicknesses derived from the second data set in drythick.dat (degradation occurs after the end of thermal pulse)

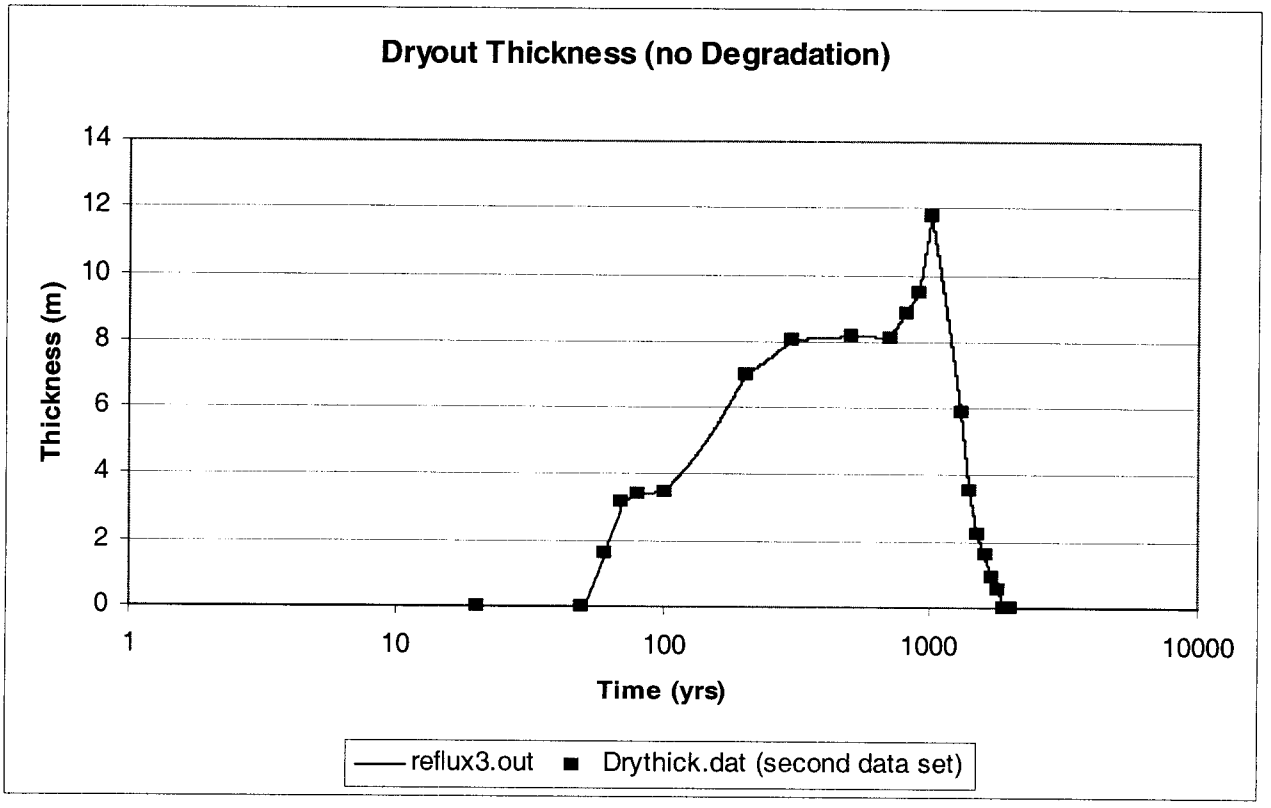
Test Results: Drift degradation does not occur prior to then end of the thermal pulse. The time for the end of the thermal pulse as defined in *drythick.dat* as 4000.00 yrs. The second data set in *drythick.dat* is chosen.

/SCR605/rung1/drythick.dat

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
: Time for the end of the thermal pulse.  This value
: is used to determine if the degraded scenario dryout
: zone thicknesses should be used or if the non-degraded
: zone thicknesses should instead be used.
 4000.0
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The following plot is a plot of the data contained in
/SCR605/rung2/drythick.dat
/SCR605/rung2/reflux3.out

The following graph is presented as evidence, that when degradation does not occur prior to the end of then thermal pulse, the proper data set in *drythick.dat* is chosen. This is provided as evidence that SCR605 has been properly implemented.



- **overall test status: PASS**

SL-3.Name: Test if the proper *drythick.dat* data set is being properly chosen when the time for the end of the thermal pulse is varied in the *drythick.dat* file

Path for run directory:

Testcase: [Spock]:/home/jmancillas/TPA/SCR605/tpa502g/rung3
[Spock]:/home/jmancillas/TPA/SCR605/tpa502g/rung4

Path for archive of results:

Testcase: SCR605/tpa502g/rung3 and SCR605/tpa502g/rung4

Archived to CD titled :SCR605 Testing

Environment variables:

Testcase : TPA_DATA=[spock]:/home/jmancillas/TPA/SCR605/tpa502g
TPA_TEST =[spock]:/home/jmancillas/TPA/SCR605/tpa502g

Special input files or modifications to input files required : itpa flag in nfenv.f is turned on

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data:

Test description: To determine if the proper *drythick.dat* data is being used by the TPA code, I will compare the *drythick.dat* data against the output data file *reflux3.out*. I will vary the time for the end of the thermal pulse to just prior to and just after the earliest degradation time for the drift. I will then examine if the proper data sets from the *drythick.dat* where properly used.

- **objective** Identify if the proper *drythick.dat* data set is used when the time for the end of the thermal pulse is changed in the file *drythick.dat.*

- **assumptions** None other than those made within the TPA code

- **constraints** None

- **output files to compare or examine** Compare the *drythick.dat* data with the *reflux3.out* data files from two different realizations

- **step by step test procedure to be used**
1) set itpa flag on to output *reflux3.out* file

3)Set the time for the end of the thermal pulse in *drythick.dat* to be 500 yrs and execute the TPA code for one realization and one subarea
4) examine the drift degradation time in *eqvdia.rlt*
5) evaluate wether the appropriate data set from *drythick.dat* was used
6)then change the time for the end of the thermal pulse to be 1000 yrs and execute the TPA code for one realization and one subarea
7)evaluate wether the appropriate data set from *drythick.dat* was used.

- pass fail criteria

1) if drift degradation time is greater than the time for the end of the thermal pulse, the reflux3.out file should contain dryout thicknesses derived from the second data set in drythick.dat (degradation occurs after the end of thermal pulse) and when the degradation time is less than the time for the end of the thermal pulse the first data set is used (degradation occurs prior to the end of the thermal pulse).

Test Results: Drift degradation occur at 606.8 yrs in both evaluations of the TPA code.

In both TPA runs (rung3 and rung4) the drift degradation time was the same, and is as shown in the following text excerpts.

SCR605/rung3/eqvdia.rlt

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
 Input file tpa.inp as supplied with TPA Version 5.0.2g Code.
 Base case.
 TPA 5.0.2g, Job started: Tue Apr  4 08:59:23 2006
 EQVDIA Results

 with the output mode specified in "tpa.inp"


REALIZATION    1


Equivalent diameters due to degradation of the drift

Equivalent Diameters, Subarea Analysis: Subarea   1

Rock Type One Drift Failure (yes=1, no=0):  1
Rock Type One Failure Time:                 7.11887E+02
Rock Type Two Drift Failure (yes=1, no=0):  1
Rock Type Two Failure Time:                 6.06805E+02
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

SCR605/rung4/eqvdia.rlt

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

```
Input file tpa.inp as supplied with TPA Version 5.0.2g Code.
 Base case.
 TPA 5.0.2g, Job started: Tue Apr  4 09:14:32 2006
 EQVDIA Results

 with the output mode specified in "tpa.inp"


REALIZATION    1


Equivalent diameters due to degradation of the drift

Equivalent Diameters, Subarea Analysis: Subarea   1

Rock Type One Drift Failure (yes=1, no=0):  1
Rock Type One Failure Time:                 7.11887E+02
Rock Type Two Drift Failure (yes=1, no=0):  1
Rock Type Two Failure Time:                 6.06805E+02
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The time for the end of the thermal pulse as defined in *drythick.dat* as 1000.00 yrs in rung3 and 500 yrs in rung4.
The following text excerpt is presented showing the time for the end of the thermal pulses
SCR605/rung3/drythick.dat

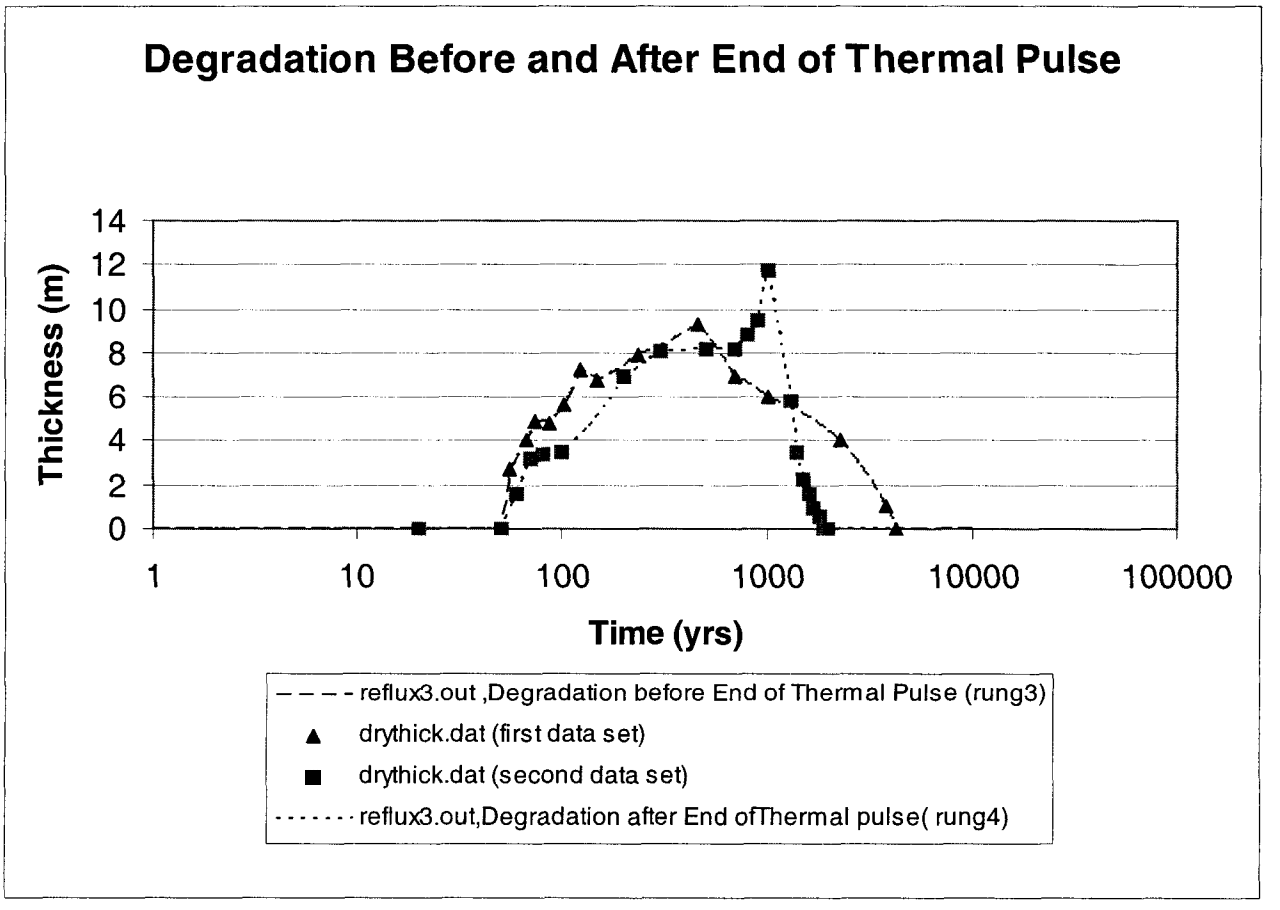
```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
: Time for the end of the thermal pulse.  This value
: is used to determine if the degraded scenario dryout
: zone thicknesses should be used or if the non-degraded
: zone thicknesses should instead be used.
1000.0
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

SCR605/rung4/drythick.dat

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
: Time for the end of the thermal pulse.  This value
: is used to determine if the degraded scenario dryout
: zone thicknesses should be used or if the non-degraded
: zone thicknesses should instead be used.
500.0
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

Since drift degradation (606.8 yrs) occurs before the end of the thermal pulse (1000 yrs) in rung3, the data in *reflux3.out* should contain data derived from the first data set in *drythick.dat*. In rung4 drift degradation (606.8 yrs) occurs after the end of the thermal pulse (500 yrs), thus the *reflux3.out* data should be derived from the second data set in *drythick.dat*.

The following plot shows the drythick.dat data sets and the reflux3.out data files from both rung3 and rung4.



This plot is presented as evidence that the data sets in *drythick.dat* are appropriately chosen when the time for the end of the thermal pulse is either after the drift degradation time (rung3) or before the drift degradation time (rung4) when the time for the thermal pulse is varied in the *drythick.dat* file.

- overall test status: PASS

ATTACHMENT B

Test Plan for TPA SCR605 (Windows)

Test Plan Name: TestPlan SCR605

Tested By: James Mancillas

Date: 4-4-2006

Host Machine: TPA

Host OS: MS Windows XP professional

Baseline Version: TPA5.0.2f

Test Version: TPA 5.0.2g

Process Level (SL) Tests

SL-1.Name: Verify that the PC version of TPA5.0.2.g has been updated to include SCR605 changes

Path for run directory:
Basecase: [Spock]:/home/jmancillas/TPA/SCR605/tpa502g
Testcase: [TPA]:\public\Mancillas\TPA\tpa502g

Path for archive of results:
Basecase : /SCR605/rung1
Testcase: \Window\runwin_g

Archived to CD titled :SCR605 Testing

Environment variables:
Basecase: TPA_DATA=[spock]:/home/jmancillas/TPA/SCR605/tpa502g
TPA_TEST =[spock]:/home/jmancillas/TPA/SCR605/tpa502g

Testcase : TPA_DATA=[TPA]:Public\Mancillas\tpa502g
TPA_TEST =[TPA]:Public\Mancillas\tpa502g

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Compare the drythick.dat files in the Unix version of TPA502g and the Windows version of TPA502g, to determine if the Windows version has been updated with SCR605. Additionally

perform a single realization run for both the Unix and Windows versions of TPA502g and compare their Peak mean dose.

- **objective** Determine if the Windows TPA code has been updated with SCR605 by comparing the drythick.dat files of the two and a single realization peak mean dose calculation

- **assumptions** None other than those made by TPA

- **constraints** None

- **output files to compare or examine** screen captures for the Windows and Unix TPA 502g output

- **step by step test procedure to be used**
  1) Run the Unix version of TPA502g and capture the screen output
  2) Run the Windows version of TPA502 and capture the screen output
  3) compare the peak mean dose reported in both both the calculations
  4) compare the drythick.dat files in the Unix and Windows versions of TPA502g

- **pass fail criteria**
  1) The peak mean dose calculations should agree between the Windows and Unix TPA502g calculations
  2) The drythick.dat files should be the same for both the Windows and Unix TPA502g codes.

Test Results

- criteria 1
The TPA code was executed on both the Windows and Unix platforms using TPA502g.
The peak mean dose calculated by the Unix version of TPA502g was 9.6549×10^{-2} rem/yr at 10000.0 yrs.

Unix results: Excerpt from run screen capture
SCR605/rung1/out

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
exec: Peak Mean Dose is 9.65490E-02 rem/yr at   10000.0 yr, based on     1
realizations.

 exec:  Run Successfully Completed
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The peak mean dose calculated by the Windows version of TPA502g was 9.6548×10^{-2} rem/yr at 10000.0 yrs

Windows results: Excerpt from run screen capture
Windows/runwin_g/out

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
exec: Peak Mean Dose is 9.65480E-02 rem/yr at   10000.0 yr, based on     1
```

```
realizations.

exec:  Run Successfully Completed

cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The results differ by 1.0×10^{-3} percent. This minimal difference is the result of rounding errors between the two computational platforms. This is presented as evidence that the TPA Windows version has been updated to include the changes from SCR605

-criteria 2

The drythick.dat files from the Unix and Windows version of TPA502g are shown bellow

Unix version:

SCR605/rung1/drythick.dat

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
: Title - drythick.dat
: Date - February 2, 2006
: Input data file for the relux3 model (nfenv.f)
: (Manepally, C., A. Sun, r. Fedors, and D. Farrell.
: "Drift-Scale Thermohydrological Process Modeling--
:  In-Drift Heat Transfer and Drift Degradation."
: CNWRA 2004-5. San Antonio, TX: CNWRA. 2004.)
:
: This file is structured to have the first data value
: as the time for the end of the thermal pulse. Then,
: it includes the block of data for the degraded case,
: and finally, the block of data for the non-degraded
: case.  The code requires the data in this order.
:
: Time for the end of the thermal pulse.  This value
: is used to determine if the degraded scenario dryout
: zone thicknesses should be used or if the non-degraded
: zone thicknesses should instead be used.
 4000.0
:
: Data applicable to the case with drift degradation.
: Data derived from METRA runs for the drift degradation case.
: (Manepally, et. al., 2004 - Table 3.1)
: Entry No.  Time(yr)   Dryout Thickness (m)
 17
 1       0.00       0.00
 2       20.00      0.00
 3       50.00      0.00
 4       55.00      2.68
 5       67.00      4.04
 6       74.00      4.92
 7       86.00      4.82
 8       102.00     5.62
 9       123.00     7.25
 10      148.00     6.75
 11      232.00     7.89
 12      456.00     9.31
 13      690.00     7.00
 14      1000.00    6.00
 15      2290.00    4.00
```

```
 16      3790.00    1.00
 17      4300.00    0.00
:
: Data applicable to the case without drift degradation.
: (Manepally, et. al., 2004 - Table 2-2 Boiling Point - 96.3 C)
: Entry No.  Time(yr)   Dryout Thickness (m)
 22
 1       0.00       0.00
 2       20.00      0.00
 3       50.00      0.00
 4       60.00      1.60
 5       70.00      3.16
 6       80.00      3.38
 7       100.00     3.47
 8       200.00     6.97
 9       300.00     8.06
 10      500.00     8.17
 11      700.00     8.13
 12      800.00     8.87
 13      900.00     9.46
 14      1000.00    11.75
 15      1300.00    5.87
 16      1400.00    3.51
 17      1500.00    2.24
 18      1600.00    1.58
 19      1700.00    0.95
 20      1800.00    0.54
 21      1900.00    0.00
 22      2000.00    0.00
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

Windows version:

Windows/runwin_g

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
: Title - drythick.dat
: Date - February 2, 2006
: Input data file for the relux3 model (nfenv.f)
: (Manepally, C., A. Sun, r. Fedors, and D. Farrell.
: "Drift-Scale Thermohydrological Process Modeling--
:  In-Drift Heat Transfer and Drift Degradation."
: CNWRA 2004-5. San Antonio, TX: CNWRA. 2004.)
:
: This file is structured to have the first data value
: as the time for the end of the thermal pulse. Then,
: it includes the block of data for the degraded case,
: and finally, the block of data for the non-degraded
: case.  The code requires the data in this order.
:
: Time for the end of the thermal pulse.  This value
: is used to determine if the degraded scenario dryout
: zone thicknesses should be used or if the non-degraded
: zone thicknesses should instead be used.
 4000.0
:
: Data applicable to the case with drift degradation.
: Data derived from METRA runs for the drift degradation case.
: (Manepally, et. al., 2004 - Table 3.1)
: Entry No.  Time(yr)   Dryout Thickness (m)
 17
 1       0.00       0.00
 2       20.00      0.00
```

```
 3        50.00       0.00
 4        55.00       2.68
 5        67.00       4.04
 6        74.00       4.92
 7        86.00       4.82
 8        102.00      5.62
 9        123.00      7.25
 10       148.00      6.75
 11       232.00      7.89
 12       456.00      9.31
 13       690.00      7.00
 14       1000.00     6.00
 15       2290.00     4.00
 16       3790.00     1.00
 17       4300.00     0.00
:
: Data applicable to the case without drift degradation.
: (Manepally, et. al., 2004 - Table 2-2 Boiling Point - 96.3 C)
: Entry No.  Time(yr)   Dryout Thickness (m)
 22
 1        0.00        0.00
 2        20.00       0.00
 3        50.00       0.00
 4        60.00       1.60
 5        70.00       3.16
 6        80.00       3.38
 7        100.00      3.47
 8        200.00      6.97
 9        300.00      8.06
 10       500.00      8.17
 11       700.00      8.13
 12       800.00      8.87
 13       900.00      9.46
 14       1000.00     11.75
 15       1300.00     5.87
 16       1400.00     3.51
 17       1500.00     2.24
 18       1600.00     1.58
 19       1700.00     0.95
 20       1800.00     0.54
 21       1900.00     0.00
 22       2000.00     0.00
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

A comparison of these files shows no differences, and is used a evidence that the Windows version of TPA502g has been properly updated with SCR605.

-Overall test status: **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 607	**2. Software Title and Version:** TPA 5.0.2	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *tpa.inp, ebsfail.f dsfail.f*

To increase the flexibility of the TPA code, failure depth thresholds for DS, WP and WeldAreas by corrosion will be added to the TPA code as user defined parameters. These parameters will allow TPA users to easily select fractional values of the components' original material thicknesses as failure criteria. The fractional values should span from 0 to 100 percent, with 100 percent corresponding to a complete material failure by corrosion required for component failure.

These failure criteria will be implemented in a manner which does not affect the thermal profile of a system.

5. Change Requested by: J. Mancillas Date:11-1-05	**6. Change Authorized by** (*Software Developer*): Ron Janetzke Date:11-4-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See Attachment A.

8. Implemented by: J. Mancillas	**Date:** 11-17-05

9. Description of Acceptance Tests:

See Attachment B for PC Acceptance Testing and Attachment C for UNIX Acceptance Testing.

10. Tested by: R. Rice	**Date:** 12-30-05 12/30/05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 607

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
Add	ebsfail	WPWeldFractionPenetrationForFailureByCorrosion[]	A fractional value to allow a failure criteria of less than 100% penetration of the WP weld area by corrosion	constant	1	1.0 corresponds to the current base case, requiring 100% penetration for failure.	O. Pensado

Add	ebsfail	WPFractionPenetrationForFailureByCorrosion[]	A fractional value to allow a failure criteria of less than 100% penetration of the WP by corrosion	constant	1	1.0 corresponds to the current base case, requiring 100% penetration for failure.	O. Pensado
Add	dsfail	DSFractionPenetrationForFailureByCorrosion[]	A fractional value to allow a failure criteria of less than 100% penetration of the DS by corrosion	constant	1	1.0 corresponds to the current base case, requiring 100% penetration for failure.	O. Pensado

ATTACHMENT A

Description of Changes for SCR-607

The parameters **WPFractionPenetratedForFailureByCorrosion[]**, **WPWeldFractionPenetratedForFailureByCorrosion[]**, and **DSFractionPenetratedForFailureByCorrosion[]** were incorporated in the TPA code to allow for the selection of a fractional thickness failures of the waste package outer burrier, waste package weld areas, and drip shields by corrosion.

These parameters were included into the *tpa.inp* file as shown in the excerpt.

```
constant
WPWeldFractionThicknessPenetratedForFailureByCorrosion[]
1.0
**
constant
WPFractionThicknessPenetratedForFailureByCorrosion[]
1.0
**
constant
DSFractionThicknessPenetratedForFailureByCorrosion[]
1.0
**
```

WPFractionThicknessPenetratedForFailureByCorrosion[] and **WPWeldFractionThicknessPenetratedForFailureByCorrosion[]** are used by *ebsfail.f* to evaluate failure criteria which are written to *ebsfail.inp*, as shown in the following excerpt from *ebsfail.f;*

```
cc jwm 11-18-05; SCR607 pass fraction thickness penetration for corrosion failure
c      write(aline(1:23),fmt='(e11.4,1x,e11.4)') cthick1,cthick2
      write(aline(1:23),fmt='(e11.4,1x,e11.4)') cthick1*wppenetration,cthick2
cc end changes; SCR607

cc SCR607 add fraction thickness penetration for corrosion failure
c      WRITE(aline(1:11), FMT = '(1pe11.4)') thickness
      WRITE(aline(1:11), FMT = '(1pe11.4)') thickness*weldpenetration
cc  end changes;SCR607
```

where *cthick1* is the thickness of the WP outer barrier, and *wppenetration* holds the value **WPFractionThicknessPenetratedForFailureByCorrosion[]**; and where *thickness* is the WP weld thickness and *weldpenetration* holds the value **WPWeldFractionThicknessPenetratedForFailureByCorrosion[]**. These values are written to ebsfail.inp, where they are used to determine EBS failure by corrosion.

DSFractionThicknessPenetratedForFailureByCorrosion[] is used by *dsfail.f* to evaluate failure criteria which are written to dsfail.inp, as shown in the following excerpt from *dsfail.f.*;

```
cc jwm 11-18-05;  SCR607 change format from float to exponential with 3 decimal places
c                 multiply ds thickness by fractional penetration for failure
c     WRITE(line7(1:18), FMT = '(F15.3, 3x)') drip_shield_thickness
      WRITE(line7(1:18), FMT = '(1PE15.3, 3x)') drip_shield_thickness*ds
     &penetration
cc end changes; SCR607
```

where *drip_shield_thickness* is the drip shield thickness and *dspenetration* holds the value **DSFractionThicknessPenetratedForFailureByCorrosion[]**. This value is written to *dsfailt.inp*, where it is used to calculate DS failure time by corrosion.

Error checking of the new parameters is performed within each routine that calls them (ie *dsfail.f* and *ebsfail.f*). This is perform in a straightforward manner, where the values are confirmed to be within the span [0,1].

Example of error testing in *dsfail.f*.

```
cc jwm 11-18-05; SCR607 add fraction thickness penetration for corrosion failure
cc               include error check to verify value between 0 and 1

      dspenetration = valuesp(i_dspenetration)

      if(dspenetration.lt.0) then
        print *, '***>>> ERROR in dsfail <<<***'
        print *,  'DSFractionThicknessPenetratedForFailureByCorrosion[]
     &out of bounds (value >1 or <0) '
        print *, 'Exiting...'
        stop
      endif

      if(dspenetration.gt.1)then
        print *,  '***>>> ERROR in dsfail <<<***'
        print *,  'DSFractionThicknessPenetratedForFailureByCorrosion[]
     &out of bounds (value >1 or <0) '
        print *, 'Exiting...'
        stop
      endif

cc end changes; SCR607
```

ATTACHMENT B

PC Acceptance Testing

Test Plan for TPA SCR#607

Test Plan Name: PC Testing of Corrosion Failure Depth Thresholds for DS, WP and Weld

Tested By: R. Rice

Date: December 30, 2005

Host Machine: Toshiba Laptop

Host OS: XP Professional

Baseline Version: 5.0.2

Test Version: 5.0.2a

System Level (SL) Tests

SL-1. Name: Basecase Corrosion Failure Depth Thresholds

Path for run directory: c:\SCR607\tpa502\run\basecase
c:\SCR607\tpa502a\run\basecase

Path for archive of results: \PC\SCR607\tpa502\run\basecase and \PC\SCR607\tpa502a\run\basecase (archived on CD named "SCR#607 Testing")

Environment variables: TPA_DATA=c:\SCR607\tpa502
TPA_TEST=c:\SCR607\tpa502

and

TPA_DATA=c:\SCR607\tpa502a
TPA_TEST=c:\SCR607\tpa502a

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Transfer of basecase (default) values for the corrosion failure depth fraction of

the drip shield, waste package, and weld from the *tpa.inp* file to the DSFAILT and FAILT input files is examined. In the basecase, there should be no changes in these input files and the temperature.

- Objective: Verify that basecase values of the drip shield, waste package, and weld corrosion failure depth fractions are correctly passed from the *tpa.inp* file to standalone code input files and that temperature calculations are not changed.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *ebsfail.inp*, *dsfailt.inp*, *ebstrh.dat*, and screenprint (*tpa.out)*

- Step by step test procedure to be used:

1. Create "run" subdirectories in both the TPA Versions 5.0.2 and 5.0.2a main source code directory.
2. In each of these run directories, create a subdirectory called "basecase".
3. Execute the TPA Version 5.0.2 and 5.0.2a codes using the basecase *tpa.inp* file (i.e., for Subarea 1 only) and capture the screenprint in the *tpa.out* file.
4. Review the "Output files to compare or examine" listed above and determine whether this test is passed or failed using the following criteria.

- Pass/Fail criteria:

Criterion 1: The FAILT input file *ebsfail.inp* should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 2: The DSFAILT input file *dsfailt.inp* should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 3: Temperatures in the *ebstrh.dat* file should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 4: Drip shield, waste package, and weld failure information in the screenprint (*tpa.out)* and at the end of the *ebstrh.dat* file should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Test Results: Files on the CD in the \PC\SCR607\tpa502\run\basecase and \PC\SCR607\tpa502a\run\basecase subdirectories contains results for this test. The results in these subdirectories indicate that the four Pass/Fail Criteria listed above were met and the test is PASSED. Test results for each of the four Pass/Fail Criteria are provided below. (Note that the text for the file comparisons ["differences"] shown

below are in the \PC\SCR607\tpa502a\run\basecase subdirectory in files with names "fc_*", where * is the name of the file being compared.)

For Criterion 1, the FAILT input file *ebsfail.inp* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
Comparing files ebsfail.inp and ..\..\..\TPA502\RUN\BASECASE\EBSFAIL.INP
FC: no differences encountered
```

Therefore, since there are no differences between the *ebsfail.inp* files for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 1 is satisfied.

For Criterion 2, the DSFAIL input file *dsfailt.inp* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
Comparing files dsfailt.inp and ..\..\..\TPA502\RUN\BASECASE\DSFAILT.INP
***** dsfailt.inp
      1.8E-06   CorrRate, m/yr, drip shield corrosion rate
    1.500E-02   DSThick, m, drip shield thickness : DripSh
         2.84   slope, dimensionless, slope of drip shield
***** ..\..\..\TPA502\RUN\BASECASE\DSFAILT.INP
      1.8E-06   CorrRate, m/yr, drip shield corrosion rate
        0.015   DSThick, m, drip shield thickness : DripSh
         2.84   slope, dimensionless, slope of drip shield
*****
```

The differences between these files is the format (i.e., 1.500E-02 versus 0.015), which is expected and shown in Attachment A. Therefore, since the only differences between the *dsfailt.inp* files for the TPA Version 5.0.2 and 5.0.2a codes is formatting, Criterion 2 is satisfied.

For Criterion 3, the file *ebstrh.dat* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
Comparing files ebstrh.dat and ..\..\..\TPA502\RUN\BASECASE\EBSTRH.DAT
FC: no differences encountered
```

Therefore, since there are no differences between the *ebstrh.dat* files for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 3 is satisfied.

For Criterion 4, the screenprint file *tpa.out* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
Comparing files tpa.out and ..\..\..\TPA502\RUN\BASECASE\TPA.OUT
***** tpa.out
==============================================================================
      exec: Welcome to TPA Version 5.0.2a
    Job started: Thu Dec 29 09:29:12 2005
==============================================================================
***** ..\..\..\TPA502\RUN\BASECASE\TPA.OUT
==============================================================================
```

```
      exec: Welcome to TPA Version 5.0.2
     Job started: Thu Dec 29 09:24:35 2005
==================================================================
*****

***** tpa.out
              Highest annual dose GW pathway
         Tc99   9.3754E-01 [mrem/yr]  at  2.863E+03 yr
         I129   4.3497E-01 [mrem/yr]  at  2.863E+03 yr
         Se79   1.1781E-02 [mrem/yr]  at  3.466E+03 yr
         Cl36   4.2736E-03 [mrem/yr]  at  2.863E+03 yr
         U234   3.1047E-03 [mrem/yr]  at  7.376E+03 yr
         U233   2.0031E-03 [mrem/yr]  at  1.000E+04 yr
        At end of TPI, annual dose GW pathway
         Tc99   5.7486E-03 [mrem/yr]
         U234   3.0417E-03 [mrem/yr]
         U233   2.0031E-03 [mrem/yr]
         I129   1.4247E-03 [mrem/yr]
         U238   8.3692E-04 [mrem/yr]
         Se79   1.1833E-04 [mrem/yr]
           sum  1.3196E-02 [mrem/yr]
exec: end realizations
***** ..\..\..\TPA502\RUN\BASECASE\TPA.OUT
              Highest annual dose GW pathway
         Tc99   9.3755E-01 [mrem/yr]  at  2.863E+03 yr
         I129   4.3497E-01 [mrem/yr]  at  2.863E+03 yr
         Se79   1.1782E-02 [mrem/yr]  at  3.466E+03 yr
         Cl36   4.2736E-03 [mrem/yr]  at  2.863E+03 yr
         U234   3.1093E-03 [mrem/yr]  at  7.376E+03 yr
         U233   2.0059E-03 [mrem/yr]  at  1.000E+04 yr
        At end of TPI, annual dose GW pathway
         Tc99   5.7487E-03 [mrem/yr]
         U234   3.0461E-03 [mrem/yr]
         U233   2.0059E-03 [mrem/yr]
         I129   1.4247E-03 [mrem/yr]
         U238   8.3803E-04 [mrem/yr]
         Se79   1.1834E-04 [mrem/yr]
           sum  1.3204E-02 [mrem/yr]
exec: end realizations
*****
```

Note that the above differences between the TPA Version 5.0.2 and 5.0.2a codes are for dose. These differences arise because DCFs were modified as part of the version change from the TPA Version 5.0.2 code to the TPA Version 5.0.2a code. Therefore, since there are no differences in failure times found in the screenprint file *tpa.out* for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 4 is satisfied.

- Overall test status: PASS

SL-2. Name: Non-basecase Corrosion Failure Depth Thresholds

Path for run directory: c:\SCR607\tpa502\run\test
c:\SCR607\tpa502a\run\test

Path for archive of results: \PC\SCR607\tpa502\run\test and \PC\SCR607\tpa502a\run\test (archived on CD named "SCR#607 Testing")

Environment variables: TPA_DATA=c:\SCR607\tpa502
TPA_TEST=c:\SCR607\tpa502

and

TPA_DATA=c:\SCR607\tpa502a
TPA_TEST=c:\SCR607\tpa502a

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only and set weld, WP, and drip shield penetration depths values at 0.001, 0.999, and 0.50 - instead of the basecase values of 1.0 - note that the weld, WP, and drip shield thicknesses in the TPA Version 5.0.2 code will need to be adjusted to 2.03e-5, 0.01998, and 0.0075 m)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Transfer of the values listed above for the corrosion failure depth fraction of the drip shield, waste package, and weld from the *tpa.inp* file to the DSFAILT and FAILT input files is examined for the TPA Version 5.0.2a code. Equivalent thicknesses are used in the TPA Version 5.0.2 code for comparison purposes. In this test, there should be no differences in values in these input files. Temperature should not be the same because of different thicknesses used in conduction calculations. Differences in the weld, WP, and dripshield thicknesses should be evident in the output files.

- Objective: Verify that values of the drip shield, waste package, and weld corrosion failure depth fractions in the TPA Version 5.0.2a code are correctly passed from the *tpa.inp* file and these values are consistent with modified thicknesses in the TPA Version 5.0.2 code. Temperatures should be affected because of the decreased equivalent thicknesses used in the TPA Version 5.0.2 code.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *ebsfail.inp*, *dsfailt.inp*, *ebstrh.dat*, screenprint (*tpa.out*), *weldfail.out*, *failt.out*, and *dsfailt.out*

- Step by step test procedure to be used:

1. Create "run" subdirectories in both the TPA Versions 5.0.2 and 5.0.2a main source code directory.
2. In each of these run directories, create a subdirectory called "test".
3. Execute the TPA Version 5.0.2 and 5.0.2a codes using the *tpa.inp* file for Subarea 1 only and the values given above. Capture the screenprint in the *tpa.out* file.
4. Review the "Output files to compare or examine" listed above and determine whether this test is passed or failed using the following criteria.

- Pass/Fail criteria:

Criterion 1: The FAILT input file *ebsfail.inp* should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 2: The DSFAILT input file *dsfailt.inp* should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 3: Temperatures in the *ebstrh.dat* file should be different for the TPA Version 5.0.2 and 5.0.2a codes; however, the temperatures from the TPA Version 5.0.2a (test) and TPA Version 5.0.2 (basecase) runs should be the same.

Criterion 4: Drip shield, waste package, and weld failure information in the screenprint (*tpa.out*) and at the end of the *ebstrh.dat* file should be consistent for the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 5: Examine the output files *weldfail.out* (for weld failure/ thickness), *failt.out* (for WP failure/thickness), and *dsfailt.out* (for drip shield failure/thickness) to confirm

the penetration depth parameters affect the thicknesses
Compare files for the TPA Version 5.0.2 ("basecase") and 5.0.2a ("test") codes.

Test Results: Files on the CD in the \PC\SCR607\tpa502\run\test and \PC\SCR607\tpa502a\run\test subdirectories contains results for this test. The results in these subdirectories indicate that the four Pass/Fail Criteria listed above were met and the test is PASSED. Test results for each of the four Pass/Fail Criteria are provided below. (Note that the text for the file comparisons ["differences"] shown below are in the \PC\SCR607\tpa502a\run\test subdirectory in files with names "fc_*", where * is the name of the file being compared.)

For Criterion 1, the FAILT input file *ebsfail.inp* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
Comparing files ebsfail.inp and ..\..\..\TPA502\RUN\TEST\EBSFAIL.INP
FC: no differences encountered
```

Therefore, since there are no differences between the *ebsfail.inp* files for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 1 is satisfied.

For Criterion 2, the DSFAIL input file *dsfailt.inp* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
Comparing files dsfailt.inp and ..\..\..\TPA502\RUN\TEST\DSFAILT.INP
***** dsfailt.inp
     1.8E-06  CorrRate, m/yr, drip shield corrosion rate
   7.500E-03  DSThick, m, drip shield thickness : DripSh
        2.84  slope, dimensionless, slope of drip shield
***** ..\..\..\TPA502\RUN\TEST\DSFAILT.INP
     1.8E-06  CorrRate, m/yr, drip shield corrosion rate
       0.007  DSThick, m, drip shield thickness : DripSh
        2.84  slope, dimensionless, slope of drip shield
*****
```

As in the previous test, the differences between these files is the format (i.e., 7.500E-03 versus 0.007), which is expected and shown in Attachment A. Therefore, since the only differences between the *dsfailt.inp* files for the TPA Version 5.0.2 and 5.0.2a codes is formatting, Criterion 2 is satisfied.

For Criterion 3, the file *ebstrh.dat* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
Comparing files ebstrh.dat and ..\..\..\TPA502\RUN\TEST\EBSTRH.DAT
Resync Failed.  Files are too different.
***** ebstrh.dat
  31    98.89370    61.33200    59.04260    0.02800    7.00000    0.00000
  32   103.51910   134.53430   111.09730    0.03790    7.00000    0.00000
  33   108.25280   150.23610   123.66010    0.04600    7.00000    0.00000
  34   113.09730   156.40490   128.41480    0.05840    7.00000    0.00000
```

35	118.05530	159.44150	130.88820	0.07580	7.00000	0.00000
36	123.12920	160.95690	132.27320	0.09920	7.00000	0.00000
37	128.32200	161.57760	132.99770	0.12950	7.00000	0.00000
38	133.63640	161.62300	133.28120	0.14090	7.00000	0.00000
39	139.07520	161.27960	133.25630	0.14210	7.00000	0.00000
40	144.64130	160.66390	133.00890	0.14440	7.00000	0.00000
41	150.33770	159.85230	132.59720	0.14740	7.00000	0.00000
42	156.16750	158.89490	132.06150	0.15100	7.00000	0.00000
43	162.13370	157.81790	131.43120	0.15530	7.00000	0.00000
44	168.23960	186.00630	130.72770	0.07890	7.00000	0.00000
45	174.48850	202.18770	129.96740	0.05570	7.00000	0.00000
46	180.88370	209.79330	129.34680	0.04770	7.00000	0.00000
47	187.42860	213.93850	128.83240	0.04400	7.00000	0.00000
48	194.12670	216.26660	128.32990	0.04200	7.00000	0.00000
49	200.98170	215.46730	128.41960	0.04270	7.00000	0.00000
50	207.99710	213.95370	128.62790	0.04390	7.00000	0.00000
51	215.17670	212.42550	128.77330	0.04530	7.00000	0.00000
52	222.52450	210.87340	128.84840	0.04670	7.00000	0.00000
53	230.04430	209.31580	128.87410	0.04820	7.00000	0.00000
54	237.74010	207.73830	128.83710	0.04970	7.00000	0.00000
55	245.61610	206.15840	128.75740	0.05140	7.00000	0.00000
56	253.67640	204.56960	128.62960	0.05310	7.00000	0.00000
57	261.92550	202.97120	128.45480	0.05480	7.00000	0.00000
58	270.36770	201.38080	128.25220	0.05670	7.00000	0.00000
59	279.00760	199.79430	128.01340	0.05860	7.00000	0.00000
60	287.84970	198.21660	127.74400	0.06060	7.00000	0.00000
61	296.89880	196.64390	127.44810	0.06260	7.00000	0.00000
62	306.15980	195.08320	127.13400	0.06470	7.00000	0.00000
63	315.63760	193.52620	126.79420	0.06690	7.00000	0.00000
64	325.33720	191.97440	126.43130	0.06920	7.00000	0.00000
65	335.26400	190.42880	126.04720	0.07160	7.00000	0.00000
66	345.42320	188.89750	125.65110	0.07400	7.00000	0.00000
67	355.82020	187.37950	125.24270	0.07660	7.00000	0.00000
68	366.46060	185.87100	124.81920	0.07920	7.00000	0.00000
69	377.35010	184.37230	124.38160	0.08190	7.00000	0.00000
70	388.49450	182.88420	123.93140	0.08470	7.00000	0.00000
71	399.89990	181.40750	123.47020	0.08760	7.00000	0.00000
72	411.57230	179.94670	123.00310	0.09060	7.00000	0.00000
73	423.51790	178.50380	122.53310	0.09370	7.00000	0.00000
74	435.74320	177.07380	122.05550	0.09680	7.00000	0.00000
75	448.25470	175.65670	121.57090	0.10010	7.00000	0.00000
76	461.05920	174.25270	121.08010	0.10350	7.00000	0.00000
77	474.16340	172.86180	120.58380	0.10690	7.00000	0.00000
78	487.57430	171.17040	119.99390	0.11140	7.00000	0.00000
79	501.29930	169.43210	119.34410	0.11610	7.00000	0.00000
80	515.34560	167.70140	118.67470	0.12110	7.00000	0.00000
81	529.72070	165.99430	118.00310	0.12630	7.00000	0.00000
82	544.43240	164.29420	117.31310	0.13180	7.00000	0.00000
83	559.48840	162.62050	116.62520	0.13740	7.00000	0.00000
84	574.89700	160.95580	115.92250	0.14330	7.00000	0.00000
85	590.66630	159.31800	115.22390	0.14940	7.00000	0.00000
86	606.80480	157.69480	114.51760	0.15580	7.00000	0.00000
87	623.32110	156.09110	113.80920	0.16240	7.00000	0.00000
88	640.22410	154.51330	113.10570	0.16920	7.00000	0.00000

89	657.52280	152.94930	112.39570	0.17630	7.00000	0.00000
90	675.22650	151.40490	111.68550	0.18370	7.00000	0.00000
91	693.34460	149.88590	110.98160	0.19130	7.00000	0.00000
92	711.88700	148.39690	110.28910	0.19910	7.00000	0.00000
93	730.86340	146.91650	109.58700	0.20730	7.00000	0.00000
94	750.28410	145.45960	108.89080	0.21580	7.00000	0.00000
95	770.15940	144.02580	108.20050	0.22450	7.00000	0.00000
96	790.50010	142.61440	107.51600	0.23350	7.00000	0.00000
97	811.31700	141.21470	106.82690	0.24280	7.00000	0.00000
98	832.62120	139.83260	106.13950	0.25250	7.00000	0.00000
99	854.42420	138.47180	105.45800	0.26250	7.00000	0.00000
100	876.73760	137.13180	104.78230	0.27280	7.00000	0.00000
101	899.57340	135.81200	104.11240	0.28340	7.00000	0.00000
102	922.94390	134.50580	103.44170	0.29430	7.00000	0.00000
103	946.86140	133.21160	102.76910	0.30570	10.67450	0.16870
104	971.33900	131.93640	102.10190	0.31740	10.67450	0.16870
105	996.38950	130.55490	101.40520	0.33080	10.67450	0.16870
106	1022.02650	129.15110	100.68420	0.34500	10.67450	0.16870
107	1048.26380	127.76480	99.96360	0.35970	10.67450	0.16870
108	1075.11530	126.39140	99.23920	0.37510	10.67450	0.16870
109	1102.59540	125.02930	98.50980	0.39110	10.67450	0.16870
110	1130.71880	123.67770	97.77510	0.40780	10.67450	0.16870
111	1159.50070	122.34910	97.04820	0.42510	10.67450	0.16870
112	1188.95640	121.03470	96.32060	0.43210	10.67450	0.16870
113	1219.10170	119.73790	95.59620	0.43850	10.67450	0.16870
114	1249.95270	118.46210	94.87890	0.44480	10.67450	0.16870
115	1281.52600	117.19850	94.16000	0.45100	10.67450	0.16870
116	1313.83850	115.94590	93.43880	0.45730	10.67450	0.16870
117	1346.90750	114.70690	92.71810	0.46350	10.67450	0.16870
118	1380.75060	113.48450	92.00150	0.46970	10.67450	0.16870
119	1415.38610	112.27190	91.28240	0.47590	10.67450	0.16870
120	1450.83240	111.07710	90.56930	0.48200	10.67450	0.16870
121	1487.10860	109.89960	89.86180	0.48810	10.67450	0.16870
122	1524.23410	108.73890	89.15980	0.49420	10.67450	0.16870
123	1562.22870	107.58450	88.45310	0.50030	10.67450	0.16870
124	1601.11280	106.44550	87.75110	0.50630	10.67450	0.16870
125	1640.90730	105.31960	87.05170	0.51230	10.67450	0.16870
126	1681.63330	104.19950	86.34800	0.51830	10.67450	0.16870
127	1723.31290	103.09370	85.64850	0.52420	10.67450	0.16870
128	1765.96820	101.99260	84.94410	0.53010	10.67450	0.16870
129	1809.62220	100.90450	84.24330	0.53590	10.67450	0.16870
130	1854.29810	99.83450	83.55150	0.54180	10.67450	0.16870

***** ..\..\..\TPA502\RUN\TEST\EBSTRH.DAT

31	98.89370	61.33200	59.04260	0.02800	7.00000	0.00000
32	103.51910	134.62300	111.09730	0.03790	7.00000	0.00000
33	108.25280	150.33510	123.66010	0.04590	7.00000	0.00000
34	113.09730	156.50150	128.41480	0.05830	7.00000	0.00000
35	118.05530	159.53380	130.88820	0.07570	7.00000	0.00000
36	123.12920	161.04480	132.27320	0.09900	7.00000	0.00000
37	128.32200	161.66150	132.99770	0.12930	7.00000	0.00000
38	133.63640	161.70340	133.28120	0.14060	7.00000	0.00000
39	139.07520	161.35680	133.25630	0.14190	7.00000	0.00000
40	144.64130	160.73850	133.00890	0.14410	7.00000	0.00000
41	150.33770	159.92440	132.59720	0.14710	7.00000	0.00000

42	156.16750	158.96510	132.06150	0.15080	7.00000	0.00000
43	162.13370	157.88740	131.43120	0.15500	7.00000	0.00000
44	168.23960	185.27070	130.72770	0.08030	7.00000	0.00000
45	174.48850	202.14900	129.96740	0.05580	7.00000	0.00000
46	180.88370	209.98080	129.34680	0.04750	7.00000	0.00000
47	187.42860	214.22580	128.83240	0.04370	7.00000	0.00000
48	194.12670	216.60510	128.32990	0.04170	7.00000	0.00000
49	200.98170	215.96120	128.37860	0.04230	7.00000	0.00000
50	207.99710	214.43850	128.58830	0.04350	7.00000	0.00000
51	215.17670	212.90140	128.73510	0.04490	7.00000	0.00000
52	222.52450	211.34080	128.81170	0.04630	7.00000	0.00000
53	230.04430	209.77490	128.83880	0.04770	7.00000	0.00000
54	237.74010	208.18920	128.80320	0.04930	7.00000	0.00000
55	245.61610	206.60150	128.72490	0.05090	7.00000	0.00000
56	253.67640	205.00490	128.59850	0.05260	7.00000	0.00000
57	261.92550	203.39910	128.42500	0.05430	7.00000	0.00000
58	270.36770	201.80140	128.22370	0.05620	7.00000	0.00000
59	279.00760	200.20770	127.98610	0.05810	7.00000	0.00000
60	287.84970	198.62300	127.71780	0.06000	7.00000	0.00000
61	296.89880	197.04350	127.42310	0.06210	7.00000	0.00000
62	306.15980	195.47620	127.11010	0.06420	7.00000	0.00000
63	315.63760	193.91270	126.77130	0.06640	7.00000	0.00000
64	325.33720	192.35460	126.40940	0.06860	7.00000	0.00000
65	335.26400	190.80270	126.02620	0.07100	7.00000	0.00000
66	345.42320	189.26530	125.63100	0.07340	7.00000	0.00000
67	355.82020	187.74120	125.22360	0.07600	7.00000	0.00000
68	366.46060	186.22680	124.80090	0.07860	7.00000	0.00000
69	377.35010	184.72230	124.36410	0.08130	7.00000	0.00000
70	388.49450	183.22850	123.91460	0.08400	7.00000	0.00000
71	399.89990	181.74630	123.45420	0.08690	7.00000	0.00000
72	411.57230	180.27990	122.98780	0.08990	7.00000	0.00000
73	423.51790	178.83170	122.51840	0.09290	7.00000	0.00000
74	435.74320	177.39640	122.04150	0.09610	7.00000	0.00000
75	448.25470	175.97410	121.55750	0.09930	7.00000	0.00000
76	461.05920	174.56500	121.06730	0.10270	7.00000	0.00000
77	474.16340	173.16910	120.57150	0.10620	7.00000	0.00000
78	487.57430	171.47140	119.98220	0.11060	7.00000	0.00000
79	501.29930	169.72700	119.33290	0.11530	7.00000	0.00000
80	515.34560	167.99020	118.66410	0.12030	7.00000	0.00000
81	529.72070	166.27710	117.99300	0.12550	7.00000	0.00000
82	544.43240	164.57130	117.30340	0.13090	7.00000	0.00000
83	559.48840	162.89190	116.61600	0.13650	7.00000	0.00000
84	574.89700	161.22160	115.91370	0.14240	7.00000	0.00000
85	590.66630	159.57840	115.21550	0.14840	7.00000	0.00000
86	606.80480	157.94990	114.50960	0.15480	7.00000	0.00000
87	623.32110	156.34110	113.80160	0.16130	7.00000	0.00000
88	640.22410	154.75810	113.09850	0.16810	7.00000	0.00000
89	657.52280	153.18920	112.38880	0.17520	7.00000	0.00000
90	675.22650	151.63990	111.67890	0.18250	7.00000	0.00000
91	693.34460	150.11620	110.97530	0.19010	7.00000	0.00000
92	711.88700	148.62250	110.28310	0.19790	7.00000	0.00000
93	730.86340	147.13760	109.58120	0.20610	7.00000	0.00000
94	750.28410	145.67630	108.88530	0.21450	7.00000	0.00000
95	770.15940	144.23810	108.19520	0.22320	7.00000	0.00000

```
 96    790.50010    142.82250    107.51100    0.23210    7.00000    0.00000
 97    811.31700    141.41860    106.82210    0.24140    7.00000    0.00000
 98    832.62120    140.03240    106.13490    0.25110    7.00000    0.00000
 99    854.42420    138.66760    105.45360    0.26100    7.00000    0.00000
100    876.73760    137.32370    104.77820    0.27120    7.00000    0.00000
101    899.57340    136.00010    104.10840    0.28180    7.00000    0.00000
102    922.94390    134.69020    103.43790    0.29280    7.00000    0.00000
103    946.86140    133.39230    102.76540    0.30410    10.67450    0.16870
104    971.33900    132.11350    102.09850    0.31580    10.67450    0.16870
105    996.38950    130.72790    101.40190    0.32910    10.67450    0.16870
106    1022.02650    129.32010    100.68110    0.34320    10.67450    0.16870
107    1048.26380    127.92980    99.96060    0.35790    10.67450    0.16870
108    1075.11530    126.55260    99.23630    0.37330    10.67450    0.16870
109    1102.59540    125.18670    98.50700    0.38920    10.67450    0.16870
110    1130.71880    123.83150    97.77250    0.40590    10.67450    0.16870
111    1159.50070    122.49920    97.04570    0.42310    10.67450    0.16870
112    1188.95640    121.18140    96.31830    0.43010    10.67450    0.16870
113    1219.10170    119.88120    95.59390    0.43640    10.67450    0.16870
114    1249.95270    118.60210    94.87670    0.44270    10.67450    0.16870
115    1281.52600    117.33530    94.15790    0.44900    10.67450    0.16870
116    1313.83850    116.07950    93.43680    0.45530    10.67450    0.16870
117    1346.90750    114.83740    92.71620    0.46150    10.67450    0.16870
118    1380.75060    113.61200    91.99970    0.46770    10.67450    0.16870
119    1415.38610    112.39640    91.28070    0.47390    10.67450    0.16870
120    1450.83240    111.19880    90.56760    0.48000    10.67450    0.16870
121    1487.10860    110.01840    89.86020    0.48620    10.67450    0.16870
122    1524.23410    108.85500    89.15830    0.49230    10.67450    0.16870
123    1562.22870    107.69790    88.45170    0.49830    10.67450    0.16870
124    1601.11280    106.55630    87.74970    0.50440    10.67450    0.16870
125    1640.90730    105.42790    87.05040    0.51040    10.67450    0.16870
126    1681.63330    104.30530    86.34670    0.51640    10.67450    0.16870
127    1723.31290    103.19700    85.64730    0.52230    10.67450    0.16870
128    1765.96820    102.09360    84.94300    0.52820    10.67450    0.16870
129    1809.62220    101.00320    84.24220    0.53400    10.67450    0.16870
130    1854.29810    99.93090    83.55040    0.53990    10.67450    0.16870
*****
```

Because the thickness used in heat conduction calculations is different in TPA Version 5.0.2 code versus the TPA Version 5.0.2a code, these different temperatures is expected. However, a comparison between the *ebstrh.dat* files from the TPA Version 5.0.2a (test) and TPA Version 5.0.2 (basecase) runs should be the same. This file comparison is shown below.

```
Comparing files ebstrh.dat and ..\..\..\TPA502\RUN\BASECASE\EBSTRH.DAT
***** ebstrh.dat
  3.000000E-02                | Weld surface fraction
  1        9.2306597405E+02   | Weld Failure Flag (1 = failure), Weld Failure Time[yr]
  0        1.0000000000E+04   | WP Failure Flag (1 = failure), WP Failure Time[yr]
***** ..\..\..\TPA502\RUN\BASECASE\EBSTRH.DAT
  3.000000E-02                | Weld surface fraction
  1        1.0160812973E+03   | Weld Failure Flag (1 = failure), Weld Failure Time[yr]
  0        1.0000000000E+04   | WP Failure Flag (1 = failure), WP Failure Time[yr]
*****
```

Note that the file *fc_ebstrh.dat_tpa502a_test_with_tpa502_basecase* contains the text from this file comparison. Also, the above difference in the files is attributable to the different weld thicknesses used in

the two tests (this thickness impacts the failure time). Therefore, since there are no differences in temperatures between the *ebstrh.dat* files for the TPA Version 5.0.2 (basecase) and 5.0.2a (test) codes, Criterion 3 is satisfied.

For Criterion 4, the screenprint file *tpa.out* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
Comparing files tpa.out and ..\..\..\TPA502\RUN\TEST\TPA.OUT
***** tpa.out
==============================================================================
      exec: Welcome to TPA Version 5.0.2a
    Job started: Thu Dec 29 11:52:37 2005
==============================================================================
***** ..\..\..\TPA502\RUN\TEST\TPA.OUT
==============================================================================
      exec: Welcome to TPA Version 5.0.2
    Job started: Thu Dec 29 13:13:22 2005
==============================================================================
*****

***** tpa.out
            Highest release rates from Sub Area 1
        Tc99    1.5319E+00 [Ci/yr/SA] at  1.854E+03 yr
        Ja241   4.9071E-01 [Ci/yr/SA] at  2.044E+03 yr
        Am241   5.4523E-02 [Ci/yr/SA] at  2.044E+03 yr
        Jp239   4.7292E-02 [Ci/yr/SA] at  5.971E+03 yr
        C14     3.8937E-02 [Ci/yr/SA] at  1.854E+03 yr
        Jp240   3.8060E-02 [Ci/yr/SA] at  4.607E+03 yr
exec: calling uzft
***** ..\..\..\TPA502\RUN\TEST\TPA.OUT
            Highest release rates from Sub Area 1
        Tc99    1.5320E+00 [Ci/yr/SA] at  1.854E+03 yr
        Ja241   4.9130E-01 [Ci/yr/SA] at  2.044E+03 yr
        Am241   5.4589E-02 [Ci/yr/SA] at  2.044E+03 yr
        Jp239   4.7295E-02 [Ci/yr/SA] at  5.971E+03 yr
        C14     3.8939E-02 [Ci/yr/SA] at  1.854E+03 yr
        Jp240   3.8064E-02 [Ci/yr/SA] at  4.607E+03 yr
exec: calling uzft
*****

***** tpa.out
        Tc99    1.2909E+00 [Ci/yr/SA] at  2.307E+03 yr
        Ja241   2.4522E-02 [Ci/yr/SA] at  3.227E+03 yr
        Jp239   2.2622E-02 [Ci/yr/SA] at  6.875E+03 yr
        Jp240   1.6597E-02 [Ci/yr/SA] at  6.407E+03 yr
        Cs135   1.0743E-02 [Ci/yr/SA] at  5.063E+03 yr
        Ja243   7.9388E-03 [Ci/yr/SA] at  3.227E+03 yr
exec: calling szft
***** ..\..\..\TPA502\RUN\TEST\TPA.OUT
        Tc99    1.2909E+00 [Ci/yr/SA] at  2.307E+03 yr
        Ja241   2.4557E-02 [Ci/yr/SA] at  3.227E+03 yr
        Jp239   2.2624E-02 [Ci/yr/SA] at  6.875E+03 yr
        Jp240   1.6598E-02 [Ci/yr/SA] at  6.407E+03 yr
```

```
        Cs135   1.0745E-02 [Ci/yr/SA] at  5.063E+03 yr
        Ja243   7.9732E-03 [Ci/yr/SA] at  3.227E+03 yr
exec: calling szft
*****

***** tpa.out
            Highest release rates from SZ
        Tc99    8.7721E-01 [Ci/yr/SA] at  2.863E+03 yr
        Se79    3.5549E-03 [Ci/yr/SA] at  3.466E+03 yr
        I129    3.2895E-03 [Ci/yr/SA] at  2.863E+03 yr
        Cl36    9.9157E-04 [Ci/yr/SA] at  2.863E+03 yr
        U234    6.1132E-05 [Ci/yr/SA] at  7.376E+03 yr
        U233    3.8970E-05 [Ci/yr/SA] at  1.000E+04 yr
exec: calling dcagw
***** ..\..\..\TPA502\RUN\TEST\TPA.OUT
            Highest release rates from SZ
        Tc99    8.7722E-01 [Ci/yr/SA] at  2.863E+03 yr
        Se79    3.5550E-03 [Ci/yr/SA] at  3.466E+03 yr
        I129    3.2894E-03 [Ci/yr/SA] at  2.863E+03 yr
        Cl36    9.9149E-04 [Ci/yr/SA] at  2.863E+03 yr
        U234    6.1142E-05 [Ci/yr/SA] at  7.376E+03 yr
        U233    3.9050E-05 [Ci/yr/SA] at  1.000E+04 yr
exec: calling dcagw
*****

***** tpa.out
            Highest annual dose GW pathway
        Tc99    9.3217E-01 [mrem/yr]  at  2.863E+03 yr
        I129    4.3127E-01 [mrem/yr]  at  2.863E+03 yr
        Se79    1.1772E-02 [mrem/yr]  at  3.466E+03 yr
        Cl36    4.2376E-03 [mrem/yr]  at  2.863E+03 yr
        U234    3.1047E-03 [mrem/yr]  at  7.376E+03 yr
        U233    2.0660E-03 [mrem/yr]  at  1.000E+04 yr
       At end of TPI, annual dose GW pathway
        Tc99    5.9494E-03 [mrem/yr]
        U234    3.0417E-03 [mrem/yr]
        U233    2.0660E-03 [mrem/yr]
        I129    1.4744E-03 [mrem/yr]
        U238    8.3692E-04 [mrem/yr]
        Se79    1.2260E-04 [mrem/yr]
          sum  1.3514E-02 [mrem/yr]
exec: end realizations
***** ..\..\..\TPA502\RUN\TEST\TPA.OUT
            Highest annual dose GW pathway
        Tc99    9.3220E-01 [mrem/yr]  at  2.863E+03 yr
        I129    4.3125E-01 [mrem/yr]  at  2.863E+03 yr
        Se79    1.1773E-02 [mrem/yr]  at  3.466E+03 yr
        Cl36    4.2373E-03 [mrem/yr]  at  2.863E+03 yr
        U234    3.1098E-03 [mrem/yr]  at  7.376E+03 yr
        U233    2.0732E-03 [mrem/yr]  at  1.000E+04 yr
       At end of TPI, annual dose GW pathway
        Tc99    5.9727E-03 [mrem/yr]
        U234    3.0466E-03 [mrem/yr]
        U233    2.0732E-03 [mrem/yr]
```

```
        I129   1.4802E-03 [mrem/yr]
        U238   8.3813E-04 [mrem/yr]
        Se79   1.2309E-04 [mrem/yr]
         sum  1.3557E-02 [mrem/yr]
exec: end realizations
*****
```

For Criterion 5, the files *weldfail.out* for the TPA Version 5.0.2 code "basecase" and 5.0.2a code "test" were compared. From TPA Version 5.0.2 code "basecase", a portion of *weldfail.out* is provided below:

```
 GENERATING MODULE: failt(weldfail)
Failure time of the weld area
1   Failure Flag (=1 if failed, 0 otherwise)
 1.0161E+03          yr, weld failure time
106  Number of time steps in this file
  Time[yr]   Rate[m/yr]  Ecorr[VSHE]  Ecrit[VSHE]  Thickness[m]
 0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   2.0300E-02

.
.
9.7134E+02   2.5000E-04  -7.5336E-03  -2.8380E-01   1.1186E-02
 9.9639E+02   2.5000E-04  -7.0329E-03  -2.7382E-01   4.9229E-03
 1.0220E+03   2.5000E-04  -6.4692E-03  -2.6368E-01  -1.4863E-03
```

From TPA Version 5.0.2 code "test", a portion of *weldfail.out* is provided below:

```
GENERATING MODULE: failt(weldfail)
 Failure time of the weld area
 1   Failure Flag (=1 if failed, 0 otherwise)
 9.2307E+02          yr, weld failure time
 103  Number of time steps in this file
   Time[yr]   Rate[m/yr]  Ecorr[VSHE]  Ecrit[VSHE]  Thickness[m]
 0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   2.0300E-05
.
.
.
8.9957E+02   2.5000E-08   0.0000E+00   0.0000E+00   1.5845E-05
 9.2294E+02   2.5000E-08   0.0000E+00   0.0000E+00   1.5261E-05
 9.4686E+02   2.5000E-04  -7.9494E-03  -2.9302E-01  -2.9747E-03
```

Note the earlier weld failure time for the "test" results compared to the ""basecase:" results.

Next, the files *failt.out* for the TPA Version 5.0.2 code "basecase" and 5.0.2a code "test" were compared. From TPA Version 5.0.2 code "basecase", a portion of *failt.out* is provided below:

```
ilayer  tstop    tcan    ecrit    ecorr  chloride  rthick     mode
     [yr]     [C]     [vshe]   [vshe]   flag      [m]
=========================================================================
===========
1      2.31    63.92   0.0000   0.0000    0   7.0000000E-02  dry oxd
1      4.67    71.49   0.0000   0.0000    0   7.0000000E-02  dry oxd
```

```
1      7.09     74.76    0.0000    0.0000    0   7.0000000E-02  dry oxd
1      9.57     76.27    0.0000    0.0000    0   7.0000000E-02  dry oxd
.
.
.
1   9543.25     60.31    0.5570    0.1022    1   6.9335669E-02  general
1   9768.98     59.91    0.5593    0.1035    1   6.9329680E-02  general
1  10000.00     59.50    0.5615    0.1047    1   6.9323671E-02  general
==========================================================================
=====
```

From TPA Version 5.0.2 code "test", a portion of *failt.out* is provided below:

```
ilayer tstop    tcan    ecrit    ecorr  chloride  rthick    mode
     [yr]     [C]     [vshe]   [vshe]   flag      [m]
==========================================================================
===========
1      2.31     63.92    0.0000    0.0000    0   6.9980000E-02  dry oxd
1      4.67     71.49    0.0000    0.0000    0   6.9980000E-02  dry oxd
1      7.09     74.76    0.0000    0.0000    0   6.9980000E-02  dry oxd
1      9.57     76.27    0.0000    0.0000    0   6.9980000E-02  dry oxd
.
.
.
1   9543.25     60.31    0.5570    0.1022    1   6.9315669E-02  general
1   9768.98     59.91    0.5593    0.1035    1   6.9309680E-02  general
1  10000.00     59.50    0.5615    0.1047    1   6.9303671E-02  general
==========================================================================
=====
```

As expected, note the decreased WP thickness for the "test" results compared to the ""basecase:" results.

Finally, the files *dsfailt.dat* for the TPA Version 5.0.2 code "basecase" and 5.0.2a code "test" were compared. From TPA Version 5.0.2 code "basecase", a portion of *dsfailt.dat* is provided below:

```
GENERATING MODULE: dsfailt
 Uniform corrosion of drip shield
 Thickness of drip shield vs time
 1  Failure Flag (=1 if failed, 0 otherwise)
 8333  yrs :  Drip shield failure time
 194  Number of time steps in this file
  Time[yr]     Thickness[m]
  0.0000E+00   1.5000E-02
  2.3102E+00   1.4996E-02
```

From TPA Version 5.0.2 code "test", a portion of *dsfailt.dat* is provided below:

```
GENERATING MODULE: dsfailt
Uniform corrosion of drip shield
Thickness of drip shield vs time
1  Failure Flag (=1 if failed, 0 otherwise)
```

```
4167  yrs :  Drip shield failure time
164  Number of time steps in this file
 Time[yr]      Thickness[m]
 0.0000E+00    7.5000E-03
 2.3102E+00    7.4958E-03
```

As expected, note the decreased DS thickness for the "test" results compared to the ""basecase:" results and that the failure is one-half (the penetration thickness was 0.5).

The TPA code output files for the weld, WP, and DS show evidence for decreased thickness and earlier failure times. Therefore, Criterion 5 is satisfied.

All Criteria are satisfied.

- Overall test status: PASS

SL-3. Name: Penetration Error Checks

Path for run directory: c:\SCR607\tpa502a\run\test1 through test3

Path for archive of results: \PC\SCR607\tpa502a\run\test1 through test3 (archived on CD named "SCR#607 Testing")

Environment variables: TPA_DATA=c:\SCR607\tpa502a
TPA_TEST=c:\SCR607\tpa502a

Special input files or modifications to input files required: *tpa.inp* (specify penetration values that are outside of acceptable range of 0 to 1)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Modify the penetration values for weld, WP, and DS to be outside of the acceptable range of 0 to 1 and demonstrate the error checking in the TPA code catches the error and stops TPA code execution with a message of the error.

- **Objective:** Verify that error check for values of the drip shield, waste package, and weld corrosion failure depth fractions work properly.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** screenprint (*tpa.out)*

- **Step by step test procedure to be used:**
  1. Modify the *tpa.inp* values for the penetration of weld to outside of 0 to 1.
  2. Run the TPA Version 5.0.2a code in "test1" and examine the screen print ijn the *tpa.out* file.
  3. Repeat steps 1 and 2 for the WP penetration in "test2".
  4. Repeat steps 1 and 2 for the DS penetration in "test3".

- **Pass/Fail criteria:**

Criterion 1: The screenprint in *tpa.out* file for test1, test2, and test3 should show TPA code execution is stopped and error message for the weld, WP, and DS penetration is printed for each case.

Test Results: Files on the CD in the \PC\SCR607\tpa502a\run\test*, where *=1,3, subdirectories contains results for this test. The results in these subdirectories indicate that Pass/Fail Criteria listed above were met and the test is PASSED. Test results for each of the four Pass/Fail Criteria are provided below.

For Criterion 1, test1 (for weld), the screenprint from the *tpa.inp* file shows an error message for the weld.

```
==========================================================================
      exec: Welcome to TPA Version 5.0.2a
    Job started: Wed Apr 12 09:25:22 2006
==========================================================================
-------------------------------------------------------------------------
  subarea  1 of  8        realization   1 of   1
-------------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:   0.0000E+00
     Mean Annual Infiltration at Start(AAI0):   5.8542E+00
exec: calling eqvdia
exec: calling nfenvFI
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
***>>> ERROR in ebsfail <<<***
WPWeldFractionThicknessPenetratedForFailureByCorrosion[] out of bounds (value >1 or <0)
Exiting...
```

For Criterion 1, test2 (for WP), the screenprint from the *tpa.inp* file shows an error message for the WP.

```
==========================================================================
      exec: Welcome to TPA Version 5.0.2a
    Job started: Wed Apr 12 09:25:48 2006
==========================================================================
-------------------------------------------------------------------------
  subarea  1 of  8        realization   1 of   1
-------------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:   0.0000E+00
     Mean Annual Infiltration at Start(AAI0):   5.8542E+00
exec: calling eqvdia
exec: calling nfenvFI
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
***>>> ERROR in ebsfail <<<***
```

```
WPFractionThicknessPenetratedForFailureByCorrosion[]  out of bounds (value >1 or <0)
Exiting...
```

For Criterion 1, test3 (for DS), the screenprint from the *tpa.inp* file shows an error message for the DS.

```
==========================================================================
      exec: Welcome to TPA Version 5.0.2a
    Job started: Wed Apr 12 09:26:10 2006
==========================================================================

--------------------------------------------------------------------------
  subarea  1 of  8        realization   1 of   1
--------------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:   0.0000E+00
     Mean Annual Infiltration at Start(AAI0):   5.8542E+00
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
***>>> ERROR in dsfail <<<***
DSFractionThicknessPenetratedForFailureByCorrosion[] out of bounds (value >1 or <0)
Exiting...
```

Therefore, since the screenprint shows the appropriate error messages for test1, test2 and test3, Criterion 1 is satisfied.

- Overall test status: PASS

ATTACHMENT C

UNIX Acceptance Testing

Test Plan for TPA SCR#607

Test Plan Name: UNIX Testing of Corrosion Failure Depth Thresholds for DS, WP and Weld

Tested By: R. Rice

Date: December 30, 2005

Host Machine: SPOCK

Host OS: Version 5.9
(SUNW, Ultra-4, sparc, sun4u)

Baseline Version: 5.0.2

Test Version: 5.0.2a

System Level (SL) Tests

SL-1. Name: Basecase Corrosion Failure Depth Thresholds

Path for run directory: /home/rrice/UNIX/SCR607/tpa502/run/basecase
/home/rrice/UNIX/SCR607/tpa502a/run/basecase

Path for archive of results: \UNIX\SCR607\tpa502\run\basecase and
\UNIX\SCR607\tpa502a\run\basecase (archived on CD named "SCR#607 Testing")

Environment variables: TPA_DATA is /home/rrice/UNIX/SCR607/tpa502/
TPA_TEST is /home/rrice/UNIX/SCR607/tpa502/

and

TPA_DATA is /home/rrice/UNIX/SCR607/tpa502a/
TPA_TEST is /home/rrice/UNIX/SCR607/tpa502a/

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Transfer of basecase (default) values for the corrosion failure depth fraction of the drip shield, waste package, and weld from the *tpa.inp* file to the DSFAILT and FAILT input files is examined. In the basecase, there should be no changes in these input files and the temperature.

- Objective: Verify that basecase values of the drip shield, waste package, and weld corrosion failure depth fractions are correctly passed from the *tpa.inp* file to standalone code input files and that temperature calculations are not changed.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *ebsfail.inp*, *dsfailt.inp*, *ebstrh.dat*, and screenprint (*tpa.out)*

- Step by step test procedure to be used:

1. Create "run" subdirectories in both the TPA Versions 5.0.2 and 5.0.2a main source code directory.
2. In each of these run directories, create a subdirectory called "basecase".
3. Execute the TPA Version 5.0.2 and 5.0.2a codes using the basecase *tpa.inp* file (i.e., for Subarea 1 only) and capture the screenprint in the *tpa.out* file.
4. Review the "Output files to compare or examine" listed above and determine whether this test is passed or failed using the following criteria.

- Pass/Fail criteria:

Criterion 1: The FAILT input file *ebsfail.inp* should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 2: The DSFAILT input file *dsfailt.inp* should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 3: Temperatures in the *ebstrh.dat* file should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 4: Drip shield, waste package, and weld failure information in the screenprint (*tpa.out)* and at the end of the *ebstrh.dat* file should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Test Results: Files on the CD in the \UNIX\SCR607\tpa502\run\basecase and \UNIX\SCR607\tpa502a\run\basecase subdirectories contains results for this test. The results in these subdirectories indicate that the four Pass/Fail Criteria listed above were met and the test is PASSED. Test results for each of the four Pass/Fail Criteria are

provided below. (Note that the text for the file comparisons ["differences"] using the UNIX "diff" utility shown below are in the \UNIX\SCR607\tpa502a\run\basecase subdirectory in files with names "diff_*", where * is the name of the file being compared.)

For Criterion 1, the FAILT input file *ebsfail.inp* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "diff" file comparison.

(This file is empty, which for the UNIX "diff" utility means that there are no differences in the files.)

Therefore, since there are no differences between the *ebsfail.inp* files for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 1 is satisfied.

For Criterion 2, the DSFAIL input file *dsfailt.inp* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "diff" file comparison.

```
7c7
<     1.500E-02   DSThick, m, drip shield thickness : DripSh
---
>        0.015   DSThick, m, drip shield thickness : DripSh
```

The differences between these files is the format (i.e., 1.500E-02 versus 0.015), which is expected and shown in Attachment A. Therefore, since the only differences between the *dsfailt.inp* files for the TPA Version 5.0.2 and 5.0.2a codes is formatting, Criterion 2 is satisfied.

For Criterion 3, the file *ebstrh.dat* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "diff" file comparison.

(This file is empty, which for the UNIX "diff" utility means that there are no differences in the files.)

Therefore, since there are no differences between the *ebstrh.dat* files for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 3 is satisfied.

For Criterion 4, the screenprint file *tpa.out* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "diff" file comparison.

```
        2,3c2,3
<       exec: Welcome to TPA Version 5.0.2a
<     Job started: Thu Dec 29 12:55:12 2005
---
>       exec: Welcome to TPA Version 5.0.2
>     Job started: Thu Dec 29 12:32:11 2005
89c89
<          Tc99   9.3754E-01 [mrem/yr]  at  2.863E+03 yr
---
>          Tc99   9.3755E-01 [mrem/yr]  at  2.863E+03 yr
91c91
<          Se79   1.1781E-02 [mrem/yr]  at  3.466E+03 yr
```

```
---
>          Se79   1.1782E-02 [mrem/yr]  at  3.466E+03 yr
93,94c93,94
<          U234   3.1047E-03 [mrem/yr]  at  7.376E+03 yr
<          U233   2.0031E-03 [mrem/yr]  at  1.000E+04 yr
---
>          U234   3.1092E-03 [mrem/yr]  at  7.376E+03 yr
>          U233   2.0059E-03 [mrem/yr]  at  1.000E+04 yr
96,98c96,98
<          Tc99   5.7486E-03 [mrem/yr]
<          U234   3.0417E-03 [mrem/yr]
<          U233   2.0031E-03 [mrem/yr]
---
>          Tc99   5.7487E-03 [mrem/yr]
>          U234   3.0461E-03 [mrem/yr]
>          U233   2.0059E-03 [mrem/yr]
100,102c100,102
<          U238   8.3692E-04 [mrem/yr]
<          Se79   1.1833E-04 [mrem/yr]
<            sum  1.3196E-02 [mrem/yr]
---
>          U238   8.3803E-04 [mrem/yr]
>          Se79   1.1834E-04 [mrem/yr]
>            sum  1.3204E-02 [mrem/yr]
```

Note that the above differences between the TPA Version 5.0.2 and 5.0.2a codes are for dose. These differences arise because DCFs were modified as part of the version change from the TPA Version 5.0.2 code to the TPA Version 5.0.2a code. Therefore, since there are no differences in failure times found in the screenprint file *tpa.out* for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 4 is satisfied.

- Overall test status: PASS

SL-2. Name: Non-basecase Corrosion Failure Depth Thresholds

Path for run directory: /home/rrice/UNIX/SCR607/tpa502/run/test
/home/rrice/UNIX/SCR607/tpa502a/run/test

Path for archive of results: \UNIX\SCR607\tpa502\run\test and \UNIX\SCR607\tpa502a\run\test
(archived on CD named "SCR#607 Testing")

Environment variables: TPA_DATA is /home/rrice/UNIX/SCR607/tpa502/
TPA_TEST is /home/rrice/UNIX/SCR607/tpa502/

and

TPA_DATA is /home/rrice/UNIX/SCR607/tpa502a/
TPA_TEST is /home/rrice/UNIX/SCR607/tpa502a/

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only and set weld, WP, and drip shield penetration depths values at 0.001, 0.999, and 0.50 - instead of the basecase values of 1.0 - note that the weld, WP, and drip shield thicknesses in the TPA Version 5.0.2 code will need to be adjusted to 2.03e-5, 0.01998, and 0.0075 m)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Transfer of the values listed above for the corrosion failure depth fraction of the drip shield, waste package, and weld from the *tpa.inp* file to the DSFAILT and FAILT input files is examined for the TPA Version 5.0.2a code. Equivalent thicknesses are used in the TPA Version 5.0.2 code for comparison purposes. In this test, there should be no differences in values in these input files. Temperature should not be the same because of different thicknesses used in conduction calculations. Differences in the weld, WP, and dripshield thicknesses should be evident in the output files.

- Objective: Verify that values of the drip shield, waste package, and weld corrosion failure depth fractions in the TPA Version 5.0.2a code are correctly passed from the *tpa.inp* file and these values are consistent with modified thicknesses in the TPA Version 5.0.2 code. Temperatures should be affected because of the decreased equivalent thicknesses used in the TPA Version 5.0.2 code.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *ebsfail.inp*, *dsfailt.inp*, *ebstrh.dat*, screenprint (*tpa.out*), *weldfail.out*, *failt.out*, and *dsfailt.out*

- Step by step test procedure to be used:

1. Create "run" subdirectories in both the TPA Versions 5.0.2 and 5.0.2a main source code directory.
2. In each of these run directories, create a subdirectory called "test".
3. Execute the TPA Version 5.0.2 and 5.0.2a codes using the *tpa.inp* file for Subarea 1 only and the values given above. Capture the screenprint in the *tpa.out* file.
4. Review the "Output files to compare or examine" listed above and determine whether this test is passed or failed using the following criteria.

- Pass/Fail criteria:

Criterion 1: The FAILT input file *ebsfail.inp* should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 2: The DSFAILT input file *dsfailt.inp* should be the same for both the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 3: Temperatures in the *ebstrh.dat* file should be different for the TPA Version 5.0.2 and 5.0.2a codes; however, the temperatures from the TPA Version 5.0.2a (test) and TPA Version 5.0.2 (basecase) runs should be the same.

Criterion 4: Drip shield, waste package, and weld failure information in the screenprint (*tpa.out*) and at the end of the *ebstrh.dat* file should be consistent for the TPA Version 5.0.2 and 5.0.2a codes.

Criterion 5: Examine the output files *weldfail.out* (for weld failure/ thickness), *failt.out* (for WP failure/thickness), and *dsfailt.out* (for drip shield failure/thickness) to confirm

the penetration depth parameters affect the thicknesses
Compare files for the TPA Version 5.0.2 ("basecase") and 5.0.2a ("test") codes.

Test Results: Files on the CD in the \UNIX\SCR607\tpa502\run\test and \UNIX\SCR607\tpa502a\run\test subdirectories contains results for this test. The results in these subdirectories indicate that the four Pass/Fail Criteria listed above were met and the test is PASSED. Test results for each of the four Pass/Fail Criteria are provided below. (Note that the text for the file comparisons ["differences"] using the UNIX "diff" utility shown below are in the \UNIX\SCR607\tpa502a\run\test subdirectory in files with names "diff_*", where * is the name of the file being compared.)

For Criterion 1, the FAILT input file *ebsfail.inp* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "diff" file comparison.

(This file is empty, which for the UNIX "diff" utility means that there are no differences in the files.)

Therefore, since there are no differences between the *ebsfail.inp* files for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 1 is satisfied.

For Criterion 2, the DSFAIL input file *dsfailt.inp* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "diff" file comparison.

```
7c7
<     7.500E-03   DSThick, m, drip shield thickness : DripSh
---
>       0.007   DSThick, m, drip shield thickness : DripSh
```

As in the previous test, the differences between these files is the format (i.e., 7.500E-03 versus 0.007), which is expected and shown in Attachment A. Therefore, since the only differences between the *dsfailt.inp* files for the TPA Version 5.0.2 and 5.0.2a codes is formatting, Criterion 2 is satisfied.

For Criterion 3, the file *ebstrh.dat* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "diff" file comparison.

```
      36,205c36,205
<  32   103.51910   134.53430   111.09730   0.03790   7.00000   0.00000
<  33   108.25280   150.23610   123.66010   0.04600   7.00000   0.00000
<  34   113.09730   156.40490   128.41480   0.05840   7.00000   0.00000
<  35   118.05530   159.44150   130.88820   0.07580   7.00000   0.00000
<  36   123.12920   160.95690   132.27320   0.09920   7.00000   0.00000
<  37   128.32200   161.57760   132.99770   0.12950   7.00000   0.00000
<  38   133.63640   161.62300   133.28120   0.14090   7.00000   0.00000
<  39   139.07520   161.27960   133.25630   0.14210   7.00000   0.00000
<  40   144.64130   160.66390   133.00890   0.14440   7.00000   0.00000
<  41   150.33770   159.85230   132.59720   0.14740   7.00000   0.00000
<  42   156.16750   158.89490   132.06150   0.15100   7.00000   0.00000
<  43   162.13370   157.81790   131.43120   0.15530   7.00000   0.00000
<  44   168.23960   186.00630   130.72770   0.07890   7.00000   0.00000
<  45   174.48850   202.18770   129.96740   0.05570   7.00000   0.00000
```

<	46	180.88370	209.79330	129.34680	0.04770	7.00000	0.00000
<	47	187.42860	213.93850	128.83240	0.04400	7.00000	0.00000
<	48	194.12670	216.26660	128.32990	0.04200	7.00000	0.00000
<	49	200.98170	215.46730	128.41960	0.04270	7.00000	0.00000
<	50	207.99710	213.95370	128.62790	0.04390	7.00000	0.00000
<	51	215.17670	212.42550	128.77330	0.04530	7.00000	0.00000
<	52	222.52450	210.87340	128.84840	0.04670	7.00000	0.00000
<	53	230.04430	209.31580	128.87410	0.04820	7.00000	0.00000
<	54	237.74010	207.73830	128.83710	0.04970	7.00000	0.00000
<	55	245.61610	206.15840	128.75740	0.05140	7.00000	0.00000
<	56	253.67640	204.56960	128.62960	0.05310	7.00000	0.00000
<	57	261.92550	202.97120	128.45480	0.05480	7.00000	0.00000
<	58	270.36770	201.38080	128.25220	0.05670	7.00000	0.00000
<	59	279.00760	199.79430	128.01340	0.05860	7.00000	0.00000
<	60	287.84970	198.21660	127.74400	0.06060	7.00000	0.00000
<	61	296.89880	196.64390	127.44810	0.06260	7.00000	0.00000
<	62	306.15980	195.08320	127.13400	0.06470	7.00000	0.00000
<	63	315.63760	193.52620	126.79420	0.06690	7.00000	0.00000
<	64	325.33720	191.97440	126.43130	0.06920	7.00000	0.00000
<	65	335.26400	190.42880	126.04720	0.07160	7.00000	0.00000
<	66	345.42320	188.89750	125.65110	0.07400	7.00000	0.00000
<	67	355.82020	187.37950	125.24270	0.07660	7.00000	0.00000
<	68	366.46060	185.87100	124.81920	0.07920	7.00000	0.00000
<	69	377.35010	184.37230	124.38160	0.08190	7.00000	0.00000
<	70	388.49450	182.88420	123.93140	0.08470	7.00000	0.00000
<	71	399.89990	181.40750	123.47020	0.08760	7.00000	0.00000
<	72	411.57230	179.94670	123.00310	0.09060	7.00000	0.00000
<	73	423.51790	178.50380	122.53310	0.09370	7.00000	0.00000
<	74	435.74320	177.07380	122.05550	0.09680	7.00000	0.00000
<	75	448.25470	175.65670	121.57090	0.10010	7.00000	0.00000
<	76	461.05920	174.25270	121.08010	0.10350	7.00000	0.00000
<	77	474.16340	172.86180	120.58380	0.10690	7.00000	0.00000
<	78	487.57430	171.17040	119.99390	0.11140	7.00000	0.00000
<	79	501.29930	169.43210	119.34410	0.11610	7.00000	0.00000
<	80	515.34560	167.70140	118.67470	0.12110	7.00000	0.00000
<	81	529.72070	165.99430	118.00310	0.12630	7.00000	0.00000
<	82	544.43240	164.29420	117.31310	0.13180	7.00000	0.00000
<	83	559.48840	162.62050	116.62520	0.13740	7.00000	0.00000
<	84	574.89700	160.95580	115.92250	0.14330	7.00000	0.00000
<	85	590.66630	159.31800	115.22390	0.14940	7.00000	0.00000
<	86	606.80480	157.69480	114.51760	0.15580	7.00000	0.00000
<	87	623.32110	156.09110	113.80920	0.16240	7.00000	0.00000
<	88	640.22410	154.51330	113.10570	0.16920	7.00000	0.00000
<	89	657.52280	152.94930	112.39570	0.17630	7.00000	0.00000
<	90	675.22650	151.40490	111.68550	0.18370	7.00000	0.00000
<	91	693.34460	149.88590	110.98160	0.19130	7.00000	0.00000
<	92	711.88700	148.39690	110.28910	0.19910	7.00000	0.00000
<	93	730.86340	146.91650	109.58700	0.20730	7.00000	0.00000
<	94	750.28410	145.45960	108.89080	0.21580	7.00000	0.00000
<	95	770.15940	144.02580	108.20050	0.22450	7.00000	0.00000
<	96	790.50010	142.61440	107.51600	0.23350	7.00000	0.00000
<	97	811.31700	141.21470	106.82690	0.24280	7.00000	0.00000
<	98	832.62120	139.83260	106.13950	0.25250	7.00000	0.00000
<	99	854.42420	138.47180	105.45800	0.26250	7.00000	0.00000

<	100	876.73760	137.13180	104.78230	0.27280	7.00000	0.00000
<	101	899.57340	135.81200	104.11240	0.28340	7.00000	0.00000
<	102	922.94390	134.50580	103.44170	0.29430	7.00000	0.00000
<	103	946.86140	133.21160	102.76910	0.30570	10.67450	0.16870
<	104	971.33900	131.93640	102.10190	0.31740	10.67450	0.16870
<	105	996.38950	130.55490	101.40520	0.33080	10.67450	0.16870
<	106	1022.02650	129.15110	100.68420	0.34500	10.67450	0.16870
<	107	1048.26380	127.76480	99.96360	0.35970	10.67450	0.16870
<	108	1075.11530	126.39140	99.23920	0.37510	10.67450	0.16870
<	109	1102.59540	125.02930	98.50980	0.39110	10.67450	0.16870
<	110	1130.71880	123.67770	97.77510	0.40780	10.67450	0.16870
<	111	1159.50070	122.34910	97.04820	0.42510	10.67450	0.16870
<	112	1188.95640	121.03470	96.32060	0.43210	10.67450	0.16870
<	113	1219.10170	119.73790	95.59620	0.43850	10.67450	0.16870
<	114	1249.95270	118.46210	94.87890	0.44480	10.67450	0.16870
<	115	1281.52600	117.19850	94.16000	0.45100	10.67450	0.16870
<	116	1313.83850	115.94590	93.43880	0.45730	10.67450	0.16870
<	117	1346.90750	114.70690	92.71810	0.46350	10.67450	0.16870
<	118	1380.75060	113.48450	92.00150	0.46970	10.67450	0.16870
<	119	1415.38610	112.27190	91.28240	0.47590	10.67450	0.16870
<	120	1450.83240	111.07710	90.56930	0.48200	10.67450	0.16870
<	121	1487.10860	109.89960	89.86180	0.48810	10.67450	0.16870
<	122	1524.23410	108.73890	89.15980	0.49420	10.67450	0.16870
<	123	1562.22870	107.58450	88.45310	0.50030	10.67450	0.16870
<	124	1601.11280	106.44550	87.75110	0.50630	10.67450	0.16870
<	125	1640.90730	105.31960	87.05170	0.51230	10.67450	0.16870
<	126	1681.63330	104.19950	86.34800	0.51830	10.67450	0.16870
<	127	1723.31290	103.09370	85.64850	0.52420	10.67450	0.16870
<	128	1765.96820	101.99260	84.94410	0.53010	10.67450	0.16870
<	129	1809.62220	100.90450	84.24330	0.53590	10.67450	0.16870
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>	34	113.09730	156.50150	128.41480	0.05830	7.00000	0.00000
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>	36	123.12920	161.04480	132.27320	0.09900	7.00000	0.00000

>	37	128.32200	161.66150	132.99770	0.12930	7.00000	0.00000
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>	42	156.16750	158.96510	132.06150	0.15080	7.00000	0.00000
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>	46	180.88370	209.98080	129.34680	0.04750	7.00000	0.00000
>	47	187.42860	214.22580	128.83240	0.04370	7.00000	0.00000
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>	129	1809.62220	101.00320	84.24220	0.53400	10.67450	0.16870
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>	143	2539.77960	89.86380	76.23560	0.58170	10.67450	0.16870
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>	173	5184.04140	72.31520	62.75120	0.65640	10.67450	0.16870
>	174	5307.71720	71.80320	62.34390	0.65860	10.67450	0.16870
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>	176	5563.82300	70.78950	61.53610	0.66300	10.67450	0.16870
>	177	5696.39000	70.28730	61.13530	0.66510	10.67450	0.16870
>	178	5832.06070	69.78940	60.73750	0.66730	10.67450	0.16870
>	179	5970.90750	69.29440	60.34150	0.66940	10.67450	0.16870
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>	183	6559.57100	67.38700	58.81950	0.67810	10.67450	0.16870
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>	187	7205.32650	65.53690	57.33780	0.68660	10.67450	0.16870
>	188	7376.32340	65.08080	56.97130	0.68870	10.67450	0.16870
>	189	7551.32370	64.62800	56.60710	0.69080	10.67450	0.16870
>	190	7730.42090	64.17860	56.24530	0.69290	10.67450	0.16870
>	191	7913.71100	63.74020	55.89360	0.69500	10.67450	0.16870
>	192	8101.29230	63.30720	55.54630	0.69710	10.67450	0.16870
>	193	8293.26500	62.87790	55.20180	0.69910	10.67450	0.16870
>	194	8489.73210	62.45180	54.85950	0.70120	10.67450	0.16870
>	195	8690.79880	62.02800	54.51860	0.70330	10.67450	0.16870
>	196	8896.57280	61.60470	54.17730	0.70540	10.67450	0.16870
>	197	9107.16420	61.18480	53.83840	0.70740	10.67450	0.16870
>	198	9322.68580	60.76890	53.50280	0.70950	10.67450	0.16870

```
> 199   9543.25310   60.35660   53.16980   0.71150   10.67450   0.16870
> 200   9768.98420   59.94780   52.83940   0.71350   10.67450   0.16870
> 201  10000.00000   59.53700   52.51160   0.71570   10.67450   0.16870
```

Because the thickness used in heat conduction calculations is different in TPA Version 5.0.2 code versus the TPA Version 5.0.2a code, these different temperatures is expected. However, a comparison between the *ebstrh.dat* files from the TPA Version 5.0.2a (test) and TPA Version 5.0.2 (basecase) runs should be the same. This file comparison is shown below.

```
208c208
<   1        9.2306597405E+02    | Weld Failure Flag (1 = failure), Weld Failure Time[yr]
---
>   1        1.0160812973E+03    | Weld Failure Flag (1 = failure), Weld Failure Time[yr]
```

Note that the file *fc_ebstrh.dat_tpa502a_test_with_tpa502_basecase* contains the text from this file comparison. Also, the above difference in the files is attributable to the different weld thicknesses used in the two tests (this thickness impacts the failure time). Therefore, since there are no differences in temperatures between the *ebstrh.dat* files for the TPA Version 5.0.2 (basecase) and 5.0.2a (test) codes, Criterion 3 is satisfied.

For Criterion 4, the screenprint file *tpa.out* for the TPA Version 5.0.2 and 5.0.2a codes was compared. The following is results of this "fc" file comparison.

```
2,3c2,3
<      exec: Welcome to TPA Version 5.0.2a
<     Job started: Thu Dec 29 13:57:05 2005
---
>      exec: Welcome to TPA Version 5.0.2
>     Job started: Thu Dec 29 13:49:51 2005
65,70c65,70
<        Tc99   1.5319E+00 [Ci/yr/SA] at  1.854E+03 yr
<        Ja241  4.9071E-01 [Ci/yr/SA] at  2.044E+03 yr
<        Am241  5.4523E-02 [Ci/yr/SA] at  2.044E+03 yr
<        Jp239  4.7292E-02 [Ci/yr/SA] at  5.971E+03 yr
<        C14    3.8937E-02 [Ci/yr/SA] at  1.854E+03 yr
<        Jp240  3.8060E-02 [Ci/yr/SA] at  4.607E+03 yr
---
>        Tc99   1.5320E+00 [Ci/yr/SA] at  1.854E+03 yr
>        Ja241  4.9130E-01 [Ci/yr/SA] at  2.044E+03 yr
>        Am241  5.4589E-02 [Ci/yr/SA] at  2.044E+03 yr
>        Jp239  4.7295E-02 [Ci/yr/SA] at  5.971E+03 yr
>        C14    3.8939E-02 [Ci/yr/SA] at  1.854E+03 yr
>        Jp240  3.8064E-02 [Ci/yr/SA] at  4.607E+03 yr
74,78c74,78
<        Ja241  2.4521E-02 [Ci/yr/SA] at  3.227E+03 yr
<        Jp239  2.2622E-02 [Ci/yr/SA] at  6.875E+03 yr
<        Jp240  1.6597E-02 [Ci/yr/SA] at  6.407E+03 yr
<        Cs135  1.0743E-02 [Ci/yr/SA] at  5.063E+03 yr
<        Ja243  7.9388E-03 [Ci/yr/SA] at  3.227E+03 yr
---
>        Ja241  2.4557E-02 [Ci/yr/SA] at  3.227E+03 yr
>        Jp239  2.2624E-02 [Ci/yr/SA] at  6.875E+03 yr
```

```
>          Jp240  1.6598E-02 [Ci/yr/SA] at  6.407E+03 yr
>          Cs135  1.0745E-02 [Ci/yr/SA] at  5.063E+03 yr
>          Ja243  7.9732E-03 [Ci/yr/SA] at  3.227E+03 yr
81,86c81,86
<          Tc99   8.7721E-01 [Ci/yr/SA] at  2.863E+03 yr
<          Se79   3.5549E-03 [Ci/yr/SA] at  3.466E+03 yr
<          I129   3.2895E-03 [Ci/yr/SA] at  2.863E+03 yr
<          Cl36   9.9157E-04 [Ci/yr/SA] at  2.863E+03 yr
<          U234   6.1132E-05 [Ci/yr/SA] at  7.376E+03 yr
<          U233   3.8970E-05 [Ci/yr/SA] at  1.000E+04 yr
---
>          Tc99   8.7722E-01 [Ci/yr/SA] at  2.863E+03 yr
>          Se79   3.5551E-03 [Ci/yr/SA] at  3.466E+03 yr
>          I129   3.2894E-03 [Ci/yr/SA] at  2.863E+03 yr
>          Cl36   9.9149E-04 [Ci/yr/SA] at  2.863E+03 yr
>          U234   6.1142E-05 [Ci/yr/SA] at  7.376E+03 yr
>          U233   3.9050E-05 [Ci/yr/SA] at  1.000E+04 yr
89,94c89,94
<          Tc99   9.3217E-01 [mrem/yr]  at  2.863E+03 yr
<          I129   4.3127E-01 [mrem/yr]  at  2.863E+03 yr
<          Se79   1.1772E-02 [mrem/yr]  at  3.466E+03 yr
<          Cl36   4.2376E-03 [mrem/yr]  at  2.863E+03 yr
<          U234   3.1047E-03 [mrem/yr]  at  7.376E+03 yr
<          U233   2.0660E-03 [mrem/yr]  at  1.000E+04 yr
---
>          Tc99   9.3220E-01 [mrem/yr]  at  2.863E+03 yr
>          I129   4.3125E-01 [mrem/yr]  at  2.863E+03 yr
>          Se79   1.1773E-02 [mrem/yr]  at  3.466E+03 yr
>          Cl36   4.2373E-03 [mrem/yr]  at  2.863E+03 yr
>          U234   3.1098E-03 [mrem/yr]  at  7.376E+03 yr
>          U233   2.0732E-03 [mrem/yr]  at  1.000E+04 yr
96,102c96,102
<          Tc99   5.9494E-03 [mrem/yr]
<          U234   3.0417E-03 [mrem/yr]
<          U233   2.0660E-03 [mrem/yr]
<          I129   1.4744E-03 [mrem/yr]
<          U238   8.3692E-04 [mrem/yr]
<          Se79   1.2260E-04 [mrem/yr]
<            sum  1.3514E-02 [mrem/yr]
---
>          Tc99   5.9727E-03 [mrem/yr]
>          U234   3.0466E-03 [mrem/yr]
>          U233   2.0732E-03 [mrem/yr]
>          I129   1.4802E-03 [mrem/yr]
>          U238   8.3813E-04 [mrem/yr]
>          Se79   1.2309E-04 [mrem/yr]
>            sum  1.3557E-02 [mrem/yr]
```

Note that the above differences between the TPA Version 5.0.2 and 5.0.2a codes are not identified as attributable to weld, WP, and drip shield failures. Therefore, since there are no differences in failure times in the screenprint file *tpa.out* for the TPA Version 5.0.2 and 5.0.2a codes, Criterion 4 is satisfied.

For Criterion 5, the files *weldfail.out* for the TPA Version 5.0.2 code "basecase" and 5.0.2a code "test" were

compared. From TPA Version 5.0.2 code "basecase", a portion of *weldfail.out* is provided below:

```
 GENERATING MODULE: failt(weldfail)
Failure time of the weld area
1   Failure Flag (=1 if failed, 0 otherwise)
 1.0161E+03          yr, weld failure time
106  Number of time steps in this file
  Time[yr]   Rate[m/yr]  Ecorr[VSHE]  Ecrit[VSHE]  Thickness[m]
 0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   2.0300E-02

.
.
9.7134E+02   2.5000E-04  -7.5336E-03  -2.8380E-01   1.1186E-02
 9.9639E+02   2.5000E-04  -7.0329E-03  -2.7382E-01   4.9229E-03
 1.0220E+03   2.5000E-04  -6.4692E-03  -2.6368E-01  -1.4863E-03
```

From TPA Version 5.0.2 code "test", a portion of *weldfail.out* is provided below:

```
GENERATING MODULE: failt(weldfail)
 Failure time of the weld area
 1   Failure Flag (=1 if failed, 0 otherwise)
  9.2307E+02          yr, weld failure time
 103  Number of time steps in this file
   Time[yr]   Rate[m/yr]  Ecorr[VSHE]  Ecrit[VSHE]  Thickness[m]
  0.0000E+00   0.0000E+00   0.0000E+00   0.0000E+00   2.0300E-05
.
.
.
8.9957E+02   2.5000E-08   0.0000E+00   0.0000E+00   1.5845E-05
 9.2294E+02   2.5000E-08   0.0000E+00   0.0000E+00   1.5261E-05
 9.4686E+02   2.5000E-04  -7.9494E-03  -2.9302E-01  -2.9747E-03
```

Note the earlier weld failure time for the "test" results compared to the ""basecase:" results.

Next, the files *failt.out* for the TPA Version 5.0.2 code "basecase" and 5.0.2a code "test" were compared. From TPA Version 5.0.2 code "basecase", a portion of *failt.out* is provided below:

```
ilayer  tstop     tcan     ecrit     ecorr  chloride  rthick     mode
      [yr]      [C]      [vshe]    [vshe]   flag      [m]
=========================================================================
===========
1      2.31     63.92    0.0000    0.0000    0   7.0000000E-02  dry oxd
1      4.67     71.49    0.0000    0.0000    0   7.0000000E-02  dry oxd
1      7.09     74.76    0.0000    0.0000    0   7.0000000E-02  dry oxd
1      9.57     76.27    0.0000    0.0000    0   7.0000000E-02  dry oxd
.
.
.
1   9543.25     60.31    0.5570    0.1022    1   6.9335669E-02  general
1   9768.98     59.91    0.5593    0.1035    1   6.9329680E-02  general
1  10000.00     59.50    0.5615    0.1047    1   6.9323671E-02  general
```

```
==========================================================================
=====
```

From TPA Version 5.0.2 code "test", a portion of *failt.out* is provided below:

```
ilayer tstop    tcan    ecrit    ecorr  chloride  rthick     mode
    [yr]    [C]    [vshe]   [vshe]  flag     [m]
==========================================================================
===========
1      2.31    63.92   0.0000   0.0000   0   6.9980000E-02  dry oxd
1      4.67    71.49   0.0000   0.0000   0   6.9980000E-02  dry oxd
1      7.09    74.76   0.0000   0.0000   0   6.9980000E-02  dry oxd
1      9.57    76.27   0.0000   0.0000   0   6.9980000E-02  dry oxd
.
.
.
1   9543.25    60.31   0.5570   0.1022   1   6.9315669E-02  general
1   9768.98    59.91   0.5593   0.1035   1   6.9309680E-02  general
1  10000.00    59.50   0.5615   0.1047   1   6.9303671E-02  general
==========================================================================
=====
```

As expected, note the decreased WP thickness for the "test" results compared to the ""basecase:" results.

Finally, the files *dsfailt.dat* for the TPA Version 5.0.2 code "basecase" and 5.0.2a code "test" were compared. From TPA Version 5.0.2 code "basecase", a portion of *dsfailt.dat* is provided below:

```
GENERATING MODULE: dsfailt
Uniform corrosion of drip shield
Thickness of drip shield vs time
1  Failure Flag (=1 if failed, 0 otherwise)
8333  yrs :  Drip shield failure time
194  Number of time steps in this file
 Time[yr]     Thickness[m]
 0.0000E+00   1.5000E-02
 2.3102E+00   1.4996E-02
```

From TPA Version 5.0.2 code "test", a portion of *dsfailt.dat* is provided below:

```
GENERATING MODULE: dsfailt
Uniform corrosion of drip shield
Thickness of drip shield vs time
1  Failure Flag (=1 if failed, 0 otherwise)
4167  yrs :  Drip shield failure time
164  Number of time steps in this file
 Time[yr]     Thickness[m]
 0.0000E+00   7.5000E-03
 2.3102E+00   7.4958E-03
```

As expected, note the decreased DS thickness for the "test" results compared to the ""basecase:" results and that the failure is one-half (the penetration thickness was 0.5).

The TPA code output files for the weld, WP, and DS show evidence for decreased thickness and earlier failure times. Therefore, Criterion 5 is satisfied.

All Criteria are satisfied.

- Overall test status: PASS

SL-3. Name: Penetration Error Checks

Path for run directory: /home/rrice/UNIX/SCR607/tpa502/run/test1 through test3

Path for archive of results: /UNIX/SCR607/tpa502a/run/test1 through test3 (archived on CD named "SCR#607 Testing")

Environment variables: TPA_DATA is /home/rrice/UNIX/SCR607/tpa502a/
TPA_TEST is /home/rrice/UNIX/SCR607/tpa502a/

Special input files or modifications to input files required: *tpa.inp* (specify penetration values that are outside of acceptable range of 0 to 1)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description: Modify the penetration values for weld, WP, and DS to be outside of the acceptable range of 0 to 1 and demonstrate the error checking in the TPA code catches the error and stops TPA code execution with a message of the error.

- **Objective:** Verify that error check for values of the drip shield, waste package, and weld corrosion failure depth fractions work properly.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** screenprint (*tpa.out)*

- **Step by step test procedure to be used:**
  1. Modify the *tpa.inp* values for the penetration of weld to outside of 0 to 1.
  2. Run the TPA Version 5.0.2a code in "test1" and examine the screen print ijn the *tpa.out* file.
  3. Repeat steps 1 and 2 for the WP penetration in "test2".
  4. Repeat steps 1 and 2 for the DS penetration in "test3".

- **Pass/Fail criteria:**

Criterion 1: The screenprint in *tpa.out* file for test1, test2, and test3 should show TPA code execution is stopped and error message for the weld, WP, and DS penetration is printed for each case.

Test Results: Files on the CD in the \PC\SCR607\tpa502a\run\test*, where *=1,3, subdirectories contains results for this test. The results in these subdirectories indicate that Pass/Fail Criteria listed above were met and the test is PASSED. Test results for each of the four Pass/Fail Criteria are provided below.

For Criterion 1, test1 (for weld), the screenprint from the *tpa.inp* file shows an error message for the weld.

```
==========================================================================
      exec: Welcome to TPA Version 5.0.2a
    Job started: Wed Apr 12 10:37:02 2006
==========================================================================

-------------------------------------------------------------------------
   subarea  1 of  8        realization   1 of   1
-------------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:   0.0000E+00
     Mean Annual Infiltration at Start(AAI0):   5.8542E+00
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
exec: calling  nfenv
exec: calling ebsfail
***>>> ERROR in ebsfail <<<***
WPWeldFractionThicknessPenetratedForFailureByCorrosion[] out of bounds (value >1 or <0)
Exiting...
```

For Criterion 1, test2 (for WP), the screenprint from the *tpa.inp* file shows an error message for the WP.

```
==========================================================================
      exec: Welcome to TPA Version 5.0.2a
    Job started: Wed Apr 12 10:37:44 2006
==========================================================================

-------------------------------------------------------------------------
   subarea  1 of  8        realization   1 of   1
-------------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:   0.0000E+00
     Mean Annual Infiltration at Start(AAI0):   5.8542E+00
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver
```

```
exec: calling  nfenv
exec: calling ebsfail
***>>> ERROR in ebsfail <<<***
WPFractionThicknessPenetratedForFailureByCorrosion[]   out of bounds (value >1 or <0)
Exiting...
```

For Criterion 1, test3 (for DS), the screenprint from the *tpa.inp* file shows an error message for the DS.

```
==========================================================================
        exec: Welcome to TPA Version 5.0.2a
      Job started: Wed Apr 12 10:38:20 2006
==========================================================================
-------------------------------------------------------------------------
   subarea   1 of   8          realization    1 of    1
-------------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
      Mean Annual Infiltration at Start(AAI0):    5.8542E+00
exec: calling eqvdia
exec: calling nfenvFl
exec: calling dsfail
***>>> ERROR in dsfail <<<***
DSFractionThicknessPenetratedForFailureByCorrosion[] out of bounds (value >1 or <0)
Exiting...
```

Therefore, since the screenprint shows the appropriate error messages for test1, test2 and test3, Criterion 1 is satisfied.

- Overall test status: PASS

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 608	**2. Software Title and Version:** TPA 5.0.2s	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *releaset.f*, *exec.f*, *ebsrel.f*, *tpa.inp*, *wpflow.def*, and *tpanames.dbs*

Release models require better integration with the drift degradation scenario. For that aim, revisions to the water contact model are proposed, allowing to track reductions in the amount of water contacting waste forms due to the presence of waste packages, drip shields, and rubble.

5. Change Requested by: O. Pensado/R. Fedors Date: 11/7/2005	**6. Change Authorized by** (*Software Developer*): Janetzke Date: 12-7-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Accomplished the following modifications: (1) calculate Fmult; (2) construct seepage factors Fr, Fd, and Fw; (3) use these four factors in RELEASET and base their use on failure times for each of the eight failure types; (4) add flag to select mechanical failure time or a time based on SEISMIC intervals, as the time for mechanical failures; (5) modify the water contact mode set in the *tpa.inp* file based on earliest failure for any failure type (except initial defectives), thus superceding the nominal failure mode for that particular failure type. These changes involved adding 12 parameters to the *tpa.inp* file and making one parameter constant instead specifying of a beta distribution.

See Attachment A for initial e-mail discussions involving these changes and the changes for *tpa.inp* parameters.

See Attachment B for a Powerpoint presentation by O. Pensado addressing these changes.

See Attachment C for additional discussion on these topics in and e-mail from O. Pensado.

8. Implemented by: R. Rice	**Date:** 3/15/2006

9. Description of Acceptance Tests:

1) Plot Fmult as a function of the deep percolation (data available in file ebsflo.dat) and verify that the functional dependence is satisfied.
2) Verify that the factors Fr, Fd, and Fw respond to the timing of drift degradation, waste package corrosion, and mechanical degradation (data available in files ebsflo.dat, driftfail.rlt, and ebsrel.rlt)
3) Activate the no-seepage-protection-credit flags to verify that protection is disabled
4) Verify that the appropriate water contact mode is activated based on the failure type.

See Attachment D for the test plan and test results.

10. Tested by: O. Pensado	**Date:** 4/12/2006

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 608

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
MODIFY FROM	EBSREL	WastePackageMultiplicationFlowFactor	See Attachment A	BETA	0.3, 1.4, 1.5, 0.8	See Attachment A	See Attachment A
MODIFY TO	EBSREL	WastePackageMultiplicationFlowFactor	See Attachment A	CONSTANT	1.0	See Attachment A	See Attachment A
ADD	EBSREL	SeepageRubbleFactor	See Attachment A	CONSTANT	1.0	See Attachment A	See Attachment A

ADD	EBSREL	SeepageEngineeringBackfillFactor	See Attachment A	CONSTANT	1.0	See Attachment A	See Attachment A
ADD	EBSREL	InitialSeepageReductionFractionByMechanicallyFailedDS	See Attachment A	CONSTANT	1.0	See Attachment A	See Attachment A
ADD	EBSREL	DSSeepageProtectionDegradationRate[1/yr]	See Attachment A	CONSTANT	0.0	See Attachment A	See Attachment A
ADD	EBSREL	FlagPartialProtectionAgainstSeepageByMechanicallyFailedDS[1=yes,0=no]	See Attachment A	IFLAG	1	See Attachment A	See Attachment A
ADD	EBSREL	InitialSeepageReductionFractionByMechanicallyFailedWP	See Attachment A	CONSTANT	0.0	See Attachment A	See Attachment A
ADD	EBSREL	WPSeepageProtectionDegradationRate[1/yr]	See Attachment A	CONSTANT	0.0	See Attachment A	See Attachment A
ADD	EBSREL	FlagPartialProtectionAgainstSeepageByMechanicallyFailedWP[1=yes,0=no]	See Attachment A	IFLAG	1	See Attachment A	See Attachment A

ADD	EBSREL	AFmultCoefficient	See Attachment A	CONSTANT	0.910758	See Attachment A	See Attachment A
ADD	EBSREL	BFmultCoefficient	See Attachment A	CONSTANT	0.210994	See Attachment A	See Attachment A
ADD	EBSREL	X0FmultCoefficient	See Attachment A	NORMAL	0.45004, 2.25004	See Attachment A	See Attachment A
ADD	EBSREL	UseTimesOrSEISMOIntervals(0=Times,1=Intervals)	See Attachment A	IFLAG	1	See Attachment A	See Attachment A

ATTACHMENT A

Text of e-mail from O. Pensado to R. Rice on Dec. 5, 2005

(Not all of the points addressed here were implemented in this SCR.)

Seepage at the drift wall boundary

1. Define fmult as a function of deep percolation

From R. Fedors:

$$fmult = \frac{a}{1 + \exp\left(-\frac{\ln Q - x_o}{b}\right)} \qquad [1]$$

where Q is the percolation flux leading up to the drift ceiling, in mm/yr. The coefficients are

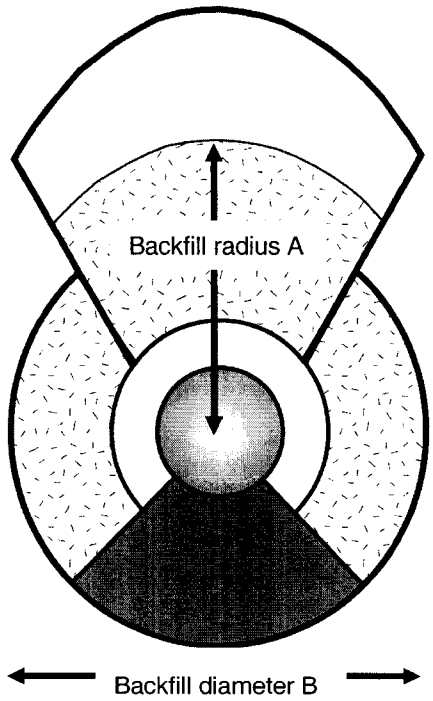
	mean	standard deviation
a	0.910758	0.021
b	0.210994	0.024
x_o	1.35004	0.30

I propose fixing a and b at the mean values and sampling x_o from a normal distribution. The quantity Q will be computed as

$$Q = \frac{1000\,\mathrm{mm/m} \times q_1 \times Fow}{\mathrm{WPlength} \times \mathrm{WPwidth}} \qquad [2]$$

where q_1 is the output of the reflux 3 module (m^3/yr per waste package in a specific subarea).

Drift degraded scenario



Equation [1] is valid for an open drift. In case of drift degradation, we will define

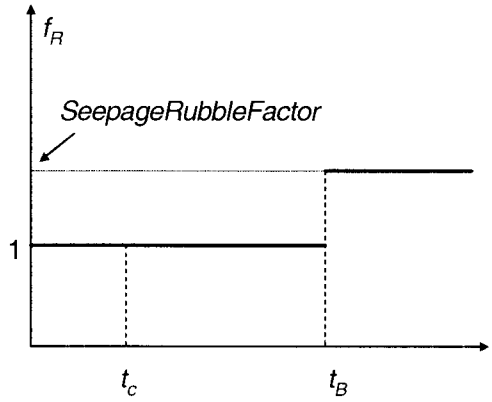
$$fmult = \begin{cases} \dfrac{a}{1+\exp\left(-\dfrac{\ln Q - x_o}{b}\right)} & \text{if } t < t_B \\ 1 \text{ otherwise} \end{cases} \qquad [4]$$

where

t_B = initial time at which the backfill diameter B equals the initial drift diameter

It is assumed that at times later than t_B, the drift wall is very irregular and is less efficient to divert deep percolation.

A new dimensionless parameter will be introduced named *SeepageRubbleFactor*. A factor f_R will be computed as indicated in the following plot



The factor f_R will multiply the *fmult* factor inside the releaset module. The parameter *SeepageRubbleFactor* will be defined by the user and could have any value. If less than one, rubble will preferentially divert seepage. If greater than one, rubble and drift wall distortion will capture additional seepage. In the basecase we will define *SeepageRubbleFactor* = 1, until technical bases are provided for a different selection.

Special Cases
Engineered backfill scenario? Do we need a separate parameter for engineered backfill?

$$f_R = SeepageEngineeringBackfillFactor$$

We will use that factor throughout the simulation if EmplacementBackfillThickness[m] is greater than 0. By design, the mechfail computations of drift and mechanical degradation are bypassed if EmplacementBackfillThickness[m] > 0.

There is no need to consider the case where drift degradation happens on top of the engineered backfill (this case is not considered in the TPA code).

Note for programmers:
The drift diameters A and B are tracked in the file *eqvdia.rlt*, which is only generated if the appropriate flag is activated. Those variables are tracked by the EXEC. I propose adding a column to the *wpflow.dat*, called fR, to track the variation of the factor f_R as a function of time.

DIVERSION BY PARTIALLY DEGRADED DRIP SHIELDS AND WASTE PACKAGES

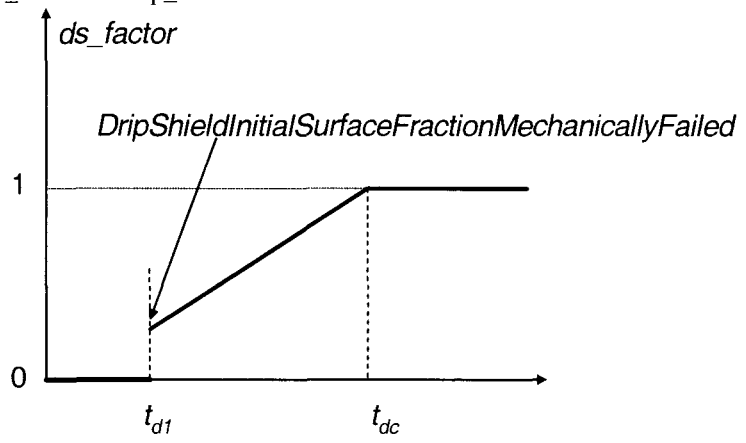
Line 839 in releaset.f (**old approach**):

```
      qin(i) = (floref(i)*flowfactr) * ctfmult(i) * ctfow(i) *
&        ds_factor * weld_wp_factor
```

New approach

```
      qin(i) = (floref(i)*flowfactr) * ctfmult(i) * ctfow(i) *
&        ds_factor(i) * wp_factor(i) * weld_wp_factor
```

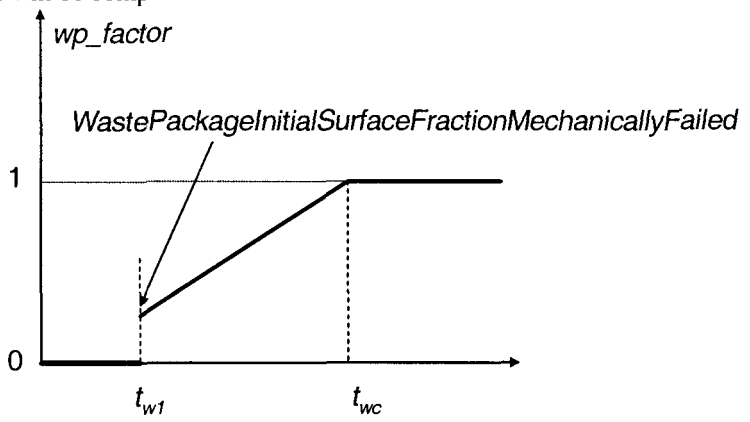
We will compute the ds_factor and wp_factor as follows



where

DripShieldInitialSurfaceFractionMechanicallyFailed user defined in *tpa.inp*
t_{d1} earliest drip shield failure time computed by MECHFAIL
t_{dc} drip shield corrosion failure time computed by DSFAIL

Analogously, wp_factor will be computed as



where

WastePackageInitialSurfaceFractionMechanicallyFailed user defined in *tpa.inp*

t_{w1} earliest waste package failure time computed by MECHFAIL

t_{wc} waste package corrosion failure time computed by FAILT

The earliest waste package failure time is defined by the input parameter

BeginningOfSEISMOWPFailureInterval1[yr]

Special cases

What if no corrosion failure happens within the simulation time?

We can select a reference time; for example, if no corrosion failure happens during the simulation time

$t_{dc} = 10^5$ years

$t_{wc} = 10^6$ years

Should the user define those times?

Initial defects?

For initially defective waste packages, we can define

wp_factor(i) * weld_wp_factor = 1.0

ADDITIONAL NOTES

Drip shields and waste packages fail as a function of time due to mechanical interactions. The fraction of failed drip shields and waste packages in a subarea are computed within the EXEC in the following block:

```
  call mechdriver( ntim, maxntime, tim(1), numberofseismicevents,
 &  timeofseismicevents(1), typeofseismicevents(1),
 &  ds_thickness(1), ds_failure_time(isa), nsa, isa,
 &  seismicfailwpsubarea(1, isa),
 &  seismicfaildssubarea(1, isa), seismicfaildriftsubarea(1, isa),
 &  seismicdsbucklingsubarea(1, isa),
 &  seismicdsplatesubarea(1, isa),
 &  seismicdsbulkheadsubarea(1, isa),
 &  seismicwptopsubarea(1, isa),
 &  seismicwpbottomsubarea(1, isa),
 &  seismicsccctopsubarea(1, isa),
 &  seismicsccbottomsubarea(1, isa), indicator_corrosion,
```

```
&   seismicdriftheightsubarea(1, isa))
```

The variables seismicfailwpsubarea(1, isa) and seismicfaildssubarea(1, isa) represent the fraction of WPs and DSs failed as a function of time. The variable seismicfailwpsubarea is also used by the cumfail procedure inside the EXEC:

```
    call cumfail( isa, ntim, tim(1),
&           corrosionfailwp(1), seismicfailwpsubarea(1, isa),
&           faultfailwp(1,isa), volcanicfailwp(1,isa),
&           cumfailwp(1), ntotalfailed,
&           numdisruptiveevents, wpsfailedtime,
&           releasewpfailedtime )
```

The cumfail procedure is used to count the number of waste packages failed by the various mechanisms in a subarea. For the seismic-drift degradation related waste package failure, the number of waste packages failed are encapsulated in a small number of simulation periods. The reason is that RELEASET is executed independently for each period. Total releases are scaled by the total number of waste packages failed in that period. The periods are defined in the following block in *tpa.inp*:

```
iconstant
NumberOfSEISMOWPFailureIntervals
4
**
constant
BeginningOfSEISMOWPFailureInterval1[yr]
0.0
**
constant
BeginningOfSEISMOWPFailureInterval2[yr]
2000.0
**
constant
BeginningOfSEISMOWPFailureInterval3[yr]
5000.0
**
constant
BeginningOfSEISMOWPFailureInterval4[yr]
10000.0
```

For long-term simulations, we need to redefine those periods.

It is not clear what BeginningOfSEISMOWPFailureInterval1[yr]=0 means. Does 0 mean time of closure?

ATTACHMENT B

Slides of PowerPoint presentation by O. Pensado on Jan. 11, 2006

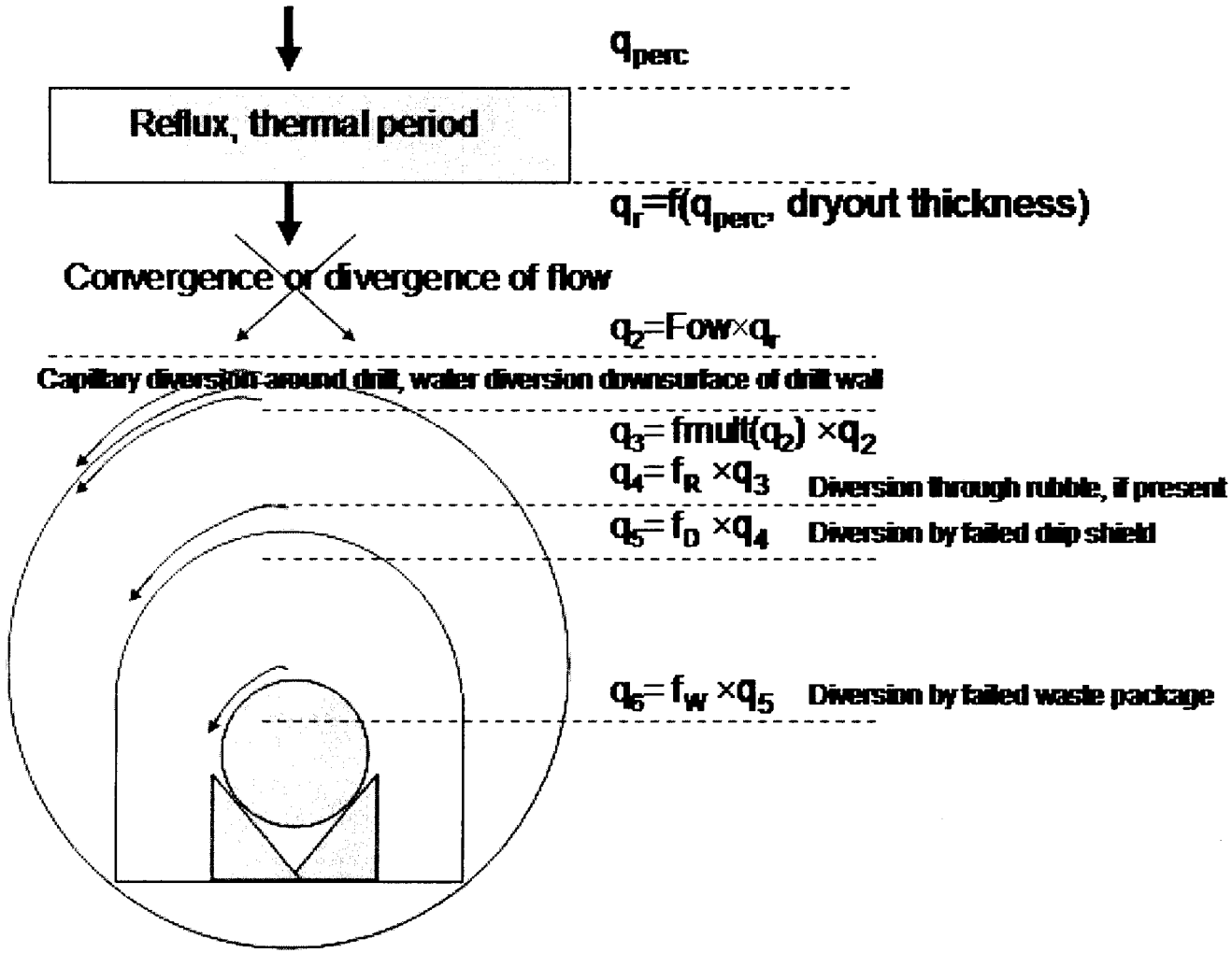
(Not all of the points addressed here were implemented in this SCR.)

Integration of seepage abstraction with drift and mechanical degradation

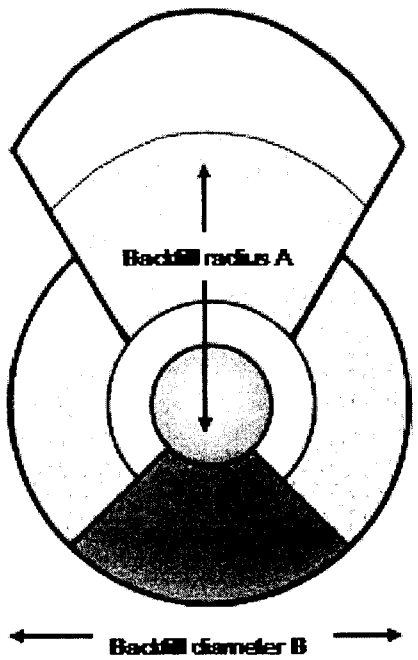
Contributors: O. Pensado, R. Fedors, R. Codell, K. Compton, R. Rice, S. Stothoff, C. Manepally

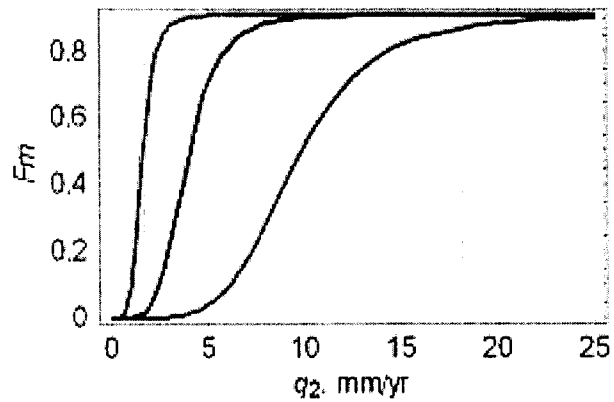
January 11, 2006

Seepage Abstraction



$fmult(q_2)$





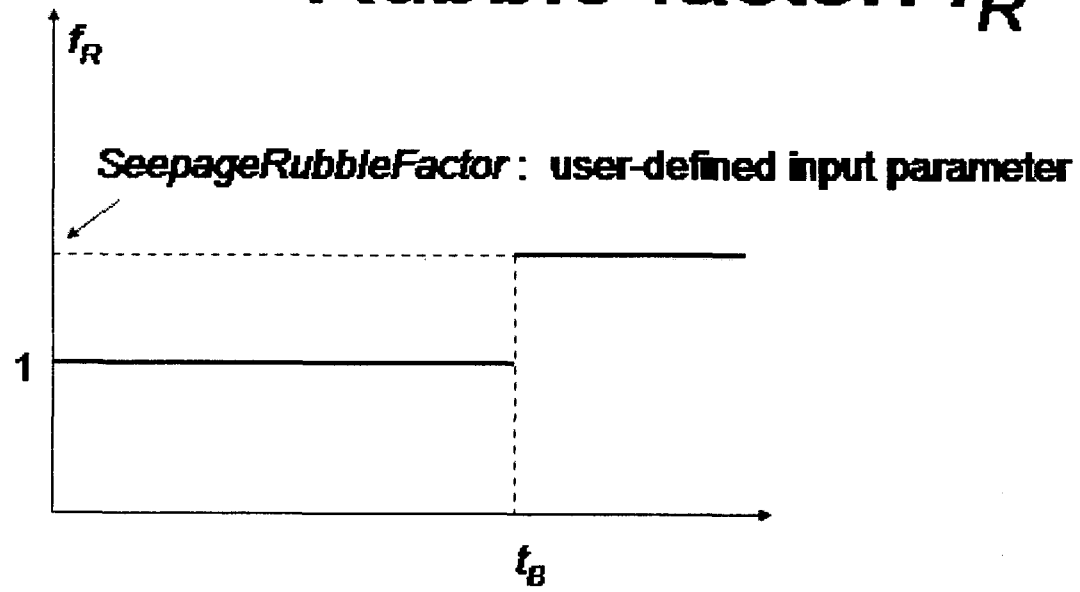
$$fmult = \begin{cases} Fm \text{ if } t < t_B \\ 1 \text{ otherwise} \end{cases}$$

t_B : time at which the backfill diameter B equals the initial drift diameter

The implicit assumption is that for times > t_B, enough asperities have accumulated on the drift wall, making it an inefficient barrier against seepage.

NOTES: WastePackageMultiplicationFlowFactor = 1. Need to update previous range provided by K. Compton. Now, all the uncertainty is carried in the function Fm.

Rubble factor: f_R

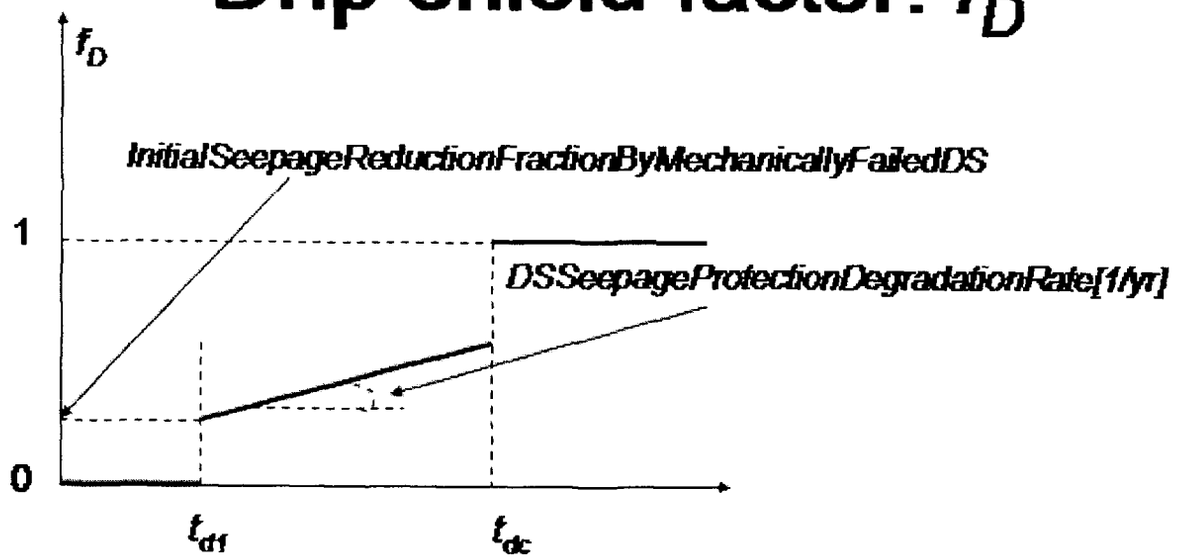


t_B : time at which the backfill diameter B equals the initial drift diameter. Distribution function for SeepageRubbleFactor will be based on empirical data to be gathered.

Special cases: engineered backfill

f_R = *SeepageEngineeringBackfillFactor* : user-defined input parameter. Activated at the time of closure.

Drip shield factor: f_D



t_{df} : earliest drip shield failure time computed by MECHFAIL

t_{dc}: corrosion failure time

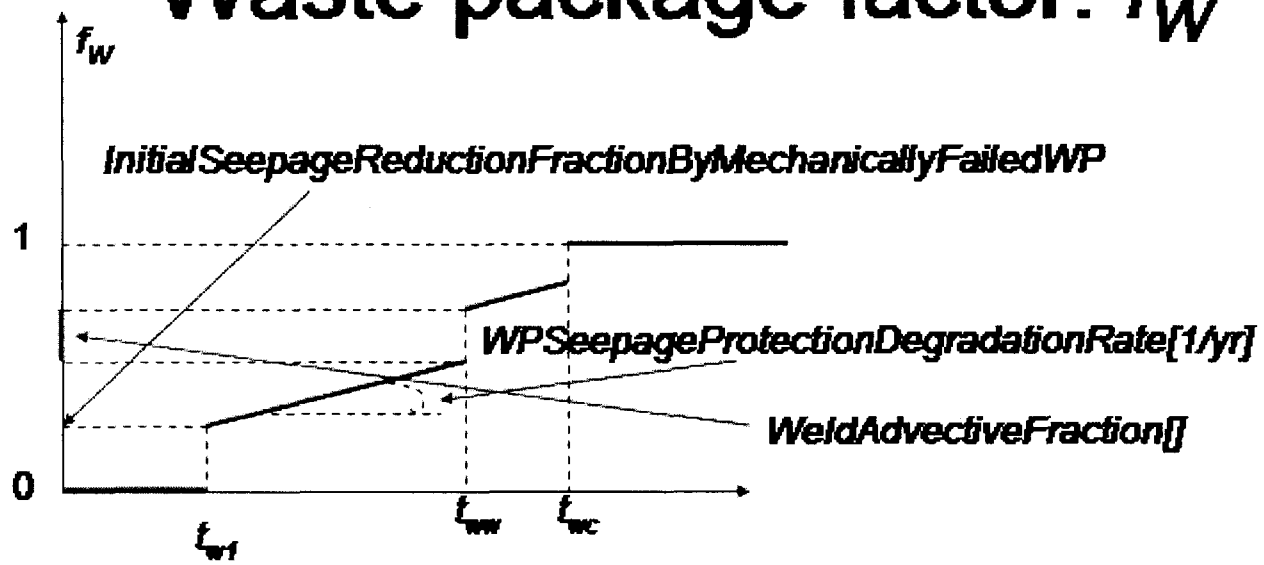
G. Adams suggested to link *InitialSeepageReductionFractionByMechanicallyFailedDS* to the fraction of drip shields located in the litophysal and non-litophysal rock units. I disagree with that proposal because the TPA code tracks seepage per wet WP. The representative DS is independent of the number of failed DSs.

Drip shield factor: f_D

- How do we define *InitialSeepageReductionFractionByMechanicallyFailedDS* and *DSSeepageProtectionDegradationRate[1/yr]*?
  - There is agreement that those factors are very uncertain. Developing solid technical bases to support defined values may not be possible.
- We will add a flag to either assign partial protection against seepage by mechanically failed drip shield or not. Removing protection can be easily implemented by defining *InitialSeepageReductionFractionByMechanicallyFailedDS* = 1. We need to add a flag to automatically adjust this value when the flag is activated.
- Flag name:
  FlagPartialProtectionAgainstSeepageByMechanicallyFailedDS[1=yes,0=no]

6

Waste package factor: f_W



t_{w1} : earliest waste package failure time computed by MECHFAIL

t_{ww}: weld failure time by corrosion

t_{wc}: general corrosion failure time (waste package body)

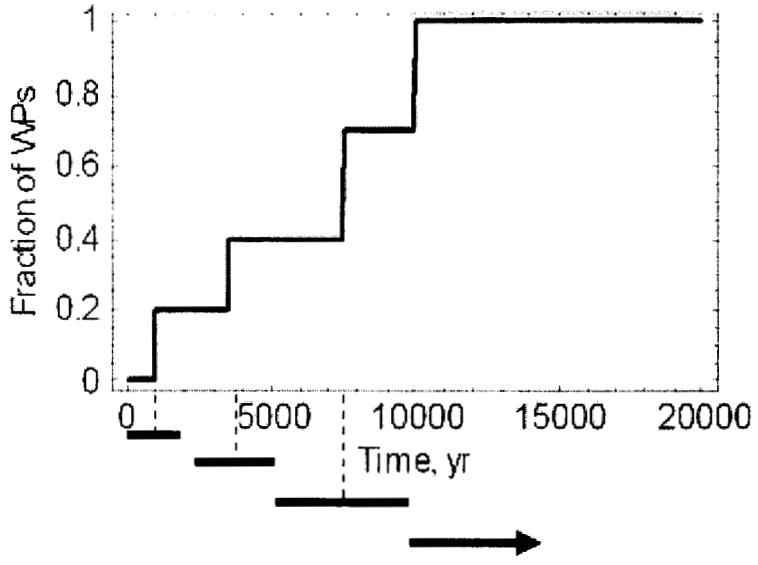
Special cases: Initially defective waste packages. In this case, $f_w = 1$ at the time of closure.

7

Waste package factor: f_W

- As in the drip shield case, there is uncertainty in the extent of the protection against seepage by a mechanically failed waste package.
- We will add a flag to assign partial protection against seepage or not
- Flag name: FlagPartialProtectionAgainstSeepageByMechanicallyFailedWP[1=yes,0=no]

Mechanical time ranges




```
iconstant
NumberOfSEISMOWPFailureIntervals
4
--
constant
BeginningOfSEISMOWPFailureInterval1[yr]
0.0
--
constant
BeginningOfSEISMOWPFailureInterval2[yr]
2000.0
--
constant
BeginningOfSEISMOWPFailureInterval3[yr]
5000.0
--
constant
BeginningOfSEISMOWPFailureInterval4[yr]
10000.0
```

We agreed that the seismic ranges lost their meaning. We will modify the TPA code to call releaset exactly at the time of mechanical failure. We may need to define another failure mode, independently of the existing seismic failure mode.

ATTACHMENT C

Text of e-mail from O. Pensado to R. Rice on Mar. 6, 2006

(The following e-mail initiated discussions on water contact mode. It was decided after discussions and e-mails that for any failure type, the water contact mode of the first failure (i.e., scenario, weld, or mechanical) would be used for that failure type. This is true for all eight failure types except initial failures which will keep the water contact mode specified in the *tpa.inp* file.)

From: Osvaldo Pensado
To: Chris Grossman, James Winterle, Bret Leslie, Timothy McCartin, Sitakanta Mohanty, Budhi Sagar, Richard Codell, Tae Ahn
Cc: 'rwrice'
Bcc:
Subject: Bathtub or flowthrough? Combined degradation processes?
Date: Mon, 06 Mar 2006 16:39:58 -0600

Fellows,

An issue was brought today to my attention that relates to the flowthrough and bathtub models in the TPA code.

In the long-term simulations, we may want to apply multiple processes before the disruptive processes. For example, we may want to allow drift degradation and corrosion to happen before an igneous or faulting event.

In the current TPA, WPs that are failed by a disruptive event are not touched by corrosion. We may want to move away from that.

According to Rob Rice, implementing such a change in the releaset module is not too difficult.

Under the new implementation, say you select "initial defects" happen at time 500,000 years. Under the new approach, mechanical and corrosion degradation of the WP would happen as usual, and then at time 500,000 years, the initial defects would kick in. Under the existing TPA, the WPs that will show defects at time 500,000 years do not experience any degradation mechanism before that time.

The only small problem in the implementation is the bathtub or flowthrough models, because these models are married to the failure type. Thus, for example, the default wetting mode for corrosion is bathtub, while for faulting is flowthrough. If the faulting event happens at time 500,000 years, after failure by corrosion, the WPs that were predestined to fail by faulting, but yet failed by corrosion, would have flowthrough as the contact mode.

To move away from that problem, I propose selecting flowthrough as the default failure mode for all of the failure types.

Now, with the higher seepage rates, there is minor difference between flowthrough and bathtub (bathtub fill times are of the order of few hundreds of years).

I would like to gather feedback on (i) whether you agree on the implementation of the combined degradation processes (e.g., corrosion before faulting), and (ii) selecting flowthrough as the default water contact mode.

I appreciate your input.

ATTACHMENT D

Test Plan for TPA SCR 608

Test Plan Name: Seepage model integration

Tested By: Osvaldo Pensado | Date: 04/11/2006

Host Machine: TPA | Host OS: Windows Server 2003

Baseline Version: | Test Version: TPA 5.02s

Process Level (PL) Tests

PL-1. Name: Fmult equation
Path for run directory: TPA\D\Public\opensado\run\
Path for archive of results: Dakath\D:\tpa\tpa5.02s\
Environment variables:
Special input files or modifications to input files required : Mean-value input file
Special diagnostic code modifications required : NA
Program modes to be used (append flags, scenario/model switches, etc.): NA
Utility scripts needed to perform the test: NA
Utility codes needed in the analysis of the test data: NA

Objective: verify that the fmult equation is well implemented. Fmult is defined as

$$fmult = \frac{a}{1+\exp\left(-\frac{\ln Q - x_o}{b}\right)} \qquad [1]$$

with

$$Q = \frac{1000\,\mathrm{mm/m} \times q_1 \times Fow}{\mathrm{WP\ length} \times \mathrm{WP\ width}} \qquad [2]$$

where q_1 is the deep field percolation, after reflux. The quantities q_1 and Fow are available in the second and fourth columns of the output file ebsflo.dat.

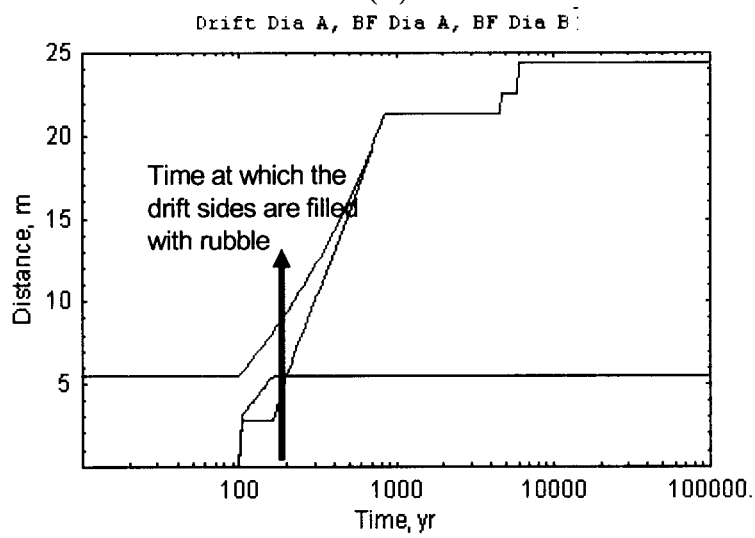
Output files: ebsflo.dat and driftfail.rlt

Procedure: A mean-value run, subarea 3 only, was completed. No additional changes to the output file were implemented. Data from ebsflo.dat were read and plotted using commercial software. To check for transition times, data from the file driftfail.rlt was checked. This run was labeled s01 (added as a prefix to the output files).

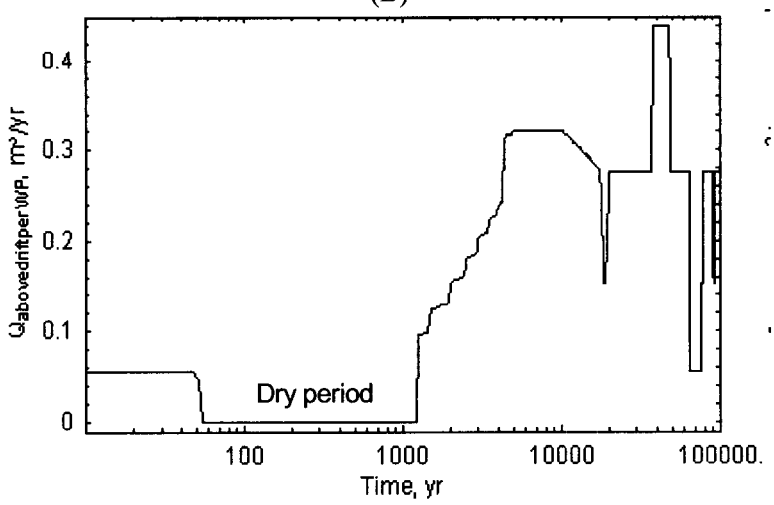
Pass criteria: A plot of fmult (third column in ebsflo.dat) versus q_1 (second column in ebsflo.dat) must produce consistent results with Eqs. [1] and [2], verified by visual inspection.

Test results:

(A)



(B)



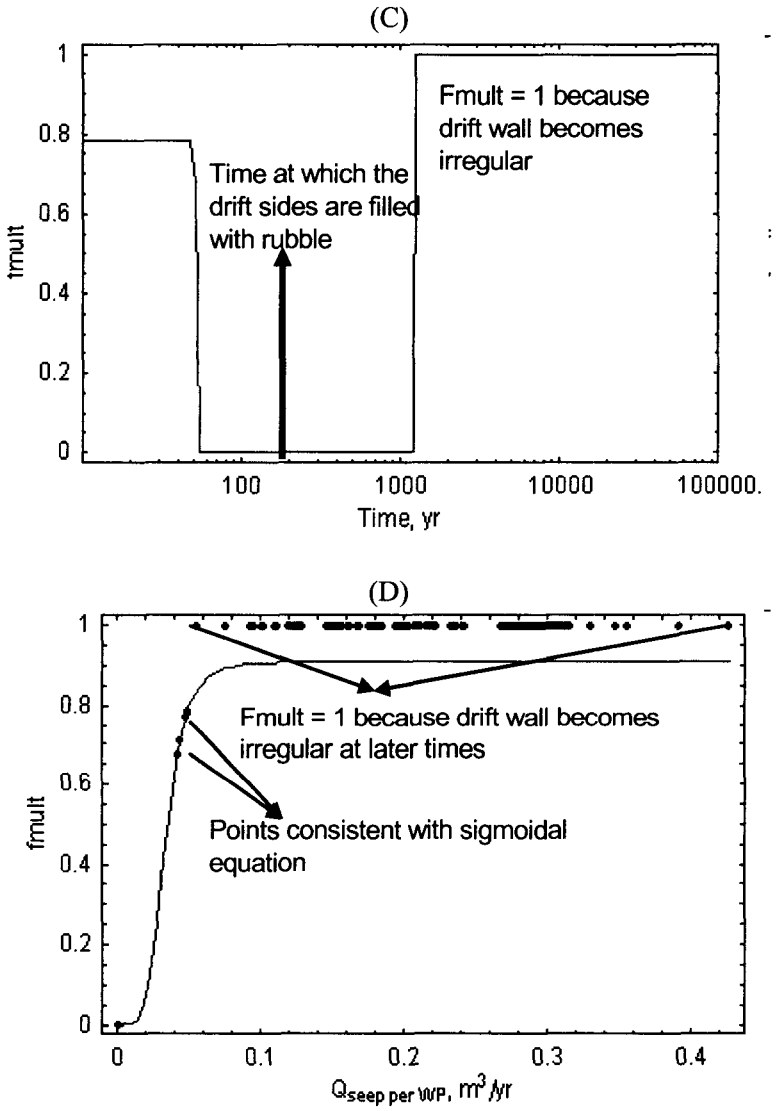


Figure 1: test s01 to verify that fmult is well computed.

Figure 1-A is a plot of data in the drift degradation file driftfail.rlt. The time at which the backfill diameter B (red line) reached the maximum value is considered the time at which the drift wall has accumulated enough irregularities so that it cannot divert water around the wall. After that time, fmult is set equal to 1. For run s01, this time is around 200 years. Figure 1-B is a plot of the deep percolation as a function of time. Rewetting occurs past 1,000 years in run s01. Figure 1-C is a plot of fmult as a function of time. Prior to 200 years, fmult is computed according to Eqs. [1] and [2]. Past the rewetting time, the drift wall is assumed too degraded, and fmult is set equal to 1. Figure 1-D is a plot of fmult versus q_1 superposed to a line computed using Eqs. [1] and [2]. This plot verifies that, for times less than 200 years, fmult is computed according to Eqs. [1] and [2]. For this run s01, release of radionuclides from the engineered barrier system only happens past the rewetting time (> 1,000 years), due to initially defective WPs. Thus, the variability of fmult is irrelevant to release and dose computations, at least in this run.

Test Status : PASS

PL-2. Name: Response of factors fr, fd, fwc, and fwm1 to timing of drift degradation, waste package corrosion, and mechanical degradation.

Path for run directory: TPA\D\Public\opensado\run\
Path for archive of results: Dakath\D:\tpa\tpa5.02s\
Environment variables:
Special input files or modifications to input files required : explained in the tests
Special diagnostic code modifications required : NA
Program modes to be used (append flags, scenario/model switches, etc.): NA
Utility scripts needed to perform the test: NA
Utility codes needed in the analysis of the test data: NA

Objective: verify that the factors fr, fd, fwc, and fwm1 respond to the timing of drift degradation, waste package corrosion, and mechanical degradation.

Output files: ebsflo.dat, driftfail.rlt, ebsnef.dat, ebsrel.rlt

Procedure: The basic mean-value file was changed to force failure of the waste package by weld corrosion, localized corrosion, and mechanical degradation. Release rate versus time curves were inspected to verify that releases respond to changes in the seepage rate (controlled by the factors fr, fd, fwc, and fwm1). Inflections in the release curves must be explainable as function of the timing of the degradation processes.

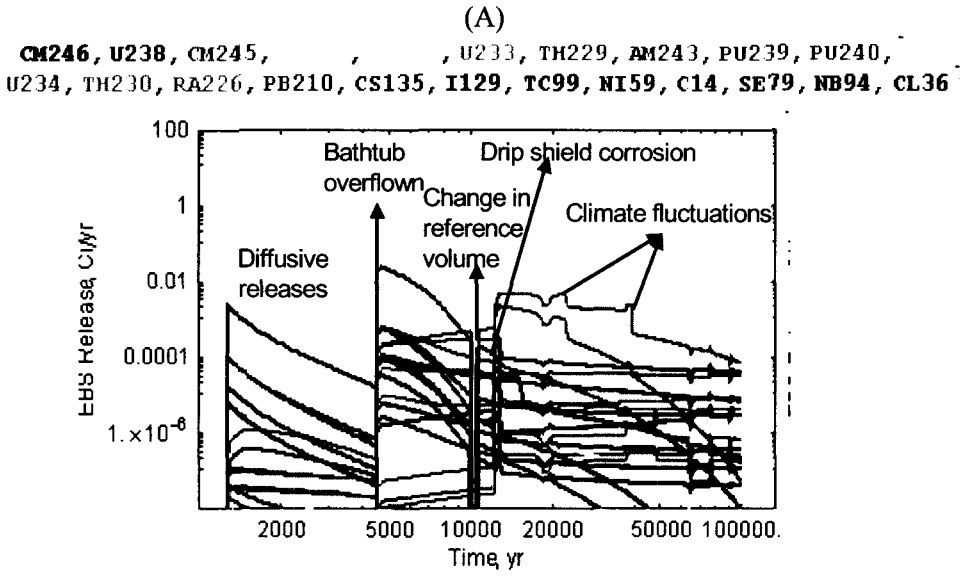
Pass criteria: Release rates must respond to changes in the seepage rates. Inflections in the release rate versus time curves must be explainable as function of the timing of the different degradation processes. No quantitative criterion was developed for this test.

Test results:

Run s03, initial defects, partial seepage protection due to rubble and a mechanically failed drip shield mean-value run, subarea 3, with the following parameter changes

SeepageRubbleFactor=0.1
InitialSeepageReductionFractionByMechFailedDS=0.01
DSSeepageProtectionDegradationRate[1/yr]=1.0E-5
InitialSeepageReductionFractionByMechFailedWP=1.0E-3
WPSeepageProtectionDegradationRate[1/yr]=1.0E-5

(A)



(B)

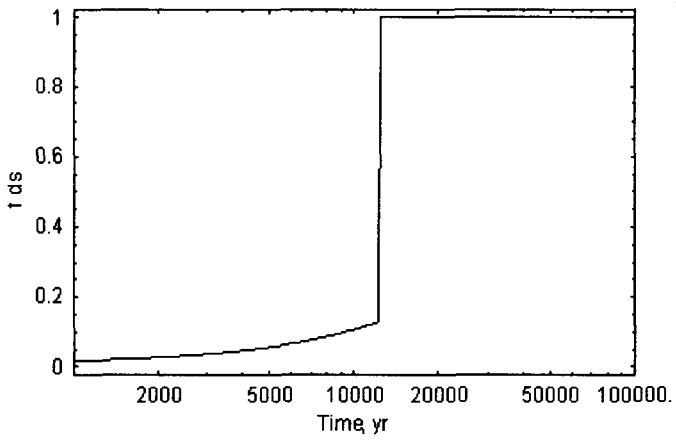


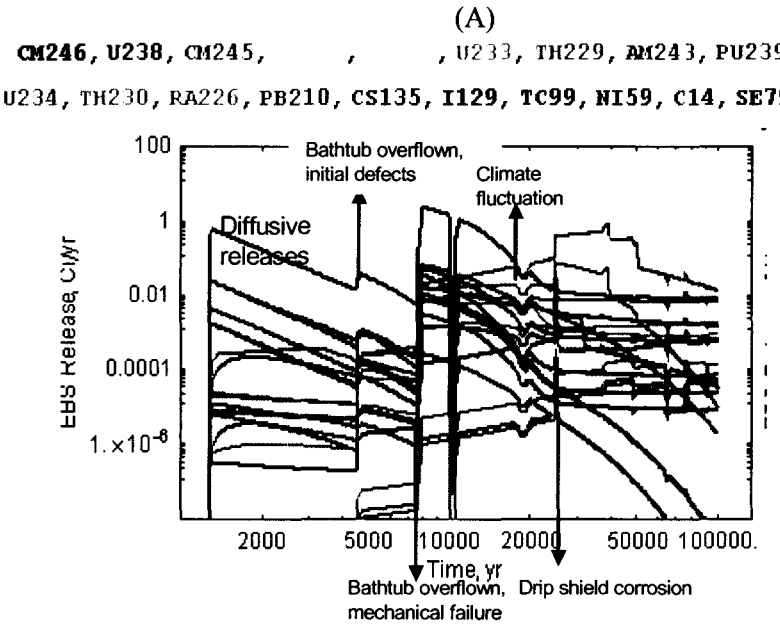
Figure 2: tests for run s03 (releases from initial defects)

All of the inflections in the release rate versus time in Figure 2-A are explainable as a function of transitions. The most notable blip occurs at 10,000 years, and it is due to the selection of a different reference volume for solubility computations, prior and after 10,000 years. For later times, a larger reference volume is selected for performance reasons. The bathtub overflown time responded to decreases in the seepage due to rubble accumulation on the drip shield and a partially protective drip shield. In this run, s03, the drip failed by corrosion at around 12,000 years, at which time the drip shield seepage factor increased to 1, as indicated in Figure 2-B. The release rate curves are consistent with intuitive trends.

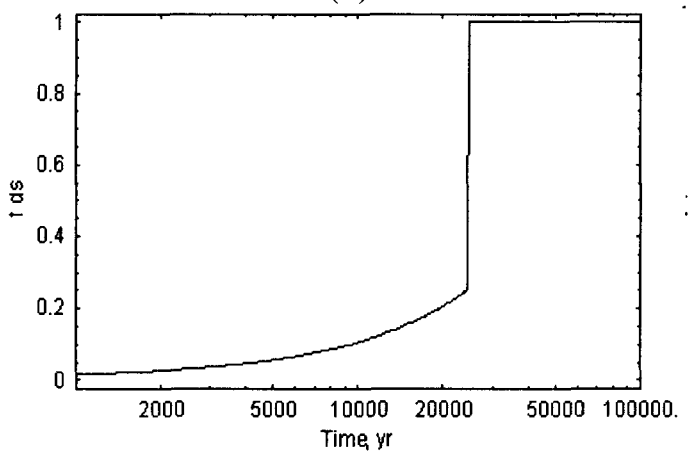
Run s04, initial defects, mechanically failed waste packages, weld corrosion
mean-value run, subarea 3, with the following parameter changes
SeepageRubbleFactor=0.1
InitialSeepageReductionFractionByMechFailedDS=0.01

DSSeepageProtectionDegradationRate[1/yr]=1.0E-5
InitialSeepageReductionFractionByMechFailedWP=1.0E-3
WPSeepageProtectionDegradationRate[1/yr]=1.0E-5
DripShieldCorrosionRate[m/yr] = 6.0E-7 (the DS corrosion rate is decreased by half, to give more time to mechanical failure)
ContactLengthSubarea_3[m]=1.0E-5 (the area is small to force failure of the WP by mechanical interaction)
EnvironmentII_NO3[mol/L] = 1.0E-3 (small nitrate to force localized corrosion)
CritChlorideConcForFirstLayer[mol/L] = 10.0 (this forbids localized corrosion of the WP body)
WeldAdvectiveFraction[] = 0.2 (the intention is making more visible the effect of weld failure on seepage)

(A)



(B)



(C)

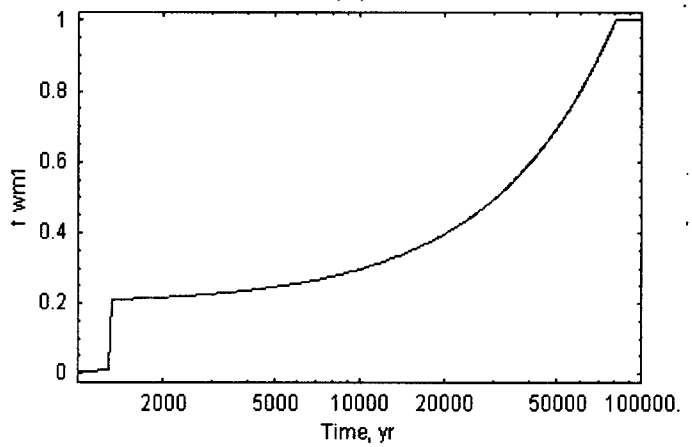


Figure 3: run s04 (initial defects, localized corrosion of the welds, mechanically failed waste packages)

All of the inflections in the release curve are explainable. In Figure 3-A, it is noted that the mechanically failed waste packages overflow after 8,000 years, later than the initially defective waste packages, because partial seepage protection for the former waste packages was assumed. Figure 3-B shows that the drip shield fails by corrosion after 20,000 years, and this coincides with an inflection point in the release curve in Figure 3-A. The seepage factor in Figure 3-C jumps to 0.2 at the time of localized corrosion penetration of the welds. This jump is not noted in the release curves because diffusive releases are assumed independent of the seepage rate. The release rate curves are consistent with intuitive trends.

Run s07, initial defects, localized corrosion of the WP (weld and body), partial seepage protection by rubble and mechanically failed drip shield

mean-value input file, subarea 3, with the following changes
SeepageRubbleFactor=0.1
InitialSeepageReductionFractionByMechFailedDS=0.01
DSSeepageProtectionDegradationRate[1/yr]=1.0E-5
InitialSeepageReductionFractionByMechFailedWP=1.0E-3
WPSeepageProtectionDegradationRate[1/yr]=1.0E-5
DripShieldCorrosionRate[m/yr] = 6.0E-7 (the DS corrosion rate is decreased by half, to give more time to mechanical failure)
EnvironmentII_NO3[mol/L] = 1.0E-3 (small nitrate to force localized corrosion)
WeldAdvectiveFraction[] = 0.2 (the intention is making more visible the effect of weld failure on seepage)
AA_1_1[C/m2/yr] = 1630.0 (low current density to force a high value of the corrosion potential)
CritChlorideConcForFirstLayer[mol/L] = 0.0 (activates localized corrosion of the WP body)

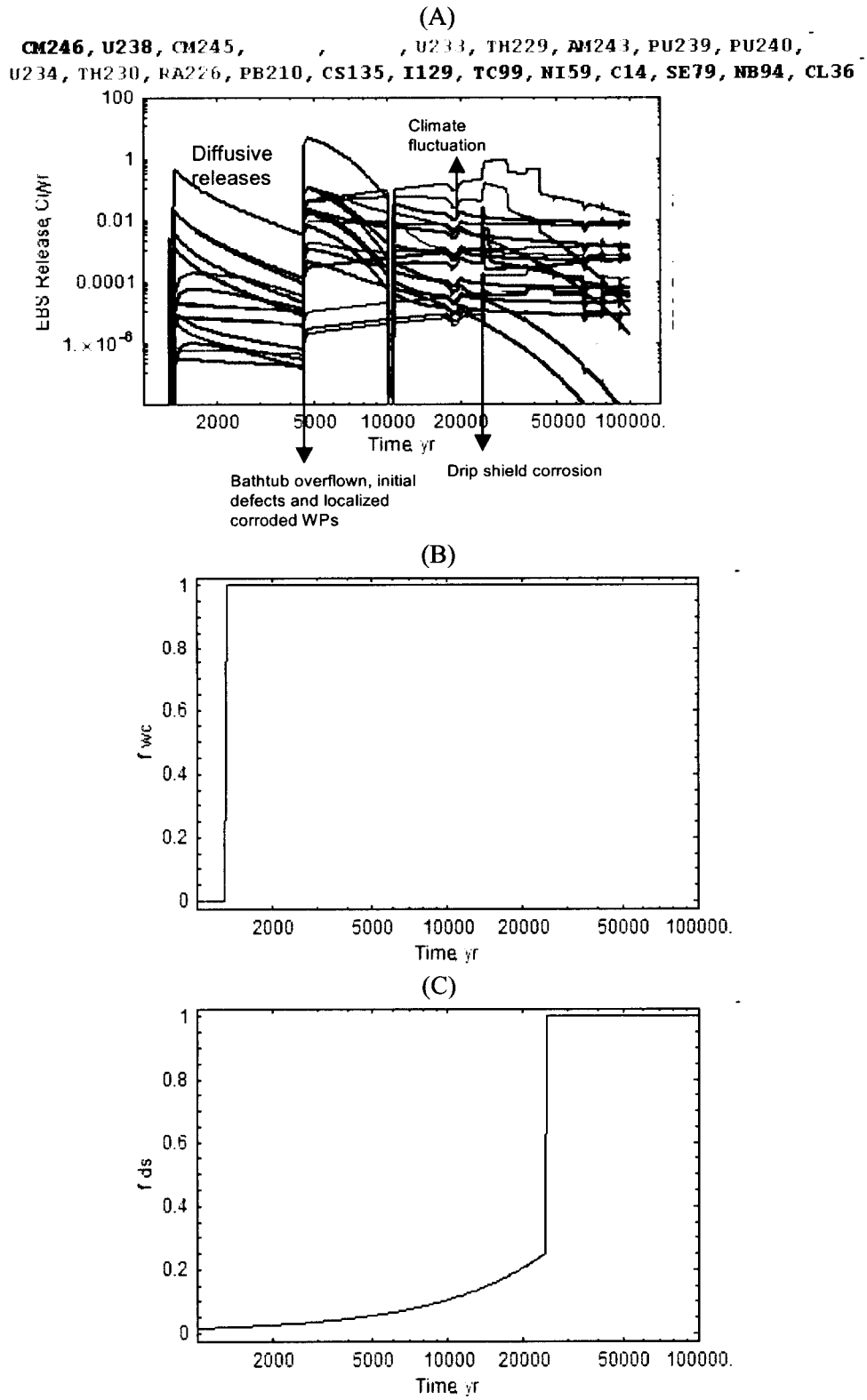


Figure 4: run s07 (initial defects, localized corrosion of the welds and waste package body)

All of the inflections in Figure 4-A are explainable. Localized corrosion occurs very early. In the conceptual design of the model, it was assumed that when corrosion of the waste package occurs, it does not offer protection against seepage anymore. Thus, the seepage factor in Figure 4-B jumps to one as soon as localized corrosion occurs. In run s07, the drip shield is fully corroded after 20,000 years, and this is consistent with the timing of the jump in Figure 4-C. To verify that the release results are reasonable, releases were compared to a run assuming 100% initially defective waste packages (DefectiveFractionOfWPs/cell = 1.0). The results of that run are displayed in Figure 5.

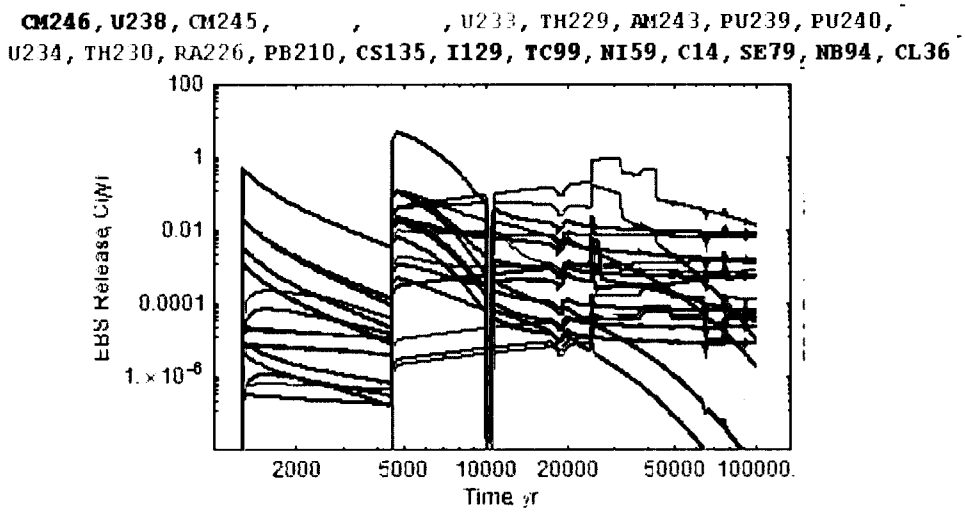


Figure 5: run s08 (100% initial defects)

The releases in Figures 5 and 4-A are clearly similar, as expected.

Test Status : PASS

PL-3. Name: Seepage protection flags

Path for run directory: TPA\D\Public\opensado\run\
Path for archive of results: Dakath\D:\tpa\tpa5.02s\
Environment variables:
Special input files or modifications to input files required : explained in the tests
Special diagnostic code modifications required : NA
Program modes to be used (append flags, scenario/model switches, etc.): NA
Utility scripts needed to perform the test: NA
Utility codes needed in the analysis of the test data: NA

Objective: verify that the flags FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no] and FlagPartialProtectionFromSeepageByMechFailedWP[1=yes,0=no] were well implemented.

Output files: ebsflo.dat, driftfail.rlt, ebsnef.dat, ebsrel.rlt

Procedure: The basic mean-value file was changed to force failure of the waste package by weld corrosion, localized corrosion, and mechanical degradation. Release rate versus time curves were inspected to verify that releases respond to changes in the seepage rate (controlled by the factors fr, fd, fwc, and fwm1). The flags were modified sequentially to verify that release rates responded to changes in the flags.

Pass criteria: Release rates must respond to changes in the seepage flags. Inflections in the release rate versus time curves must be explainable as function of the timing of the different degradation processes. No quantitative criterion was developed for this test.

Test results:

Run s06

SeepageRubbleFactor=0.1
InitialSeepageReductionFractionByMechFailedDS=0.01
DSSeepageProtectionDegradationRate[1/yr]=1.0E-5
InitialSeepageReductionFractionByMechFailedWP=1.0E-3
WPSeepageProtectionDegradationRate[1/yr]=1.0E-5
DripShieldCorrosionRate[m/yr] = 6.0E-7 (the DS corrosion rate is decreased by half, to give more time to mechanical failure)
ContactLengthSubarea_3[m]=1.0E-5 (the area is small to force failure of the WP by mechanical interaction)
EnvironmentII_NO3[mol/L] = 1.0E-3 (small nitrate to force localized corrosion)
WeldAdvectiveFraction[] = 0.2 (the intention is making more visible the effect of weld failure on seepage)
AA_1_1[C/m2/yr] = 1630.0 (low current density to force a high value of the corrosion potential)
CritChlorideConcForFirstLayer[mol/L] = 0.0 (activates LC of the WP body)

Run s06b, same as Run s06 with the following changes

FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no]=0

Run s06c, same as Run s06 with the following changes

FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no]=1
FlagPartialProtectionFromSeepageByMechFailedWP[1=yes,0=no]=0

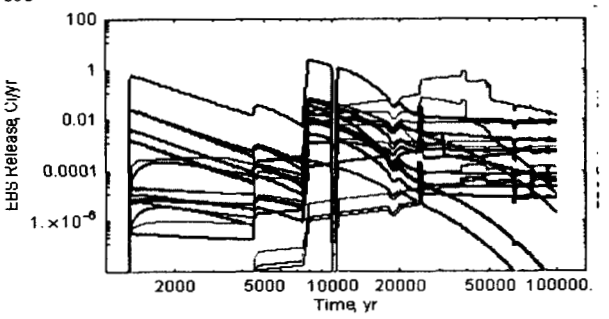
Run s06d, same as Run s06 with the following changes

FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no]=0
FlagPartialProtectionFromSeepageByMechFailedWP[1=yes,0=no]=0

Run s08b, same as Run s06 with the following changes

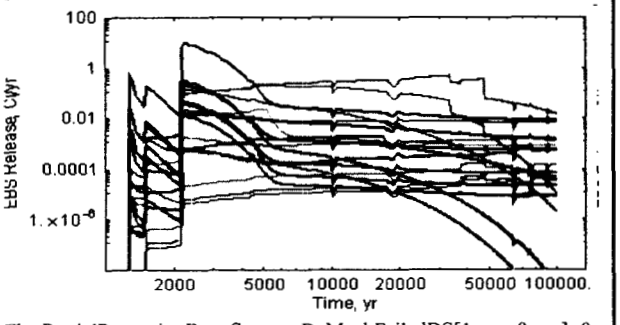
ContactLengthSubarea_3[m] = 0.5 (avoid mechanical degradation of the WP)
DefectiveFractionOfWPs/cell = 1.0
FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no] = 0

s06



Waste packages fail early due to mechanical degradation. The jump at 5,000 and 8,000 years are due to bathtub overflow in initially defective and mechanically failed waste packages, respectively.

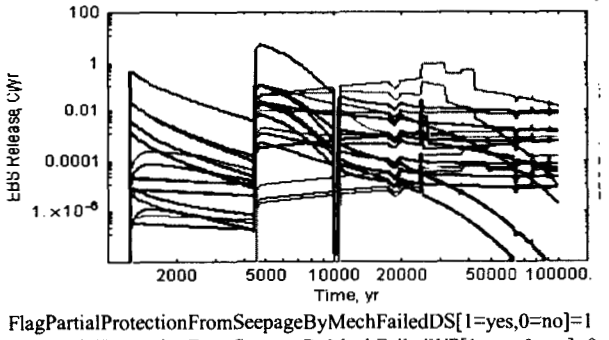
s06b



FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no]=0

There is no seepage protection by mechanically failed drip shield, but there is partial protection by a mechanically failed WP. The inflections at 1,500 and 2,000 years are due to due to bathtub overflow in initially defective and mechanically failed waste packages, respectively. The overflow times occur earlier than in run s06, due to the lack of seepage reduction by the drip shield.

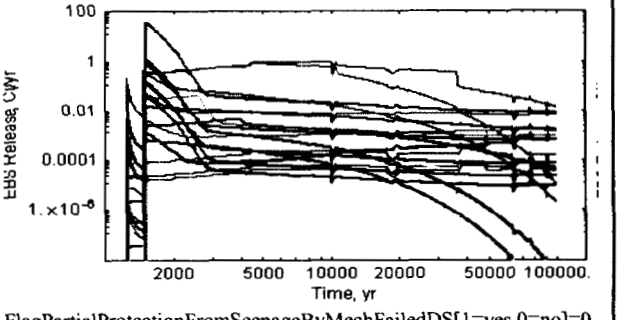
s06c



FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no]=1
FlagPartialProtectionFromSeepageByMechFailedWP[1=yes,0=no]=0

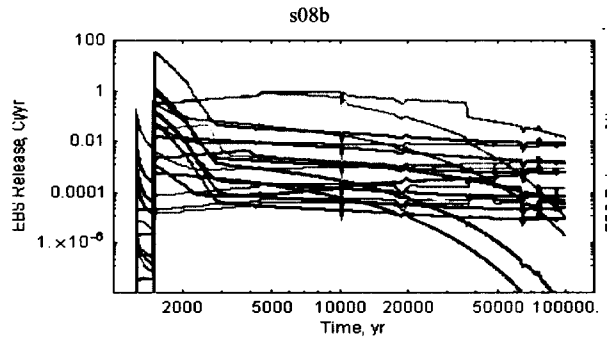
In this case, both the initially defective and the mechanicall failed waste packages overflow at the same time, at around 5,000 years. Overflow occurs at the same time because both kinds of packages experience the same amount of seepage.

s06d



FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no]=0
FlagPartialProtectionFromSeepageByMechFailedWP[1=yes,0=no]=0

In this case, both the initially defective and the mechanicall failed waste packages overflow at the same time, at around 1,500 years. Overflow occurs at the same time because both kinds of packages experience the same amount of seepage. These releases must be comparable to those derived assuming 100% of initially failed waste packages and no-seepage protection (run s08b).



FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no]=0
FlagPartialProtectionFromSeepageByMechFailedWP[1=yes,0=no]=0
DefectiveFractionOfWPs/cell = 1.0

This run was completed to compare to releases from run s06d. Indeed, both release rates are comparable, which is consistent with expectations.

Figure 6: test 3

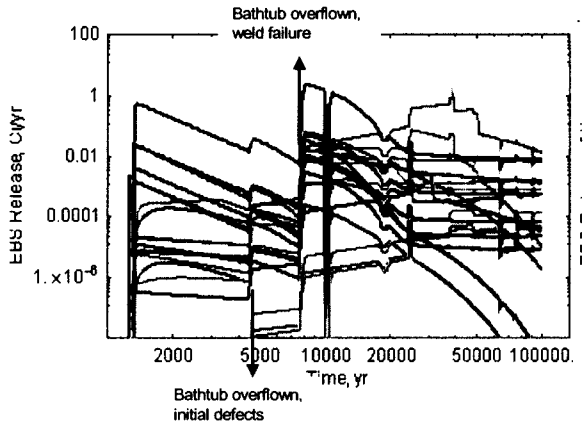
By model design, WPs failed by mechanical degradation do not experience corrosion degradation at later times, other than weld corrosion. This approach was selected as a simplification. In a regular run, general corrosion is not expected to fail WPs in one-million years. If localized corrosion occurs, it will occur in the first few thousands of years, before the onset of mechanical degradation. After the localized corrosion failure time, the model assumes no further protection against seepage by the WP, if it occurs before mechanical failure. If mechanical failure occurs first, localized corrosion of the WP body is ignored. This case will occur very infrequently in the TPA realizations, but run s06 (Figure 5-A) is a representative of this case. The seepage model needs refinement. It is proposed to consider partial protection against seepage by a localized corroded WP. It is necessary to discuss whether seepage protection should degrade as a function of time if the waste package has been affected by weld or localized corrosion. It probably may be appropriate to allow degradation only if seismic events are enabled. These recommendations are proposed as model refinement. Current model limitations are due to the model design, and are not due to an implementation error. It is recommended discuss model refinements during the beta testing period.

Test Status : PASS

PL-4. Name: Water Contact Mode
Path for run directory: TPA\D\Public\opensado\run\
Path for archive of results: Dakath\D:\tpa\tpa5.02s\
Environment variables:
Special input files or modifications to input files required : explained in the tests
Special diagnostic code modifications required : NA
Program modes to be used (append flags, scenario/model switches, etc.): NA
Utility scripts needed to perform the test: NA
Utility codes needed in the analysis of the test data: NA
Objective: verify that the appropriate water contact model is activated.
Output files: ebsflo.dat, driftfail.rlt, ebsnef.dat, ebsrel.rlt
Procedure: The basic mean-value file was changed to force failure of the waste package by weld corrosion. Volcanic (intrusive) events and faulting events were forced to occur at specific times, before and after the time of weld failure. If the event occurs before weld corrosion, flowthrough must be selected as the water contact mode (default mode for faulting and igneous). In contrast, if the event happens after weld failure, bathtub (default for corrosion) must be selected as the water contact mode.
Pass criteria: Release rate curves and the file ebsrel.rlt were inspected for consistency in the water contact mode. No quantitative criterion was developed for this test.

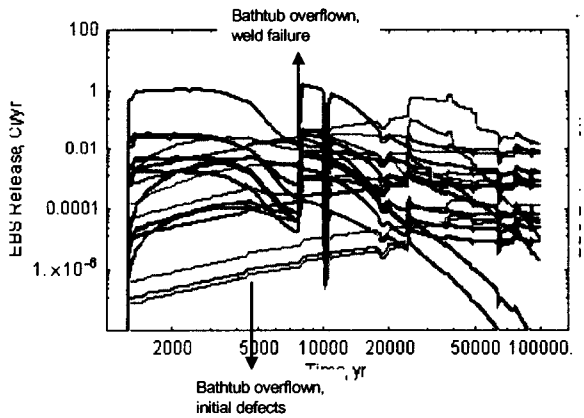
Test results:
Run s09, localized corrosion of the welds
SeepageRubbleFactor=0.1
InitialSeepageReductionFractionByMechFailedDS=0.01
DSSeepageProtectionDegradationRate[1/yr]=1.0E-5
InitialSeepageReductionFractionByMechFailedWP=1.0E-3
WPSeepageProtectionDegradationRate[1/yr]=1.0E-5
DripShieldCorrosionRate[m/yr] = 6.0E-7 (the DS corrosion rate is decreased by half, to give more time to mechanical failure)
ContactLengthSubarea_3[m]=0.5 (no mechanical failure of the WP)
EnvironmentII_NO3[mol/L] = 1.0E-3 (small nitrate to force localized corrosion)
CritChlorideConcForFirstLayer[mol/L] = 10.0 (this kills LC of the WP body)
WeldAdvectiveFraction[] = 0.2 (the intention is making more visible the effect of weld failure on seepage)
Run s09b, same as run s09 with the following changes
VolcanismDisruptiveScenarioFlag(yes=1,no=0) = 1
TimeOfNextVolcanicEventinRegionOfInterest[yr] = 1000.0
SubareaOfVolcanicEvent[] = 3
ExtrusiveEventFlag(extrusive=1,intrusive=0) = 0
Run s09c, same as run s09 with the following changes
VolcanismDisruptiveScenarioFlag(yes=1,no=0) = 1
TimeOfNextVolcanicEventinRegionOfInterest[yr] = 3000.0
SubareaOfVolcanicEvent[] = 3
ExtrusiveEventFlag(extrusive=1,intrusive=0) = 0
Run s09d, same as run s09 with the following changes
FaultingDisruptiveScenarioFlag(yes=1,no=0) = 1
TimeOfNextFaultingEventinRegionOfInterest[yr] = 1000.0
Run s09e, same as run s09 with the following changes
FaultingDisruptiveScenarioFlag(yes=1,no=0) = 1
TimeOfNextFaultingEventinRegionOfInterest[yr] = 3000.0

Run s09



Releases come from initial defects and weld corrosion failure. Time of weld failure = 1,300 years.

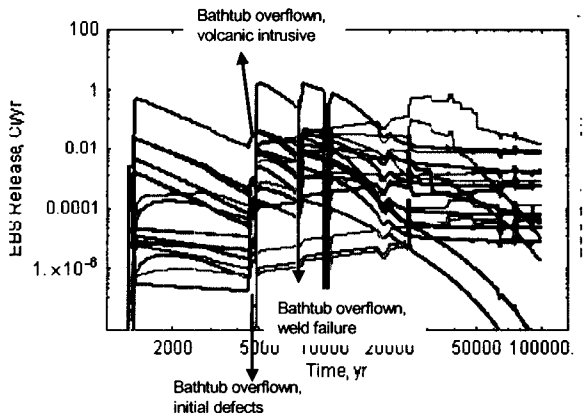
Run s09b



TimeOfNextVolcanicEventinRegionOfInterest[yr] = 1000.0

Because the event happens at 1,000 years, and the default water contact model for volcanic intrusion is flowthrough, releases occur immediately after rewetting. The volcanic event only fails a fraction of the waste packages (33%). The other waste packages fail on the welds at 1,300 years.

Run s09c



TimeOfNextVolcanicEventinRegionOfInteres t[yr] = 3000.0

Since the volcanic event happens at 3,000 years, and weld failure occurs at 1,300 years, the activated water contact mode for the waste packages failed by the igneous event is bathtub (default water contact mode for corrosion). The other waste packages, affected exclusively by weld corrosion, produce identical releases as the corresponding ones in run s09b.

Figure 6: test 4.

Runs s09d and s09e (faulting test) produced practically identical release rates as run s09. This is because only one waste package was computed to fail due to faulting, which releases are shadowed by the initial defects and the weld corrosion. However, the files s09d_ebsrel.rlt and s09e_ebsrel.rlt show that the appropriate water contact mode was selected. A portion of those files is reproduced as follows:

run s09d (TimeOfNextFaultingEventinRegionOfInterest[yr] = 1000.0)

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	11	1.2500E+03	3.3253E+03	1.2815E+03	4.6068E+03
2	1	1.2500E+03	0.0000E+00	1.2815E+03	**1.2815E+03 FTHROUGH**
3	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2078	1.3156E+03	6.5668E+03	1.3469E+03	7.9137E+03

run s09e (TimeOfNextFaultingEventinRegionOfInterest[yr] = 3000.0)

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	11	1.2500E+03	3.3253E+03	1.2815E+03	4.6068E+03
2	1	1.3156E+03	3.5982E+03	1.3469E+03	**4.9451E+03 BATH**
3	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.2500E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2078	1.3156E+03	6.5668E+03	1.3469E+03	7.9137E+03

The type 2 corresponds to faulting. In both cases, 1 waste package failed. In run s09d, flowthrough (default for faulting) was activated because the faulting event occurred before weld corrosion. In run s09e, bathtub (default for corrosion) was activated because weld corrosion occurred before the faulting event.

Based on these test results, it is concluded that the water contact mode is selected according to the model specification.

Test Status : PASS

OVERALL TEST STATUS (PASS/FAIL): PASS

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 609	**2. Software Title and Version:** TPA 5.0.2s	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): (See list, 'Affected Software Modules/Files' attached)

The current TPA abstraction of mechanical waste package failures is based on drip-shield design features that have since been superceded and further interaction analysis. Therefore, the abstraction for drip shield mechanical failure and waste package mechanical failure from interaction between the drip shield and waste package needs to be updated to reflect the current design information and abstraction described by :Drip Shield-Waste Package Mechanical Interaction prepared by L.Ibarra, G. Ofoegbu, R.Kazban, F. Ferrante and A. Chowdhury at CNWRA, January 2006

5. Change Requested by: L. Ibarra Date: 2-15-2006	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 2-15-2006

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Replaced the existing mechanical failure abstraction with a new abstraction. Drift failure was separated out and included in a DRIFTFAIL module implemented under SCR610. Mechanical failure of the drip shield and waste package were implemented in the new MECHFAIL module implemented under this SCR. Specific changes are included in 'Description of Change(s) or Problem Resolution' attached.

8. Implemented by: G. Adams	**Date:** 3-15-2006

9. Description of Acceptance Tests:

See Attachments A and B

10. Tested by: J. Mangillas	**Date:** 4-13-2006

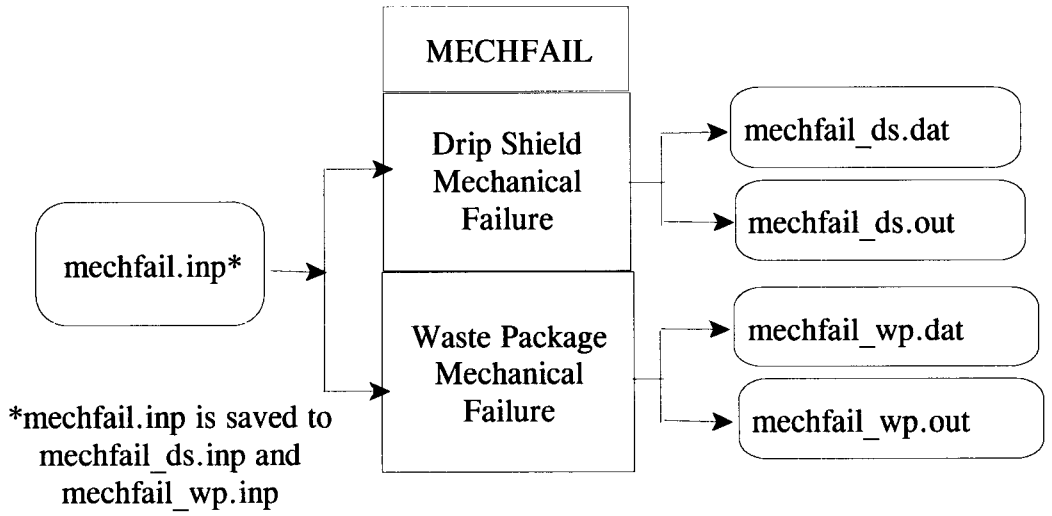
CNWRA Form TOP-5 (05/2000)

Affected Software Modules/Files

ashplumo.f
cumfail.h
ebsfail.def
ebsfail.f
ebsfail.h
ebsrel.f
exec.f
execa.i
failt.f
fileunit.f
fileutil.f
getdsfailure.h (remove)
getdsfailure.t (remove)
mechadj.i (remove)
mechdrive.f (add)
mechfail.f
putfailwp.h
releaset.f
sampler.f
seismo2.f (remove)
tpa.inp
wpsfail.res

Description of Change(s) or Problem Resolution

The mechanical failure abstraction was implemented as a standalone code module contained in files mechfail.f/mechfail.exe. The module is invoked twice per subarea by the tpa executive. When the module is first invoked, it is used to generate the fraction of drip shields that fail versus time. When it is invoked the second time, it is used to generate the fraction of waste packages that fail versus time. This information is included in files mechfail_ds.dat for drip shield failures and mechfail_wp.dat for waste package failures. A diagram of the standalone mechanical failure module is shown below.



The MECHFAIL driver is contained in file mechdrive.f and is used to interface the MECHFAIL module to the tpa code. The driver creates the mechfail.inp file from either mechfail_ds.def or mechfail_wp.def and saves the input file to either mechfail_ds.inp or mechfail_wp.inp. Within the ".def" files is a debug flag defined as: `:Debug flag (1=debug, 0=no debug)`. If the debug flag is set to 1, then the files mechfail_ds.out and mechfail_wp.out are created. The driver obtains drip shield failure versus time information from mechfail_ds.dat and waste package failure versus time information from mechfail_wp.dat. The failure data is passed back to the executive through the driver's parameter list.

As part of the changes for the MECHFAIL module, the waste package corrosion failure module (EBSFAIL/FAILT) had to be moved and modified. The waste package corrosion module was modified to generate waste package outer layer thickness versus time. This module was moved to execute prior to the second call to MECHFAIL so that waste package outer layer thickness could be supplied to the MECHFAIL module.

A partial list showing the tpa code module execution order is as follows:

DRIFTFAIL –> NFENVFL –> DSFAIL –> MECHFAIL (Drip Shield) –> NFENV –> EBSFAIL –>MECHFAIL (Waste Package)

UPDATE REQUIREMENTS for TPA.INP

SCR 609

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
Modify	sampler	SeismicHazardCurveforSEISMO	Parameters used to estimate the mean annual probability of exceedence. From the sampled values, the peak ground velocity, peak ground acceleration, and compaction factor are also determined.	hazardcurve	5 4.0 10000 5.0 100000 6.0 1000000 7.0 10000000 8.0 100000000		

Modify from ContactAngle[degrees] to ContactAngleSubarea_1[degrees]	MECHFAIL	ContactAngleSubarea_1{2..10}[degrees]	Angle between the drip shield components (bulkhead and longitudinal stiffners) and the waste package outer shell	normal	-30.8, 30.8	Ibarra,L., T. Wilt, G. Ofoegbu, R. Kazban, F. Ferrante, and A. Chowdhury. "Drip Shield - Waste Package Mechanical Interaction"	
Add	MECHFAIL	ContactLengthSubarea_1{2..10}[m]	Parameter used to obtain an equivalent pressure from the plane strain model	normal	0.192, 0.808	same	
Add	MECHFAIL	DripShieldBulkheadTributaryArea[m^2]	Parameter used to obtain the waste package outer shell vertical load carrying capacity. It is the tributary area to the drip shield bulkhead.	constant	2.3	same	
Add	MECHFAIL	DripShieldHorizToVertLoadRatioRock1{2}Subarea_1{2..10}	Parameter used to estimate the drip shield vertical load carrying	beta	0.0, 1.0, 9.8306	same	

Add	MECHFAIL	DripShieldCreepThreshold[]	Parameter used to estimate the drip shield creeping multiplier. It is the creeping threshold (with respect to the yielding stress) for creeping failure of the drip shield.	uniform	0.9, 1.2	same	
Add	MECHFAIL	DynamicAmplificationFactor[]	Parameter used to estimate the increase in vertical pressure on the drip shield or waste package during a seismic event.	constant	1.0	same	
Delete		DeflectionDepth[m]					
Delete		BulkheadThickness[m]					
Delete		WastePackageOuterBarrierUltimateTensileStrength[MPa]					
Delete		ThicknessRockfallRubbleAboveDripShieldCrown[m]					
Delete		NumberOfBlockSizePoints[]					

Delete		DripShieldToWastePackageClearance[m]					
Delete		DripShieldCrownRadius[m]					
Delete		DripShieldPlateCreepFactor[]					
Delete		DripShieldBulkHeadCreepFactor[]					
Delete		DripShieldPlateYieldStress[MPa]					
Delete		DripShieldBulkHeadYieldStress[MPa]					
Delete		DripShieldPlateCreepCoefficient[]					
Delete		DripShieldBulkHeadCreepCoefficient[]					
Delete		DripShieldBulkHeadCreepCoefficient[]					
Delete		DripShieldPlateCreepExponent[]					
Delete		DripShieldBulkHeadCreepExponent[]					
Delete		DripShieldPlateFailureLogStrain[]					

Delete		DripShieldBulkHeadFailureLogStrain[]					
Delete		WastePackageOuterBarrierYieldStress[MPa]					
Delete		WastePackageOuterBarrierFailureLogStrain[]					
Delete		StartingBlockPointerOne_1{2..10}[]					
Delete		StartingBlockPointerTwo_1{2..10}[]					
Delete		DripShieldBucklingLoadSubarea_1{2..10}[kg/m]					

Attachment A

Test Plan for TPA SCR609

Test Plan Name: SCR609 Testing

Tested By: James Mancillas Date:

Host Machine: TPA Host OS: MS Windows XP SP2

Baseline Version: TPA5.0.2.j Test Version TPA 5.0.2.s

Process Level (PL) Tests

PL-1. Name : Evaluate source code changes and basic execution of the TPA code.

Path for run directory:
Basecase: [TPA]:Public\SCR609\run1
Testcase: [TPA]:Public\SCR609\runs1

Path for archive of results:
Testcase: SCR609\runs1

Archived to CD titled :SCR609 Testing

Environment variables:
Basecase: TPA_DATA=[TPA]:Public\SCR609\tpa502j
TPA_TEST =[TPA]:Public\SCR609\tpa502j

Testcase : TPA_DATA=[TPA]:Public\SCR609\tpa502s
TPA_TEST =[TPA]:Public\SCR609\tpa502s

Special input files or modification to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Default

Utility scripts needed to perform the test: none

Utility codes needed in the analysis of the test data: none

Test description: The drift degradation and mechanical interactions previously calculated in the stand alone module *mechfail.f* in the TPA version tpa502j are now calculated using two stand alone modules.

The first called *driftfail.f* calculates the vertical pressures resulting from drift degradation and the second is a revised *mechfail.f* module.

-Objective This test will examine the changes to the *tpa.inp* file associated with mechfail alterations and examine the changes to the *exec.f* module

-Assumptions None other than those made within the TPA code

-Constraints None

-Output files to compare or examine

-Step-by-step test procedure to be used

1) examine the tpa.inp file for parameter changes outlined by SCR609.
2) examine the exec.f for proper calling of the new *mechfail.f* and *driftfail.f* modules
3) execute a run of the testcase TPA code and examine the screen capture for the call and return from the mechfail module.

-pass fail criteria

1) The *tpa.inp* file should include the parameter changes outlined by this SCR
2) The *exec.f* module should contain an updated *driftfail.f* and *mechfail.f* calling functions.
3) A realization of the TPA code should properly occur with basecase parameter values in the *tpa.inp* file.

Test Results

-criterion 1

The following text are excerpts from the *tpa.inp* file in tpa502s which are associated with SCR609

```
**          ***>>> MECHFAIL <<<***
**
**hazardcurve
**SeismicHazardCurveforSEISMO
**6
**0.1316 1000
**0.1911 2000
**0.4257 10000
**1.0753 100000
**2.4625 1000000
**5.531  10000000
**
**rwj SCR609
hazardcurve
SeismicHazardCurveforSEISMO
5
4.0 10000
5.0 100000
6.0 1000000
7.0 10000000
8.0 100000000
**
constant
SeedForRandomNumberForSEISMO
```

```
1456789101.0
**
normal
ContactAngleSubarea_1[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_2[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_3[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_4[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_5[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_6[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_7[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_8[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_9[degrees]
-30.8, 30.8
**
normal
ContactAngleSubarea_10[degrees]
-30.8, 30.8
**
normal
ContactLengthSubarea_1[m]
0.192, 0.808
**
normal
ContactLengthSubarea_2[m]
0.192, 0.808
**
normal
ContactLengthSubarea_3[m]
0.192, 0.808
**
normal
ContactLengthSubarea_4[m]
0.192, 0.808
**
normal
ContactLengthSubarea_5[m]
0.192, 0.808
**
normal
ContactLengthSubarea_6[m]
```

The distribution of the contact angles are adjusted to account for bounded distributions in the TPA code. 30.8 is equivalent to three sigmas

The distribution of the contact lengths are adjusted to account for the bounded distributions in the TPA code. 0.808 is equivalent to three sigma values

```
0.192, 0.808
**
normal
ContactLengthSubarea_7[m]
0.192, 0.808
**
normal
ContactLengthSubarea_8[m]
0.192, 0.808
**
normal
ContactLengthSubarea_9[m]
0.192, 0.808
**
normal
ContactLengthSubarea_10[m]
0.192, 0.808
**
constant
DripShieldBulkheadTributaryArea[m^2]
2.3
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_1[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_2[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_3[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_4[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_5[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_6[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_7[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_8[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_9[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock1Subarea_10[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_1[]
```

The two shape values 9.8306 and 9.8306 produce a beta distribution with a mean = 0.5 and sig = 0.11

```
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_2[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_3[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_4[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_5[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_6[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_7[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_8[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_9[]
0.0, 1.0, 9.8306, 9.8306
**
beta
DripShieldHorizToVertLoadRatioRock2Subarea_10[]
0.0, 1.0, 9.8306, 9.8306
**
uniform
DripShieldCreepThreshold[]
0.9, 1.2
**
** GA 3-30-06; SCR609
constant
DynamicAmplificationFactor[]
1.0
```

These parameters and their values are consistent with those requested by SCR609. The Following parameters are no longer present in the *tpa.inp* file contained with tpa502s.

DeflectionDepth[m]
BulkheadThickness[m]
WastePackageOuterBarrierUltimateTensileStrength[MPa]
ThicknessRockfallRubbleAboveDripShieldCrown[m]
NumberOfBlockSizePoints[]
DripShieldToWastePackageClearance[m]
DripShieldCrownRadius[m]
DripShieldPlateCreepFactor[]
DripShieldPlateYieldStress[MPa]
DripShieldPlateCreepCoefficient[]
DripShieldBulkHeadCreepCoefficient[]

DripShieldPlateCreepExponent[]
DripShieldPlateFailureLogStrain[]
WastePackageOuterBarrierYieldStress[MPa]
WastePackageOuterBarrierFailureLogStrain[]
StartingBlockPointerOne_1{2..10}[]
StartingBlockPointerTwo_1{2..10}[]
DripShieldBucklingLoadSubarea_1{2..10}[kg/m]

These changes are presented as evidence that this SCR has been implemented properly. A file containing a file comparison of the basecase and testcase tpa versions is *SCR609\files_diff\tpa.inp_fc*

-criterion 2

The following text shows the new function call for the mechanical failure stand alone code. The calling function is named *mechdriver*.

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc

c     GADAMS SCR609 3-7-2006: Moved drip shield mechanical failure
c     code to before near field environment (chemistry)

c     Mechanical Failure Scenario - Drip Shield Mechanical Failure
      IF(iflagmechanical .EQ. 1) THEN
        print '(a)',  ' exec: calling mechdriver (drip shield)'

        call mechdriver_ds(ntim, tim(1), ds_thickness(1),
     &    tempdsiA(1), tempdsiB(1),
     &    vert_pressure1_subarea(1, isa),
     &    vert_pressure2_subarea(1, isa),
     &    vert_pressure1_seismic(1, isa),
     &    vert_pressure2_seismic(1, isa),
     &    numberofseismicevents, timeofseismicevents(1),
     &    dmape(1), pga(1), nsa, isa, ds_failure_time(isa),
     &    dmechfaildssubarea(1, isa),
     &    dmechfaildssubareacorrosion(1, isa),
     &    dmechfaildssubareastatic(1, isa),
     &    dmechfaildssubareadynamic(1, isa), indicator_corrosion,
     &    ids_static1(1), ids_static2(1), ids_dynamic1(1),
     &    ids_dynamic2(1), ids_static1_seis(1), ids_static2_seis(1),
     &    ids_dynamic1_seis(1), ids_dynamic2_seis(1))
      endif
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The following excerpt shows the stand alone call for the *driftfail.f* module. The calling function is named *driftdriver*.

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc


c       GADAMS SCR609 3-14-2006: Replaced eqvdia with driftfail
c        call eqvdia( ntim, tim(1),
c     &    numberofseismicevents, timeofseismicevents(1),
```

```
c     &    typeofseismicevents(1), nsa, isa,
c     &    equivdriftdiaAsubarea(1, isa), equivdriftdiaBsubarea(1, isa),
c     &    equivbfdiaAsubarea(1, isa), equivbfdiaBsubarea(1, isa),
c     &    driftheightsubarea(1, isa), drift_flag_one, drift_time_one,
c     &    drift_flag_two, drift_time_two)
        call driftdriver( ntim, tim(1),
     &    numberofseismicevents, timeofseismicevents(1),
     &    nsa, isa,
     &    equivdriftdiaAsubarea(1, isa), equivdriftdiaBsubarea(1, isa),
*****

***** TPA502J\exec.f
     &    equivbfdiaAsubarea(1, isa), equivbfdiaBsubarea(1, isa),
     &    driftheightsubarea(1, isa), drift_flag_one, drift_time_one,
     &    drift_flag_two, drift_time_two)
c       GADAMS SCR605 2-2-2006: End of change
***** TPA502S\EXEC.F
     &    equivbfdiaAsubarea(1, isa), equivbfdiaBsubarea(1, isa),
     &    driftheightsubarea(1, isa), driftfailsubarea(1, isa),
     &    drift_flag_one, drift_time_one,
     &    drift_flag_two, drift_time_two,
     &    vert_pressure1_subarea(1, isa),
     &    vert_pressure2_subarea(1, isa),
     &    vert_pressure1_seismic(1, isa),
     &    vert_pressure2_seismic(1, isa), pga(1), cf)
c       GADAMS SCR609 3-14-2006: End of change
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The complete comparison of the basecase and testcase exec.f modules is contained in SCR609\files_diff\exec.f_fc.

These excerpts are presented as evidence that SCR609 has implemented properly

-criterion 3

The following text is an excerpt from a screen capture of the successful execution of the testcase TPA code.

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
-----------------------------------------------------------------------
    subarea  10 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of Weld failure =     1783.2  yr
     *** No Corrosion WP Failure ***
exec: calling mechdriver (waste package)
exec: failed WPs from INITIAL   event =      6 at time =      0.0 yr
 *** failed WPs:  6   out of  1747  ***
exec: calling ebsrel
```

```
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                 Highest release rates from Sub Area 10
             Tc99     3.0058E+00 [Ci/yr/SA] at  3.076E+03 yr
             Ja241    1.9795E-01 [Ci/yr/SA] at  3.004E+03 yr
             C14      1.5409E-01 [Ci/yr/SA] at  3.076E+03 yr
             Ja243    8.2456E-02 [Ci/yr/SA] at  4.499E+03 yr
             Cs135    5.9062E-02 [Ci/yr/SA] at  7.038E+03 yr
             Np237    1.9527E-02 [Ci/yr/SA] at  3.076E+03 yr
exec: calling uzft
                      Highest release rates from UZ
             Tc99     2.1960E+00 [Ci/yr/SA] at  4.394E+03 yr
             I129     9.9518E-03 [Ci/yr/SA] at  4.394E+03 yr
             Se79     8.4020E-03 [Ci/yr/SA] at  6.113E+03 yr
             Cl36     4.6683E-03 [Ci/yr/SA] at  4.394E+03 yr
     The remaining  29   nuclide(s) have zero release
exec: calling szft
                      Highest release rates from SZ
             Tc99     2.1150E+00 [Ci/yr/SA] at  4.830E+03 yr
             I129     9.5996E-03 [Ci/yr/SA] at  4.830E+03 yr
             Se79     8.1095E-03 [Ci/yr/SA] at  7.038E+03 yr
             Cl36     4.4986E-03 [Ci/yr/SA] at  4.830E+03 yr
     The remaining  29  nuclide(s) have zero release
exec: calling dcagw
                      Highest annual dose GW pathway
             Tc99     1.1251E+01 [mrem/yr]  at  3.004E+03 yr
             I129     2.9426E+00 [mrem/yr]  at  3.903E+03 yr
             Se79     7.6619E-02 [mrem/yr]  at  5.308E+03 yr
             Cl36     5.4264E-02 [mrem/yr]  at  3.903E+03 yr
             U238     5.4263E-26 [mrem/yr]  at  1.000E+04 yr
     The remaining  17   nuclide(s) have zero release
           At end of TPI, annual dose GW pathway
             Tc99     1.7660E-01 [mrem/yr]
             I129     3.4081E-02 [mrem/yr]
             Se79     3.3671E-03 [mrem/yr]
             Cl36     5.7701E-04 [mrem/yr]
             U238     5.4263E-26 [mrem/yr]
                sum   2.1463E-01 [mrem/yr]
     The remaining  17   nuclide(s) have zero release
exec: end realizations

exec: Peak Mean Dose is 1.31570E-02 rem/yr at    3465.9 yr, based on     1
realizations.
Ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

This excerpt shows that the executive module called both the driftfail and mechfail stand alone modules were called, and that the TPA code successfully executed.
This is provided as evidence that SCR609 has been properly implemented.

The complete screen capture is in the file
SCR609\runs1\out.

-overall test status: **PASS**

System Level (SL) Tests

SL-1. Name :Test drip shield and waste package failure flags with no seismic events.

Path for run directory:
Testcase: [TPA]:Public\SCR609\mech_fail\run1

Path for archive of results:
Testcase: SCR609\mech_fail\run1

Archived to CD titled :SCR609 Testing

Environment variables:

Testcase : TPA_DATA=[TPA]:Public\SCR609\tpa502s
TPA_TEST =[TPA]:Public\SCR609\tpa502s

Special input files or modification to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Seismic flag turned off

Utility scripts needed to perform the test: none

Utility codes needed in the analysis of the test data: MS Excel

Test description: The mechfail.f module evaluates the failure status of the dripshield (DS) and waste package outer barrier (WP). The status of the DS and WP is determined by a comparison of the vertical pressure and the capacity of the DS and WP. This test evaluates if the status of the DS and WP is properly evaluated by the mechfail module under static conditions.

-Objective Determine if the status of the DS and WP is properly returned during static conditions

-Assumptions None other than those made within the TPA code

-Constraints None

-Output files to compare or examine mechfail_ds.dat, mechfail_wp.dat debug output file from mechfail module

-Step-by-step test procedure to be used

1) Perform a single subarea realization.
2) save the mechfail_ds.inp and mechfail_wp.inp files into two subdirectories
   SCR609\mech_fail\run1\DS_failure

SCR609\mech_fail\run1\WP_failure

3) Place a copy of the stand alone code mecfail.e into each of those directories.

4) The mechfail_ds.inp and mechfail_wp.inp file are then renamed mechfail.inp in their respective directories and the debug flag option is turned on.

5) The mechfail.e is then executed in each directory and the screen output is captured. The screen output is a result of the debug flag being set to on.

6) The DS and WP capacities will then be compared to MS Excel calculations.

7) The DS and WP failure status will then be compared to MS Excel status calculations for comparison.

-pass fail criteria

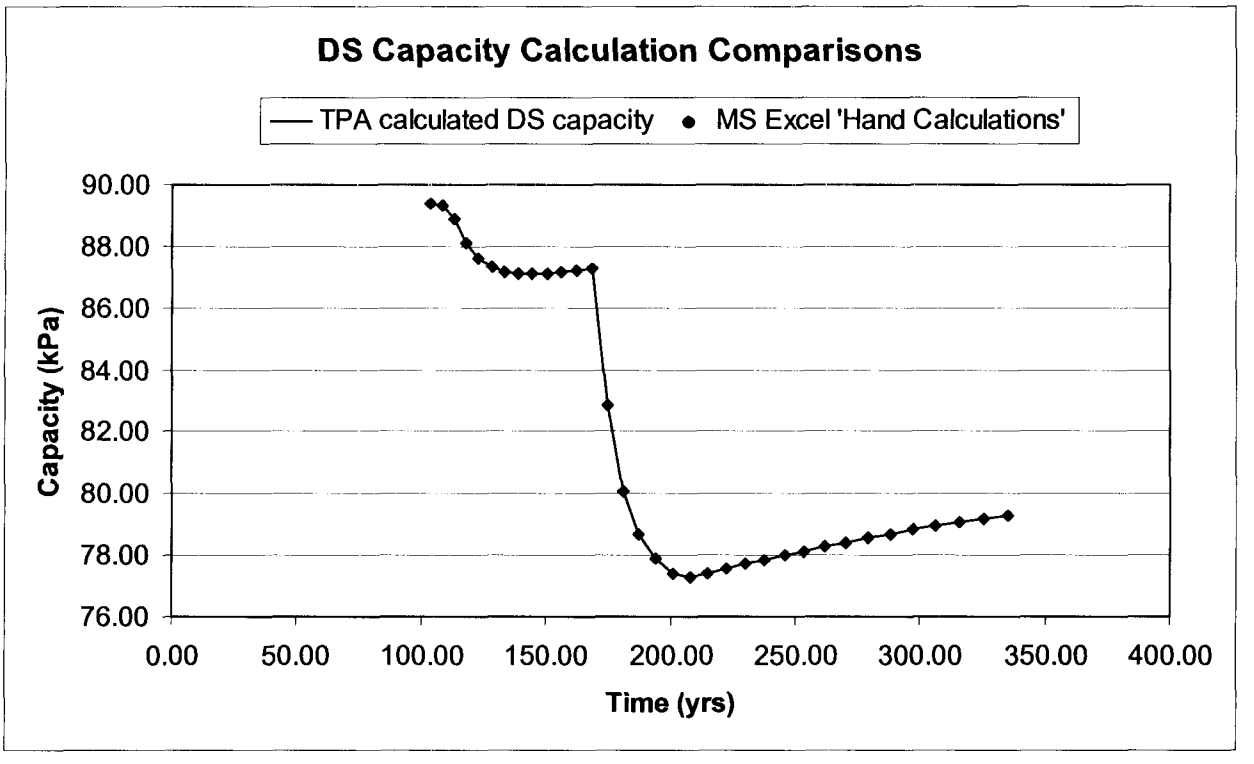
1) The DS and WP capacities calculated by mechfail.e should be the same as those generated by the MS Excel Worksheet using the same input parameters.

2) The failure status of the DS and WP should be the same as that calculated by the MS Excel Worksheet using the same applied vertical pressures.

Test Results

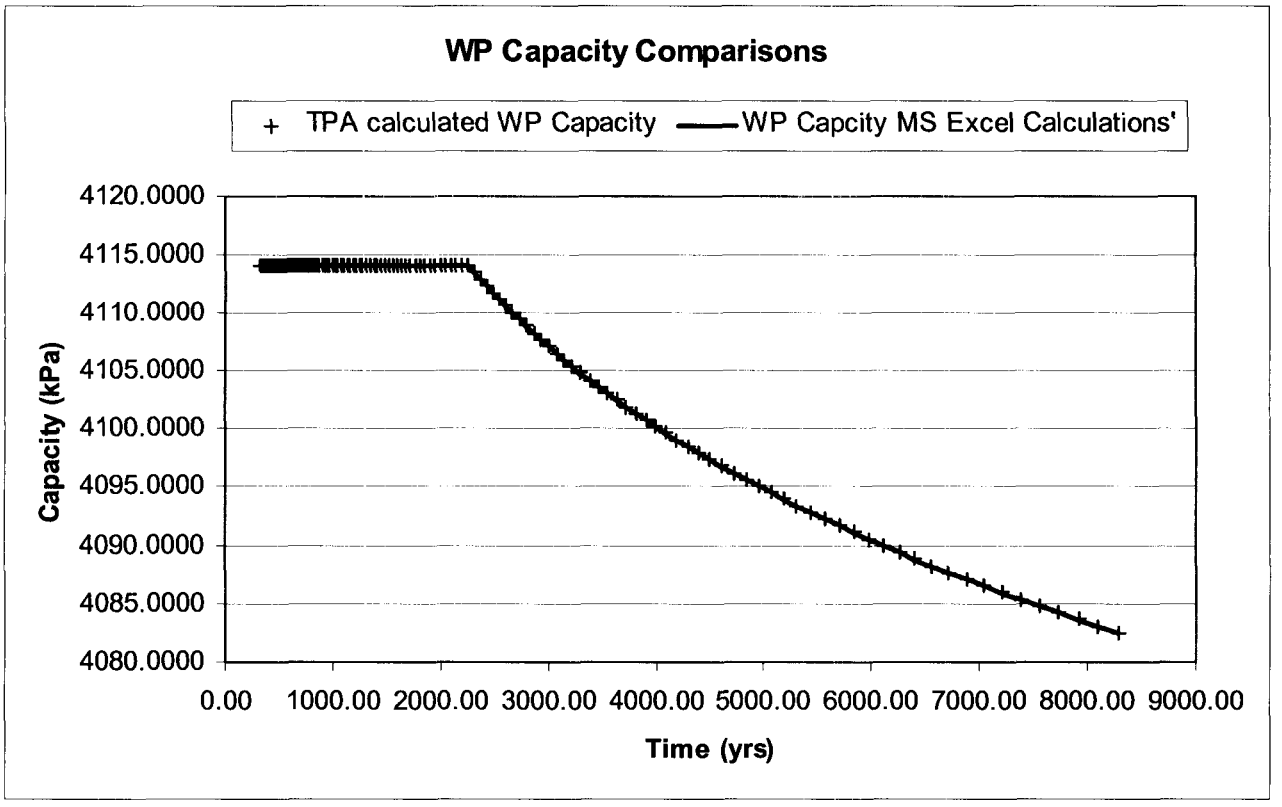
-criterion 1

The following plot shows the comparison of DS capacity for rock type one, as determined by the mechfail module to that calculated in the Excel Worksheet titled:
SCR609\mech_fail\run1\DS_failure\DS_failure no Seismic.



The drip shield capacity is a function of the DS temperature, thickness and creep factors. The correlation between the TPA calculations and the MS Excel worksheet calculations are presented as evidence that the DS capacity calculations are properly implemented. The fitting parameters for the capacity functions are located in the file *mechfail_ds.def.*

The following plot show the comparison of the WP capacity for rock type one as determined by the mechfail module to that calculated by hand using a MS Excel Worksheet titled:
SCR609\mech_fail\run1\WP_failure\WP_failure no Seismic



The WP capacity is a function of WP thickness, contact angle, contact length and tributary area. This capacity calculation was repeated using a MS Excel worksheet. The parameter values were obtained from the *mechfail.inp* file (WP thickness, contact angle , contact length and tributary area). The capacity functions were obtained from the DS-WP Mechanical interaction report. The correlation between the TPA calculations and the MS Excel calculations provide evidence that the WP capacity calculations were properly implemented. The fitting parameters for the capacity functions are located in the file *mechfail_wp.def.*

In both the DS and WP capacities the hand calculations agree with the *mechfail.e* results. In the mechfail module the calculations are repeated for rock type two using the same algorithms, so the testing of the first

rock type should be a sufficient test of the capacity calculations. This is presented as evidence that SCR609 has been properly implemented.

It is pointed out that the WP capacity is determined only for the period from which DS failure occurs to the time at which the DS has been corroded to a thickness of zero and can no longer interact with the WP. After that time the DS WP interaction no longer exists and can not fail the WP (In the preceding WP analysis the time at which the DS was corroded to a zero thichness was about 8300 yrs.). This is explained in the DS WP Mechanical Interaction report Jan 2006.

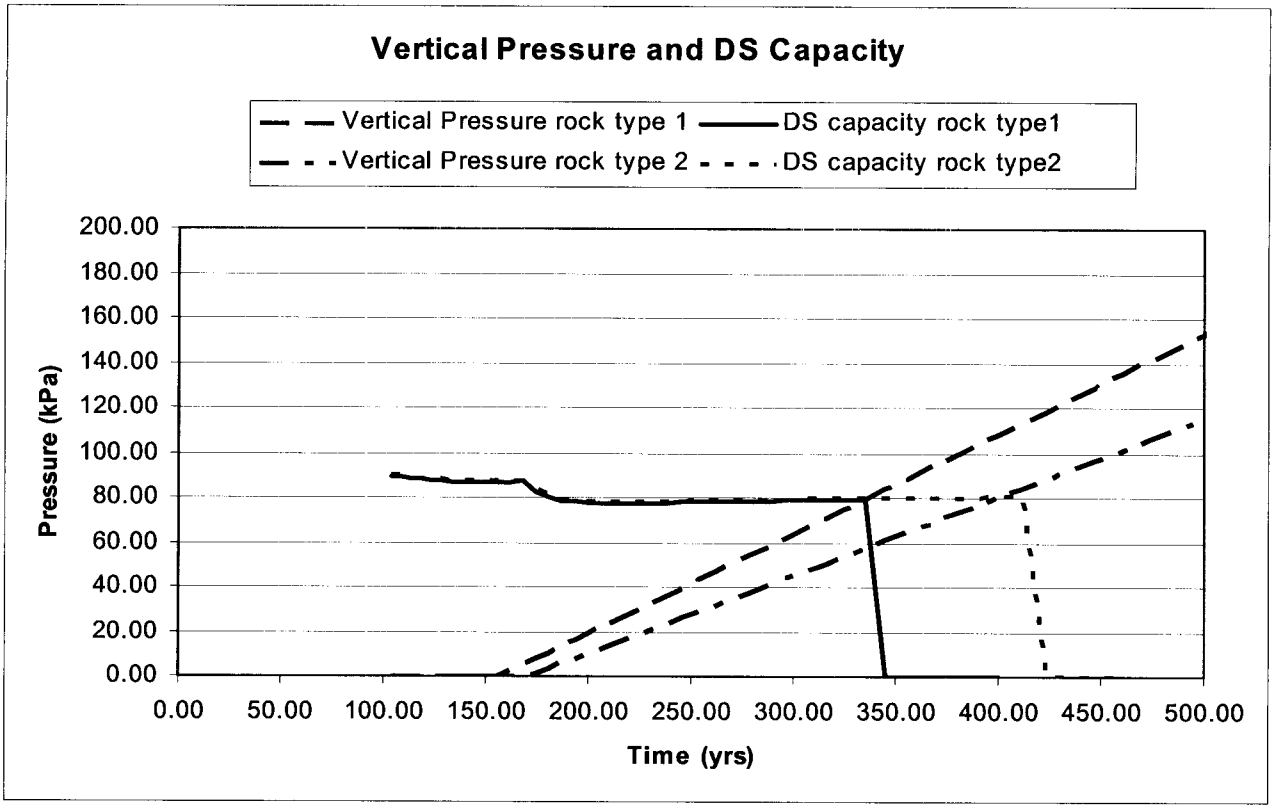
* comment: THE DS corrosion rate for DS-WP interaction analysis may be non-conservative, subsequent versions of the TPA code will address this issue.

-criterion 2 evidence

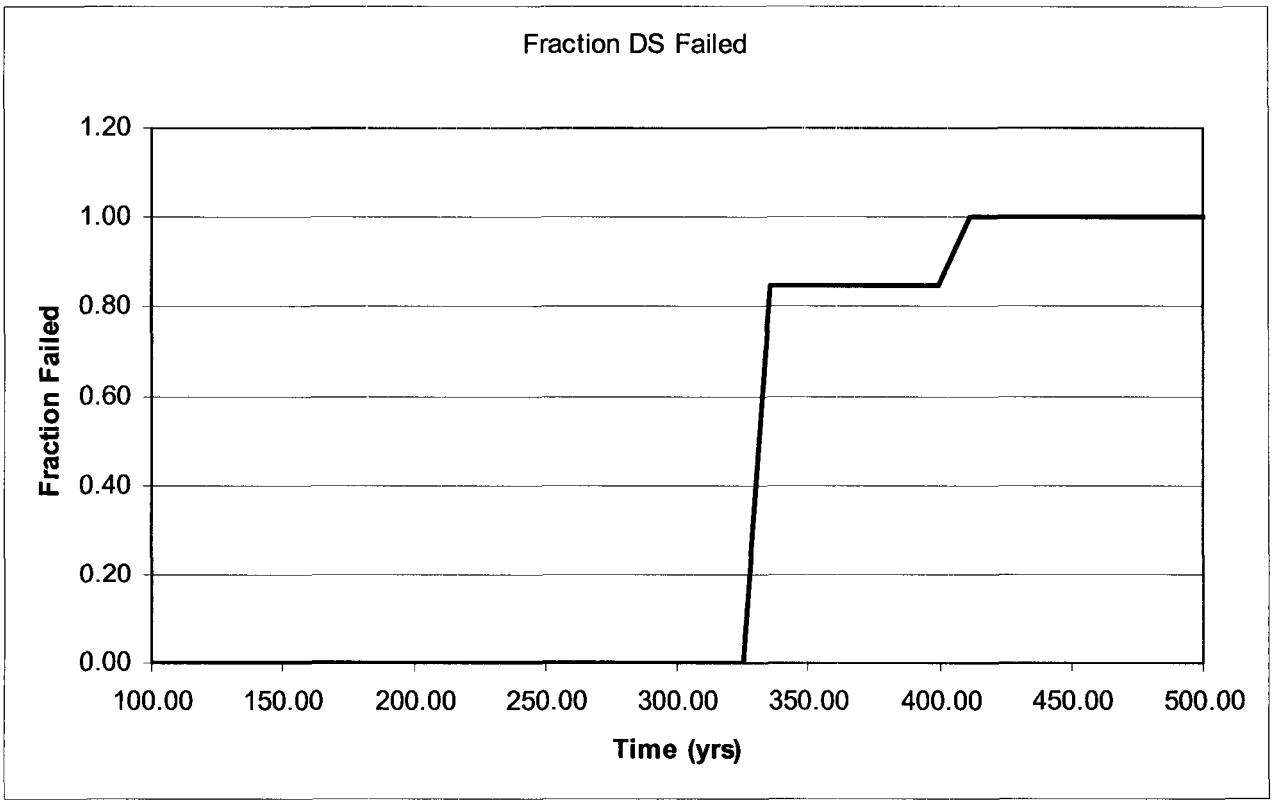
The failure status of the DS and WP s are compared between the mechfail module and hand calculations using MS Excel.

The DS is failed when the vertical pressure on the DS exceeds the DS capacity. The following plot shows the DS capacity and vertical pressures as a function of time.
SCR609\mech_fail\run1\DS_failure\DS_failure no Seismic
In this plot the failure of DS 1 occurs at a time of 335 yrs and DS 2 fails at a time of 412 yrs.
The following plot shows the fraction of DS failure as determined by the mechfail module.

Note: The capacity of the DS drops immediately to zero at the time of failure. In the Vertical Pressure and DS Capacity plot the capacity appears to have a slight delay as it decreases to zero, this however is just an artifact of the time stepping in the TPA code.



The failure time of the DS as reported by the mechfail module corresponds to the same time as that determined by hand calculations in the MS Excel Worksheet.
SCR609\mech_fail\run1\DS_failure\DS_failure no Seismic.



The failure of the WP under static conditions is not achievable under normal simulation conditions and was not tested. The fraction of WP failed during this testing was returned by the mechfail module as being zero. This is fully consistent with the WP design.
The non failure of the WP as reported by the mechfail module corresponds to that determined by hand calculations in the MS Excel Worksheet.
SCR609\mech_fail\run1\WP_failure\WP_failure no Seismic

Note: The DS fails immediately at the time of failure. In the Fraction DS Failed plot the fractions failed appears to have a slight delay at the time of DS failures, this however is just an artifact of the time stepping in the TPA code.

The capacities and failure status of the DS and WP are consistent with hand calculations and are presented as evidence that SCR609 was implemented properly.

-overall test status: **PASS**

SL-2. Name :Test drip shield and waste package failures during seismic events.

Path for run directory:
Testcase: [TPA]:Public\SCR609\mech_fail\run2

Path for archive of results:
Testcase: SCR609\mech_fail\run2

Archived to CD titled :SCR609 Testing

Environment variables:

Testcase : TPA_DATA=[TPA]:Public\SCR609\tpa502s
TPA_TEST =[TPA]:Public\SCR609\tpa502s

Special input files or modification to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Drift degradation flag is disabled

Utility scripts needed to perform the test: none

Utility codes needed in the analysis of the test data: none

Test description: The DS and WP can fail due to seismic induced pressures in which the ground shaking will magnify the static pressure applied on the DS or WP

-Objective Execute the *mechfail.e* module under conditions which will result in DS and WP failure due to Seismic activity

-Assumptions None other than those contained within the TPA code

-Constraints None

-Output files to compare or examine debug screen capture of the *mechfail.e* module

-Step-by-step test procedure to be used

1) Perform a single subarea realization.
2) save the mechfail_ds.inp and mechfail_wp.inp files into two subdirectories
   SCR609\mech_fail\run2\DS_failure
   SCR609\mech_fail\run2\WP_failure
3) Place a copy of the stand alone code mecfail.e into each of those directories.
4) The mechfail_ds.inp and mechfail_wp.inp file are then renamed mechfail.inp in their respective directories and the debug flag option is turned on.
5) Modify the mechfail.inp file as necessary to induce a discernable seismically induced failure.

6) The mechfail.e is then executed in each directory and the screen output is captured. The screen output is a result of the debug flag being set to on.
6) The Dynamic vertical pressures generated by the mechfail.e module will then be compared to hand calculated dynamic vertical pressures.
7) The DS and WP failure status will then be compared to MS Excel status calculations for comparison.

-pass fail criteria

1) the dynamic pressure of the seismic events and the status of the DS should be properly returned by the *mechfail.e* module.
2)the dynamic pressure of the seismic events and the status of the WP should be properly returned by the *mechfail.e* module.

Test Results

-criterion 1

To test the DS capacity under seismic conditions the drift degradation flag was deactivated. The TPA code was run for one realization and for one subarea. The mech_fail_ds.inp file was then saved to the directory SCR609\mech_fail\run2\DS_failure\. The sampled parameters were such that the DS failed immediately after a seismic event because of the resultant static load from accumulated rubble. The failure occurred after the first seismic event, but not during the seismic event.

To test for failures during seismic events these files (*mechfail.inp* and *mechfail.e*) were copied to the directory
SCR609\mech_fail\run2\DS_failure\test\.
The mechfail.inp file was then modified to have a static vertical pressure for the first seismic event. The pressure was changed from 0.00 (no rubble) to 50 kPa (simulated load) and the time of the first seismic event was moved to 461.1 yrs (to ensure a seismic event occurred before DS was compromised by corrosion)

This resulted in a dynamic vertical pressure of (1+.752)*50*1.5=131.4 kPa,(1.5 was used for the dynamic amplification factor (to ensure dynamic pressures would be sufficient to fail DS) and 0.752 is the PGA of the first seismic event, which produces a vertical pressure greater than the DS capacities for rock types 1 and 2, which were respectively 83.5 and 84.3 kPa.

Under these conditions the mechfail.e module returned the appropriate Seismic dynamic pressures DS failure times and DS failure cause.
These results are recorded in the files
SCR609\mech_fail\run2\DS_failure\test\mechfail.dat
SCR609\mech_fail\run2\DS_failure\test\out (debug screen capture)
and summarized on an MS Excel Worksheet
SCR609\mech_fail\run2\DS_failure\test\DS_failures Seismic

These results are presented as evidence that SCR609 has been properly implemented.

- Criterion 2

To test the WP capacity under seismic conditions the drift degradation flag was deactivated. The TPA code was run for one realization and for one subarea. The mechfail_ds.inp file was then saved to the directory SCR609\mechfail\run2\WP_failure. Under the sampled conditions the WP did not fail.

To test for failures during seismic events these files (*mechfail.inp* and *mechfail.e*) were copied to the directory SCR609\mech_fail\run2\WP_failure\test\. The *mechfail.inp* file was then modified to have a PGA of 7.32 for the third seismic event (of thirteen). Under these conditions the WP experienced Dynamic pressures of 4378.79 kPa and 4449.63 kPa in grid elements one and two. The WP capacities for both grid elements at the time of the third seismic event were 4093.86 kPa. The mechfail module properly calculated the dynamic vertical pressures and returned the proper failed status of the WP at the correct time.
These calculations and results are summarized in the MS Excel Worksheet titled WP_failures Seismic in the directory *SCR609\mech_fail\run2\WP_failure\test\WP_failures Seismic.*

These results are presented as evidence that SCR609 was properly implemented

-overall test status: **PASS**

SL-3. Name :Drip shield failure when seismic event with MAPE <1e-5

Path for run directory:
Testcase: [TPA]:Public\SCR609\mech_fail\run3

Path for archive of results:
Testcase: SCR609\mech_fail\run3

Archived to CD titled :SCR609 Testing

Environment variables:

Testcase : TPA_DATA=[TPA]:Public\SCR609\tpa502s
TPA_TEST =[TPA]:Public\SCR609\tpa502s

Special input files or modification to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Drift degradation flag is disabled

Utility scripts needed to perform the test: none

Utility codes needed in the analysis of the test data: none

Test description: The DS should be failed when the MAPE of a seismic event is less than 1e-5

-Objective Execute the *mechfail.e* module under conditions which will result in DS due to the MAPE being less than 1e-5 and not because of static or dynamic pressures

-Assumptions None other than those contained within the TPA code

-Constraints None

-Output files to compare or examine debug screen capture of the *mechfail.e* module

-Step-by-step test procedure to be used:

1) Perform a single subarea realization.
2) save the mechfail_ds.inp into the subdirectory
SCR609\mech_fail\run3\DS_failure

3) Place a copy of the stand alone code mecfail.e into the directory.
4) The mechfail_ds.inp is then renamed mechfail.inp and the debug flag option is turned on.
5) Modify the mechfail.inp file as necessary to induce a discernable seismically induced failure due to a MAPE <1e-5.

-pass fail criteria

1) the mechfail.e module returns a DS failure status when a seismic event with a MAPE<1e-5.

The following text is an excerpt from the mechfail.f module
SCR609\tpa502s\codes\mechfail.f

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
          IF(dmapeValue .GT. 0.0D0 .AND. dmapeValue .LE. 1.0D-5)THEN
c           Drip shield collapses
            bdsFailure = .TRUE.
            bdsFailureDynamic = .TRUE.
          ELSEIF(dmapeValue .GT. 1.0D-5 .AND.
     &           dmapeValue .LE. 1.0D-4)THEN
            IF(dvertPress .GT. ds_yield) THEN
c             Drip shield collapses
              bdsFailure = .TRUE.
              bdsFailureDynamic = .TRUE.
            ELSE
c             Seismic algorithm
              IF(dvert_press_dyn .GT. ds_capacity)THEN
                bdsFailure = .TRUE.
                bdsFailureDynamic = .TRUE.
              ENDIF
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

This text depicts the logic loop that checks for the mape value and fails the DS if it is less than or equal to 1e-5.

This is presented as evidence that SCR609 has been properly implemented.

This requirement was also tested by modifying a mechfail.inp file for DS failure analysis.
The input file was modified to have the first seismic event to have a MAPE of less than 1e-5
Because the drift degradation flag has been turn off, there is no static or dynamic vertical pressure for the first seismic event (this is because there is no rubble accumulation on the DS until after the first seismic event). Thus the only way that the DS can fail during the first seismic event (with no drift degradation) is because of the MAPE requirement.
The modified mechfail.inp file used for this test is in the directory
SCR609\mech_fail\run3\DS_failure\mechfail.inp. The first seismic event is at 461.4 yrs with a MAPE of 9.9e-6.

Executing the mechfail.e module the module returned a DS failure at the time of the seismic event as shown in the following text
SCR609\mech_fail\run3\DS_failure\mechfail_ds.dat

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
          Time        DS Stat1       DS Stat2        DS Dyn1        DS Dyn2
    4.61143E+02   0.00000E+00   0.00000E+00   1.00000E+00   1.00000E+00
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

This excerpt shows that the DS was dynamically failed at the time of the seismic event.

An examination of the screen capture of the debug file shows that the static and dynamic pressures at the time of the seismic event are 0.00kPa. Thus the DS was failed because of the MAPE requirement.

These results has been summarized in the MS Excel Worksheet
SCR609\mech_fail\run3\DS_failure\DS_failure MAPE.

These results are presented as evidence that SCR609 has be properly implemented.

-overall test status: **PASS**

Attachment B

Test Plan for TPA SCR609

Test Plan Name: SCR609 Platform testing

Tested By: James Mancillas Date: 4-11-06

Windows Machine: TPA Windows OS: MS Windows XP SP2
Unix Machine : Spock UNIX OS : SUNOS 5.9

Baseline Version: TPA5.0.2.s windows Test Version TPA 5.0.2.s unix

System Level (PL) Tests

SL-1. Name : Compare Windows and Unix TPA5.0.2.s basecase results.

Path for run directory windows:
Windows: [TPA]:Public\SCR609\runs1
Unix : [spock]:/home/jmancillas/TPA/run2

Path for archive of results:
Windows: SCR609\runs1
Unix : Unix\run2\

Archived to CD titled :SCR609 Testing

Environment variables:
Windows: TPA_DATA=[TPA]:Public\SCR609\tpa502s
TPA_TEST =[TPA]:Public\SCR609\tpa502s

Unix : TPA_DATA=[spock]:/home/jmancillas/TPA/tpa502s
TPA_TEST =[spock]:/home/jmancillas/TPA/tpa502s

Special input files or modification to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Default

Utility scripts needed to perform the test: none

Utility codes needed in the analysis of the test data: none

Test description: Compare the results of the Windows and UNIX versions of the TPA code version 5.0.2s

-Objective Ensure that the two versions of the code produce the same general results.

-Assumptions None other than those made within the TPA code

-Constraints None

-Output files to compare or examine Screen capture from both versions of the code during a basecase execution

-Step-by-step test procedure to be used

1) execute the windows version of the code and capture the screen output
2) execute the unix version of the code and capture the screen output
3) compare the peak mean dose and times from the two verions

-pass fail criteria

1) the peak mean dose and times calculated by the two versions should agree within the limits of mathematic processing differences between computational platforms (rounding errors).

Test Results

The following text depicts the peak mean doses calculated by the windows and unix versions of tpa502s

SCR609\runs1\out

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
exec: end realizations

exec: Peak Mean Dose is 1.31570E-02 rem/yr at    3465.9 yr, based on     1
realizations.

exec:  Run Successfully Completed
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

Unix\run2\out

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
 exec: end realizations

 exec: Peak Mean Dose is 1.31610E-02 rem/yr at    3465.9 yr, based on     1
realizations.

 exec:  Run Successfully Completed
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The two different platform calculations agree within a 0.03% difference in peak mean dose at a time of 3465.9 yrs. This minor difference in peak mean dose is expected and is attributed to rounding differences

between computational platforms.

These results are presented as evidence that SCR609 has been properly implemented.

-overall test status: **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 612	**2. Software Title and Version:** TPA 5.0.2	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *reader.f, tpa.inp, tpa_include.inp*

Input parameters such as **LogCO2PartialPressure_AllUZ_SZLayers[atm]** and **pH_AllUZ_SZLayers[StandardUnits]** are critical to the function of their respective models and the models are sensitive the actual values provided, therefore their modification should be restricted to the model expert. As such, it is desired to move the specification of these and similar parameters outside of the default *tpa.inp* input file.

5. Change Requested by: Ron Janetzke Date: 10-28-05	**6. Change Authorized by** (*Software Developer*): Ron Janetzke Date: 10-28-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

A new keyword called include was added to the *reader.f* module. This permits the reference to one or more include files in the *tpa.inp* file. They may appear as a keyword entry, with an additional line for the file name specification in single quotes, between the title lines and the endoffile keyword. The keyword may be used more than once, however only one level of nesting is permitted, that is the include file can not have an include keyword within it. The following is how it is used in the tpa.inp file.

```
**
include
'tpa_include.inp'
**
```

See attachment A for the list of modification to the *reader.f* file.

See attachment B for the listing of the new *tpa_include.inp* file.

8. Implemented by: Ron Janetzke	**Date:** 11-28-05

9. Description of Acceptance Tests:

See attachment C for Acceptance Test (unix platform)

See attachment D for Acceptance Test (PC platform)

10. Tested by: Jose Menchaca	**Date:** 12-22-05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 612

Status (*ADD, DELETE, MODIFY TO, MODIFY FROM)*	Module	Parameter Name	Description (*Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)*	Distribution	Range	Justification *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	Source

ATTACHMENT A

```
3c3
< c File Date:          11/18/05
---
> c File Date:          11/29/05
134a135,140
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
>       logical lexist
>       integer includefileunit
>       character*40 includefilename
>       integer trimlen
>
226c232,236
<       iunit = igetunitnumber('exec    ')
---
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
> cc    iunit = igetunitnumber('exec    ')
>       inpunit = igetunitnumber('exec    ')
>       includefileunit = igetunitnumber('exec    ')
>       iunit = inpunit
1527a1538,1585
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
>        elseif( pdftype .eq. 'include' ) then
>         if (iunit .eq. includefileunit) then
>             print *, ' '
>             print *, ' ***>>> Error in  reader <<<*** '
>             print *, ' "include" keyword can only be nested to' //
>      &                ' one level.'
>             print *, ' include file = ', includefilename
>             print *, ' see line ', iline
>             print *, ' '
>             CALL QUERYSTOP()
>         endif
>
>
>         read( iunit, *) includefilename
>         itrimlen = trimlen(includefilename)
>
>         call clearchar(80,aline)
>         aline='cp ' // dpath // 'data/' //
>      &         includefilename(1:itrimlen) // ' .'
>         istatus = zportsh(aline)
>
>         if( istatus .ne. 0 ) then
>             print *, ' ***>>> Error in  reader <<<*** '
>             print *, ' istatus .ne. 0 '
>             print *, ' istatus = zportsh( ' // aline
>             print *, ' istatus = ', istatus
>             CALL QUERYSTOP()
>         endif
>
>         inquire( file = includefilename, EXIST=lexist)
>
>         if (.NOT. lexist) then
>          print *, ' '
>          print *, ' ***>>> Error in Reader <<<*** '
>          print *, ' Include file not found.'
```

```
>          print *, ' file name = ', includefilename
>          print *, ' Look on Line Number = ', iline
>          print *, ' '
>          CALL QUERYSTOP()
>         endif
>
>         open (unit=includefileunit, file=includefilename, status='old')
>         iunit = includefileunit
>         inpline = iline
>         iline = 0
> cc End SCR612
>
1575,1580c1633,1656
<  955  print *, ' '
<       print *, ' ***>>> Error in Reader <<<*** '
<       print *, ' need to use keyword: endoffile '
<       print *, ' as last line to be read in the tpa.inp file '
<       print *, ' '
<       CALL QUERYSTOP()
---
>
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
> cc955  print *, ' '
> cc      print *, ' ***>>> Error in Reader <<<*** '
> cc      print *, ' need to use keyword: endoffile '
> cc      print *, ' as last line to be read in the tpa.inp file '
> ccc     print *, ' '
> cc      CALL QUERYSTOP()
>
>  955  if ( iunit .eq. inpunit) then
>         print *, ' '
>         print *, ' ***>>> Error in Reader <<<*** '
>         print *, ' need to use keyword: endoffile '
>         print *, ' as last line to be read in the tpa.inp file '
>         print *, ' '
>         CALL QUERYSTOP()
>       else
>         iline = inpline
>         iunit = inpunit
>         close (includefileunit)
>       end if
>       go to 50
> cc End SCR612
>
1581a1658,1664
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
>       if ( iunit .eq. includefileunit) then
>         iline = inpline
>         iunit = inpunit
>         close (includefileunit)
>         go to 50
>       end if
2113c2196,2199
<       call writemeanvalues(iunit)
---
> cc rwj 11-28-05; SCR612
> cc    call writemeanvalues(iunit)
>       call writemeanvalues(iunit, includefileunit, includefilename)
```

```
>
3879c3965,3968
<       subroutine writemeanvalues( iunit )
---
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
> cc    subroutine writemeanvalues( iunit )
>       subroutine writemeanvalues( inpunit, includefileunit,
>      &                            includefilename)
3892c3981,3984
< c       INPUT:    iunit = integer, input unit for tpa.inp
---
> c       INPUT:    inpunit = integer, input unit for tpa.inp
> c                 includefileunit = integer, input unit for tpa.inp
> c                                   include file.
> c                 includefilename = character*(*), buffer for file name.
3917a4010,4014
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
>       integer includefileunit
>       character*(*) includefilename
>       integer inpunit
>
3954a4052,4053
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
>       iunit = inpunit
4021c4120,4122
<         read( iunit, '(a80)' ) line
---
> cc rwj 11-28-05; SCR612
> cc      read( iunit, '(a80)' ) line
>         read( iunit, '(a80)' , END=900) line
4425a4527,4532
> cc rwj 11-28-05; SCR612  Enable tpa.inp include file.
>        elseif( pdftype .eq. 'include' ) then
>         read ( iunit, *) includefilename
>         open (unit=includefileunit, file=includefilename, status='old')
>         iunit = includefileunit
>
4458a4566,4575
> cc rwj 11-28-05; SCR612
>       go to 999
>
>   900 continue
>       close (includefileunit)
>       iunit = inpunit
>
>   999 continue
> cc End SCR612
>
```

ATTACHMENT B

```
**
**          ***>>>  Importance Analysis Flags  <<<***
**
iflag
ImportanceAnalysisFlag(yes=1,no=0)
0
**
**iflag
**SubsystemNaturalStudy
**0
**
**iflag
**BarrierBiosphereStudy
**0
**
**iflag
**ComponentPrecipitationStudy
**0
**
**iflag
**BarrierUpperUnsaturatedZoneStudy
**0
**
**iflag
**ComponentTivaCanyonStudy
**0
**
**iflag
**BarrierLowerUnsaturatedZoneStudy
**0
**
**iflag
**ComponentTSwStudy
**0
**
**iflag
**ComponentCHnvStudy
**0
**
**iflag
**ComponentCHnzStudy
**0
**
**iflag
**ComponentPPwStudy
**0
**
**iflag
**ComponentUCFStudy
**0
**
**iflag
**ComponentBFwStudy
**0
```

```
**
**iflag
**BarrierSaturatedZoneStudy
**0
**
**iflag
**Component_STFF_SAV_Study
**0
**
**iflag
**BarrierReceptorGroupStudy
**0
**
**iflag
**ComponentWellWaterStudy
**0
**
**iflag
**SubsystemEngineeredStudy
**0
**
**iflag
**BarrierDriftStudy
**0
**
**iflag
**ComponentBackfillStudy
**0
**
**iflag
**ComponentDripShieldStudy
**0
**
**iflag
**BarrierInvertStudy
**0
**
**iflag
**ComponentInvertStudy
**0
**
**iflag
**BarrierWastePackageStudy
**0
**
**iflag
**ComponentInnerContainerStudy
**0
**
**iflag
**ComponentOuterContainerStudy
**0
**
**iflag
**ComponentBathTubStudy
**0
**
**iflag
```

```
**BarrierSpentFuelDissolutionStudy
**0
**
**iflag
**ComponentSpentFuelDissolutionStudy
**0
**
**          ***>>> Subarea Size  <<<***
**
subarea
8
Subarea 1 (Top Left)
547388., 4080177.
547535., 4080514.
547582., 4079221.
547344., 4079145.
547388., 4080177.
Subarea 2
547535., 4080514.
547729., 4080945.
547955., 4079338.
547582., 4079221.
547535., 4080514.
Subarea 3
547729., 4080945.
549746., 4081578.
549068., 4079692.
547955., 4079338.
547729., 4080945.
Subarea 4
547344., 4079145.
547582., 4079221.
547606., 4078449.
547454., 4078398.
547344., 4079145.
Subarea 5
547582., 4079221.
547955., 4079338.
548058., 4078605.
547606., 4078453.
547582., 4079221.
Subarea 6
547955., 4079338.
548608., 4079543.
548555., 4078768.
548058., 4078601.
547955., 4079338.
Subarea 7
547801., 4078310.
548544., 4078551.
548525., 4078130.
547800., 4077891.
547801., 4078310.
Subarea 8
547800., 4077891.
548525., 4078130.
548467., 4077034.
547797., 4076825.
```

```
547800., 4077891.
**
usersuppliedpwisecdf
LogCO2PartialPressure_AllUZ_SZLayers[atm]
19
-3.9,  0.0
-3.7,  0.037
-3.5,  0.071
-3.3,  0.124
-3.2,  0.159
-2.9,  0.298
-2.7,  0.413
-2.56, 0.5
-2.4,  0.599
-2.2,  0.713
-1.9,  0.849
-1.8,  0.882
-1.6,  0.933
-1.4,  0.965
-1.2,  0.983
-1.0,  0.993
-0.8,  0.997
-0.6,  0.999
-0.5,  1.0
**
usersuppliedpwisecdf
pH_AllUZ_SZLayers[StandardUnits]
18
6.5,  0.0
6.63, 0.018
6.81, 0.036
6.98, 0.067
7.15, 0.114
7.33, 0.185
7.5,  0.273
7.68, 0.385
7.85, 0.5
8.02, 0.615
8.2,  0.727
8.37, 0.815
8.55, 0.886
8.72, 0.933
8.89, 0.964
9.07, 0.982
9.24, 0.992
9.4,  1.0
**
```

Attachment C

Test Plan for TPA SCR#612

Test Plan Name: Include File Test

Tested By: Jose M. Menchaca | Date: Dec 22, 2005

Host Machine: SUN Ultra-4 server: Spock | Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0.2 | Test Version: TPA 5.0.2a

Process Level (PL) Tests

PL-1. Name: Test of reader.f

Path for run directory: ~jmench/tpa502a/SCR612/

Path for archive of results: R:\unix_tpa502a/SCR612/
Note: The R: drive is the designated CD drive for stu2560.

Environment variables: setenv TPA_TEST ~/tpa502a
setenv TPA_DATA ~/tpa502a

Special input files or modifications to input files required :
For running comparisons to tpa502 the tpa502a gnewdf.dat file must be used instead of the tpa502 gnewdf.dat file.

Pertinent Lines in the tpa.inp file:
For assuring that the "include" keyword is working properly, a run must be executed with the actual entries inserted into the tpa.inp file at the location of the "include" keyword with the keyword and following filename commented out. For comparison tests with tpa502, this requires moving the location of the pertinent sections just after the UZFT subsection of the tpa.inp file. This is required to generate an lhs.out file with the same sampled parameter order as generated in the basecase run.

Special diagnostic code modifications required:

Program modes to be used (append flags, scenario/model switches, etc.):

Utility scripts needed to perform the test:

Utility codes needed in the analysis of the test data:
The "difference" utility on unix

Test Description:

Moving parameters and subarea coordinates from tpa.inp file to tpa_include.inp file

Test 1.

The parameters, LogCO2PartialPressure_AllUZ_SZLayers[atm] and pH_AllUZ_SZLayers[StandardUnits] and the subarea coordinates are now contained in the tpa_include.inp file with an "include" keyword in the tpa.inp that references the file. The first test should determine whether removing these items from the tpa.inp file has any effect on the output.

To accomplish this, run a basecase run with an unmodified tpa.inp file. A second basecase run with the contents of the tpa_include.inp copied into the tpa.inp file and the keyword "include" and file name "tpa_include.inp" commented out.

The results of the two runs should be identical. This can be verified using the following command

```
diff -r tpa502a/SCR612/bcrUsingIncludeFile tpa502a/SCR612bcrWithNoIncludeFile
```

PASS

Tests 2.

Running a basecase run will generate three constant value files that are variations based on the tpa.inp file, tpameans.out, tpamax.out, and tpamin.out. These are constant value tpa.inp files with all of the sampled parameters set to constants at their mean value, maximum value, and minimum value respectively. The tpa code should generate these files with the mean, maximum, and minimum data embedded in the tpa.inp, i.e. without referring to an include file.

To test if this is done correctly, a visual inspection of each file will verify that the values for the LogCO2PartialPressure_AllUZ_SZLayers[atm] and pH_AllUZ_SZLayers[StandardUnits] sampled parameters are set to their mean value, max value and minimum value in their respective files.

PASS

Test 3.

Single vector runs of the three constant value files should be executed to verify that there are no system level errors in the file generation. A failure to run is not guaranteed since the extreme input values generated in the tpamax.out and tpamin.out files could cause errors not based on system level problems. To test if the files were generated correctly, copy each of the constant value files to its own subfolder and run each for a single realization. The runs should complete successfully.

PASS

Tests 4.

The final test compares the output of the TPA version 5.0.2 with the output of TPA Version 5.0.2a. This requires some file manipulation since the Version 5.0.2a gnewdf.dat data file must replace the Version 5.0.2 file. Additionally the order and location of the LogCO2PartialPressure_AllUZ_SZLayers[atm] and pH_AllUZ_SZLayers[StandardUnits] sampled parameters and subarea coordinates must be moved to match the location in the Version 5.0.2a tpa.inp file.

Running a basecase run for each version under the conditions described above will verify that the outputs are identical (within a given tolerance).

This can be verified using the following command

```
diff tpa502/SCR612/bcrWithRearrangedTPAINPandTPA502AgnewdfDat tpa502a/SCR612/bcrUsingIncludeFile
```

PASS

Attachment D
Test Plan for TPA SCR#612

Test Plan Name: Include File Test

Tested By: Jose M. Menchaca

Date: Dec 22, 2005

Host Machine: AMD Opteron PC

Host OS: MS Windows Server 2003 Version 5.2

Baseline Version: TPA 5.0.2

Test Version: TPA 5.0.2a

Process Level (PL) Tests

PL-1. Name: Test of reader.f

Path for run directory: D:\JMenchaca\tpa502a\SCR612\

Path for archive of results: R:\pc_tpa502a\SCR612\
Note: The R: drive is the designated CD drive for stu2560.

Environment variables: set TPA_TEST=u:\tpa502a
set TPA_DATA=u:\tpa502a (for Tests 1 and 3)
or
set TPA_DATA=d:\JMenchaca\tpa502a (for Test 4)

Special input files or modifications to input files required :
For running comparisons to tpa502 the tpa502a gnewdf.dat file must be used instead of the tpa502 gnewdf.dat file.

Pertinent Lines in the tpa.inp file:
For assuring that the "include" keyword is working properly, a run must be executed with the actual entries inserted into the tpa.inp file at the location of the "include" keyword with the keyword and following filename commented out. For comparison tests with tpa502, this requires moving the location of the pertinent sections just after the UZFT subsection of the tpa.inp file. This is required to generate an lhs.out file with the same sampled parameter order as generated in the

basecase run.

Special diagnostic code modifications required: N/A

Program modes to be used (append flags, scenario/model switches, etc.):

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data:
The "file compare" utility on PC

Test Description:

Moving parameters and subarea coordinates from tpa.inp file to tpa_include.inp file

Test 1.

The parameters, LogCO2PartialPressure_AllUZ_SZLayers[atm] and pH_AllUZ_SZLayers[StandardUnits] and the subarea coordinates are now contained in the tpa_include.inp file with an "include" keyword in the tpa.inp that references the file. The first test should determine whether removing these items from the tpa.inp file has any effect on the output.

To accomplish this, run a basecase run with an unmodified tpa.inp file. A second basecase run with the contents of the tpa_include.inp copied into the tpa.inp file and the keyword "include" and file name "tpa_include.inp" commented out.

The results of the two runs should be identical. This can be verified using the following command on a PC platform

```
fc tpa502a\SCR612\basecaseRun\* tpa502a\SCR612\basecaseWithNoIncludeFile\*
```

PASS

Tests 2.

Running a basecase run will generate three constant value files that are variations based on the tpa.inp file, tpameans.out, tpamax.out, and tpamin.out. These are constant value tpa.inp files with all of the sampled parameters set to constants at their mean value, maximum value, and minimum value respectively. The tpa code should generate these files with the mean, maximum, and minimum data embedded in the tpa.inp, i.e. without referring to an include file.

To test if this is done correctly, a visual inspection of each file will verify that the values for the LogCO2PartialPressure_AllUZ_SZLayers[atm] and pH_AllUZ_SZLayers[StandardUnits] sampled parameters are set to their mean value, max value and minimum value in their respective files.

PASS

Test 3.

Single vector runs of the three constant value files should be executed to verify that there are no system level errors in the file generation. A failure to run is not guaranteed since the extreme input values generated in the tpamax.out and tpamin.out files could cause errors not based on system level problems. To test if the files were generated correctly, copy each of the constant value files to its own subfolder and run each for a single realization. The runs should complete successfully.

PASS

Tests 4.

The final test compares the output of the TPA version 5.0.2 with the output of TPA Version 5.0.2a. This requires some file manipulation since the Version 5.0.2a gnewdf.dat data file must replace the Version 5.0.2 file. Additionally the order and location of the LogCO2PartialPressure_AllUZ_SZLayers[atm] and pH_AllUZ_SZLayers[StandardUnits] sampled parameters and subarea coordinates must be moved to match the location in the Version 5.0.2a tpa.inp file.

Running a basecase run for each version under the conditions described above will verify that the outputs are identical (within a given tolerance).

This can be verified using the following command

```
fc tpa502\SCR612\basecaseRun\* tpa502a\SCR612\basecaseRun\*
```

PASS

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 614	2. Software Title and Version: TPA 5.0.2m TPA 5.0.2o	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *uzft.f, tpa.inp, tpanames.dbs, nefmks.f*

V5.0.2m

A limitation of the current TPA code is that long run times are often encountered for some realizations as a result of the NEFTRAN transport code needing to use extremely small timesteps to simulate short travel times. This issue is addressed in the current TPA code by bypassing unsaturated zone transport calculations altogether for realizations where the calculated unsaturated zone groundwater travel time is less than 20 years. Complete bypassing of unsaturated zone transport, however, may bias total-system results. To address this issue, modifications may be required to either the TPA code or the NEFTRAN transport code. The preferred approach, however, would be to limit the ranges of the TPA code input parameters in a manner that avoids realizations with unrealistically short groundwater travel times through the unsaturated zone. For example, the current approach of sampling the CHnv layer thickness (previously constant) now seems to increase the likelihood of sampling layer thickness values that are too thin to be considered in the NEFTRAN calculations. Criteria for selecting NEFTRAN transport legs will be reviewed to ensure consistency with the sampling of CHnv and CHnz layer thicknesses.

V5.0.2o

Additionally, unsaturated zone transport is bypassed in certain realizations as a result of limitations of the NEFTRAN radionuclide transport code. If it is not possible to eliminate such realizations, it will be necessary to modify the abstraction to account for colloid filtration in the unsaturated zone, even in the realizations that bypass unsaturated zone transport.

5. Change Requested by: O. Osidele Date: 11-4-2005	6. Change Authorized by (*Software Developer*): R. Janetzke Date: 11-4-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment A.

8. Implemented by: R. Rice	Date: 3-27-2006

9. Description of Acceptance Tests:

See Attachment C

10. Tested by: O.Osidele	Date: 4-10-2006

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 614

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
ADD	UZFT	UZVelocity(0=average,1=time-dependent)	This parameter allows the user an option to have an average velocity in UZ NEFTRAN, instead of time-dependent velocities read from the *NEFII.VEL* file	IFLAG	1	A value of 1 allows for the use of time-dependent velocities in UZ NEFTRAN; this default value is chosen because it is consistent with the previous versions of the TPA code	Request by T. McCartin (Attachment B)

MODIFY FROM	UZFT	PermanentLossColloidFilterFactor_CHnv[]	For the CHnv unit, the fraction of mass removed from transport in the matrix; this factor is applied prior to spawning NEFTRAN; the filter factor was derived based on assuming only the CHnv layer is present and represents the proportion of colloids trapped by the unit	constant	0.5	The filter factor for a single layer was chosen assuming no other layers are present because the approach implemented in the UZFT module is to choose the nonzero length layer with the highest filter factor and apply that value to the released mass	D Pickett, Scientific Notebook 133, pp. 67-70 and 85-90
MODIFY TO	UZFT	PermanentLossColloidFilterFactor_CHnv[]	(same as above)	constant	0.57	(same as above)	(same as above)
MODIFY FROM	UZFT	PermanentLossColloidFilterFactor_CHnz[]	(same as above, except for the CHnz unit)	constant	0.57	(same as above)	(same as above)
MODIFY TO	UZFT	PermanentLossColloidFilterFactor_CHnz[]	(same as above, except for the CHnz unit)	constant	0.75	(same as above)	(same as above)

MODIFY FROM	UZFT	PermanentLossColloidFilterFactor_PPw_[]	(same as above, except for the PPw unit)	constant	0.19	(same as above)	(same as above)
MODIFY TO	UZFT	PermanentLossColloidFilterFactor_PPw_[]	(same as above, except for the PPw unit)	constant	0.41	(same as above)	(same as above)
MODIFY FROM	UZFT	PermanentLossColloidFilterFactor_UCF_[]	(same as above, except for the UCF unit)	constant	0.25	(same as above)	(same as above)
MODIFY TO	UZFT	PermanentLossColloidFilterFactor_UCF_[]	(same as above, except for the UCF unit)	constant	0.51	(same as above)	(same as above)
MODIFY FROM	UZFT	PermanentLossColloidFilterFactor_BFw_[]	(same as above, except for the BFw unit)	constant	0.18	(same as above)	(same as above)
MODIFY TO	UZFT	PermanentLossColloidFilterFactor_BFw_[]	(same as above, except for the BFw unit)	constant	0.66	(same as above)	(same as above)

MODIFY FROM	UZFT	CHnvThickness_1SubArea[m]	Thickness of the CHnv unit underlying Subarea 1	triangular	0.0, 27.7, 66.9	The lower limit of the distribution was 0; however, because of formatting of the NEFTRAN input file *nefii.inp*, a value between 0.0 and 0.05 m causes 0.0 to be written and a NEFTRAN error is generated; to avoid this condition, the lower limit was adjusted to have a minimum value of 0.05 m.	N/A
MODIFY TO	UZFT	CHnvThickness_1SubArea[m]	Thickness of the CHnv unit underlying Subarea 1	triangular	0.05, 27.7, 66.9	(same as above)	N/A
MODIFY FROM	UZFT	CHnvThickness_2SubArea[m]	Thickness of the CHnv unit underlying Subarea 2	triangular	0.0, 16.4, 77.8	(same as above)	N/A
MODIFY TO	UZFT	CHnvThickness_2SubArea[m]	Thickness of the CHnv unit underlying Subarea 2	triangular	0.05, 16.4, 77.8	(same as above)	N/A

MODIFY FROM	UZFT	CHnvThickness_3SubArea[m]	Thickness of the CHnv unit underlying Subarea 3	triangular	0.0, 4.2, 9.1	(same as above)	N/A
MODIFY TO	UZFT	CHnvThickness_3SubArea[m]	Thickness of the CHnv unit underlying Subarea 3	triangular	0.05, 4.2, 9.1	(same as above)	N/A
MODIFY FROM	UZFT	CHnvThickness_4SubArea[m]	Thickness of the CHnv unit underlying Subarea 4	triangular	0.0, 4.2, 9.1	(same as above)	N/A
MODIFY TO	UZFT	CHnvThickness_4SubArea[m]	Thickness of the CHnv unit underlying Subarea 4	triangular	0.05, 4.2, 9.1	(same as above)	N/A
MODIFY FROM	UZFT	CHnvThickness_5SubArea[m]	Thickness of the CHnv unit underlying Subarea 5	triangular	0.0, 4.2, 9.1	(same as above)	N/A
MODIFY TO	UZFT	CHnvThickness_5SubArea[m]	Thickness of the CHnv unit underlying Subarea 5	triangular	0.05, 4.2, 9.1	(same as above)	N/A

ATTACHMENT A

Changes implemented in TPA Version 5.0.2m code are:
(a) determine and store the non-zero length matrix layer with greatest conductivity in a layer loop, instead of time-step loop, since it will be the same matrix layer at all time steps
(b) adjust the "infil" array proportionally by the "highestmatfraction" array to account for matrix flow; carry forward the flow to use it to calculate travel times/velocities for NEFTRAN
(c) for the layer determined in (a), force that layer to be a matrix leg in NEFTRAN
(d) if every layer has travel time less than "gwttmin," reset the length of the layer determined in (a) so that the travel time of the layer is equal to "gwttmin"
(e) use the "PermanentLossColloidFilterFactor" for the non-zero length layer that has the highest value; modify data in the *tpa.inp* file to use values that are specific to each layer and not dependent on the filtration in the preceding layer.
(f) remove code that sets Chnv thickness to zero if a value less than 2m is sampled
(g) reformat NEFTRAN output to have more precision in output times (increase from 4 to 6 decimal places)
(h) add check for UZ layers with zero thickness so they are not used in flux splitting or colloid filtration
(i) implement a flag in the *tpa.inp* file to allow the user to select using either average or time-dependent velocities in a NEFTRAN run; use the velocity of the first kept layer for the repository leg velocity; ensure the length of the first kept layer from the *tpa.inp* file is equal to the sum of the repository layer length and the adjusted length of that kept layer (these lengths are written to the *nefii.inp* file); and ensure the dispersivities of the repository leg and the first kept layer are consistent with their lengths and using either average or time-dependent velocities
(j) because of NEFTRAN formatting requirements, do not allow the user to specify a UZ thickness less than 5 cm (0.05 m); reset data in the *tpa.inp* file so that minimum thicknesses are 5 cm; note that zero thickness is allowed to preclude its inclusion in the *tpa.inp* file.

Changes implemented in TPA Version 502o code are to skip UZ NEFTRAN if the user has specified zero thickness for all layers in a subarea.

ATTACHMENT B

File attached to e-mail from T. McCartin to J. Winterle (and forwarded to R. Rice) on Jan. 17, 2006

Suggested Changes to UZFT

1) **Provide for use of average velocity or time dependent velocity based on a input flag specified in tpa.inp**

   A) **read the integer parameter called "iaveuz" in tpa.inp where a value of '0' indicates use of average velocities and "1" indicates the use of time dependent velocities**

   B) **this parameter is used in subroutine prenefmks**

2) **Revise repository velocity to be the same velocity as the first kept layer (currently the repository velocity is the first non-zero velocity, which will in all cases be the velocity of the Topopah Springs unit that is present in all subareas and will in all likelihood be fracture flow a very high velocity). The reason to do this change is: (1) the repository leg is used as a source term for the initial layer (or leg in NEFTRAN speak) of the tranport path and should be representative of the properties of this first leg of the transport path or the first kept leg; and (2) currently the retardation values for the repository leg are specified as the same properties as the first kept leg - thus the velocities should be the same.**

   A) **at lines 2298-2302 where the time dependent velocities are accepted for a layer lines have been added to save the repository velocities with the same values as the first accepted layer**

```
        if (INC .eq. 1) then
repvel(itm) = vell(itime,N)
endif
```

   B) **comment out the previous determination of the repository velocity at lines 2336 - 2341**

```
c  tjm change 12/29/2005
c   this do loop removed and repvel calculated above
c   (note that the DMIN1 test was incorrect in using
c    the 'repleg' as if it was a velocity)
c
c        do inonzero=1,nlyeru
c          if (vell(itime,inonzero) .gt. 0.0d0) then
c           repvel(itm) = DMIN1(vell(itime,inonzero), repleg)
c          goto 427
c          endif
c        enddo
```

C) Use the parameter 'iaveuz' to set the NEFTRAN input flag for using time-dependent velocities at lines 2580-2581

```
C       WRITE(i3,'(I5,5X,A)') 1,
          WRITE(i3,'(I5,5X,A)') iaveuz,
      &              'NEFII.VEL, UNIT 11,TIME-DEPENDENT '//
      &              'VELOCITIES READ FROM'
```

(D) Use the parameter 'iaveuz' to set the NEFTRAN input flag for reading a time-dependent velocity file lines 2628

```
c
c         WRITE(i3,'(I5,5X,A)') 1,'VELOCITY FIELDS FROM UNIT 11'
          WRITE(i3,'(I5,5X,A)') iaveuz,'VELOCITY FIELDS FROM UNIT 11'
```

3) Revise the length of the first leg such that the combined thickness of the first leg and the repository leg (set to 1 meter) is equal to the thickness of the first kept layer or leg.

A) do the correction in the '900' Do Loop at lines 2781 - 2786

```
     DO 900 II=1,NEFLEG
c
c  tjm change 1/6/2006
     if (II .eq. 1) then
    WRITE(i3,'(I2,5X,I2,5X,I2,4(3X,F7.1))') II+1,II+1,II+2,
   &                    (NEFLEN(II)- REPLEG),0.0,0.0,0.0
    else
c
c end tjm change except for endif statement below
c
     WRITE(i3,'(I2,5X,I2,5X,I2,4(3X,F7.1))') II+1,II+1,II+2,
    &                          NEFLEN(II),0.0,0.0,0.0
c
     endif
c
900 CONTINUE
```

4) Need to ensure the dispersivity and velocities for the repository leg are are consistent with the first kept layer or leg

```
c tjm change 12/30/2005
c  replace the repvelocity with the velocity of the first kept layer
c  and the dispersivity used for the first kept layer (with a minimum
c  of 0.01 - note repository leg lenght is hard wired to 1.0)
c  which is consistent with the other properties retained for the
c  repository leg (e.g., porosity, Kd)
c  and this is now the average velocity and can be used for the
c  average velocity - steady state run
c
     REPDISPER = DMAX1(0.01d0,REPLEG*DISPER(1)/NEFLEN(1))
c
c  Note: if this is an average velocity simulation only the
C       dispersion of the first leg will be used for the composite
C       leg, thus the dispersion length should be what was calculated
C       for the first leg
c     IF (iaveuz .eq. 0) REPDISPER = DISPER(1)
```

```
C
    WRITE(i3,'(I3,X,e10.4,3X,F5.1,5X,I2,3X,E10.3,2X,E10.3,2X,E10.3,2X,
   &     E10.3)') 1,REPDISPER,SPASTP,0,MOISTC(1),0.0,0.0,
   &     NEFVEL(1)

c    &     repvel(1)
c
c tjm change end
```

5) Need to adjust the dispersion for the second leg to account for the reduced length - only needed for time dependent velocity (average velocity will use first leg dispersion only)

A) revise Do Loop 901; lines 2799 - 2805

```
    DO 901 II=1,NEFLEG
c
c tjm change 1/6/2006 - need to account for the reduction of dispersion length in
c the first kept leg due to the repository leg length being substracted from
c  the first kept leg length
c
    if (II .eq. 1) then

     DISPER(1) = (NEFLEN(1) - REPLEG)*DISPER(1)/NEFLEN(1)
c
c  need to recheck the minimum values
c
      if (NEFLEN(1) .GE. 40.0) then
       DISPER(1) = DMAX1(0.1d0, DISPER(1))
      else
       DISPER(1) = DMAX1(0.01d0, DISPER(1))
      endif
     endif
c
c   end tjm change
c
    WRITE(i3,'(I3,X,e10.4,3X,F5.1,5X,I2,3X,E10.3,2X,E10.3,2X,E10.3,2X,
   &  E10.3)') II+1,DISPER(II),SPASTP,0,MOISTC(II),0.0,0.0,
   &          NEFVEL(II)

  901 CONTINUE
```

ATTACHMENT C

PC Acceptance Testing

Test Plan for TPA SCR 611

Test Plan Name: PC Testing of Unsaturated Zone Transport Abstraction

Tested By: O. Osidele

Date: April 10, 2006

Host Machine: TPA

Host OS: XP Professional

Baseline Version: 5.0.2m

Test Versions: 5.0.2q and 5.0.2r

Process Level (PL) Tests

PL-1. Name: Matrix-Fracture Flux Splitting and Ground Water Travel Time

Path for run directory:
d:\oosidele\run_tpa502m
d:\oosidele\run_tpa502r

Path for archive of results:
\scr614_test\PC\Test1
(archived on CD named "Test Plan for SCR 614")

Environment variables:
TPA_TEST=d:\oosidele\tpa502m
TPA_DATA=d:\oosidele\tpa502m
TPA_TEST=d:\oosidele\tpa502r
TPA_DATA=d:\oosidele\tpa502r

Special input files or modifications to input files required:
tpa.inp: run ten realizations; set thickness of CHnv layer to zero

Special diagnostic code modifications required :
Print statements added to *uzft.f* to display: (i) the media type assigned to each UZ layer, (ii) the matrix conductivity calculated for each existing (non-zero thickness) layer; (iii) the layer with the highest matrix conductivity; (iv) the "infil" value and fracture fraction at each time step; (v) the layer kept for the NEFTRAN input file and the travel time in the kept layer; (vi) the reset layer thickness; (vii) the total UZ travel time; and (viii) the travel times in the layers included in the NEFTRAN input file.

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description:
Determination of UZ layer with highest matrix conductivity; calculation of fraction for splitting flux between matrix and fracture media; if necessary, resetting the thickness of the layer with highest matrix conductivity for inclusion in NEFTRAN input file.

Objective:
Verify that the layer with highest matrix conductivity is: (i) used in calculating the matrix fraction; (ii) kept for inclusion in the NEFTRAN input file; and (iii) assigned a greater thickness if its travel time is less than 20 years.

Assumptions: None

Constraints: None

Output files to compare or examine: Screen print (*tpa.out*)

Step by step test procedure to be used:
1. Execute ten realizations of the test code with the specified modifications using the basecase *tpa.inp* file and capture the screenprint in the *tpa.out* file.
2. Set the CHnv layer thickness to zero in *tpa.inp*.
3. Repeat step 1 to force selection of a different layer with the highest matrix conductivity.
4. Examine the *tpa.out* file generated from steps 1 and 3.

Pass/Fail criteria:
1. The fracture fraction printed to screen should equal one minus the ratio of the highest matrix conductivity to the "infil" value at each time step. If the highest matrix conductivity exceeds the "infil" value, then the fracture fraction printed should be zero.
2. The kept matrix layer (indexed by its sequence number) should match the layer determined earlier to have the highest matrix conductivity.
3. If the travel time printed for this kept leg is less than 20, then a reset stament should follow indicating the augmented kayer thickness.

Test Results:

Files on the CD in the *\scr614_test\PC\Test1* subdirectory contain results for this test run. The relevant parts (from realization #1, subarea #2) of the screenprint (*\run_tpa502r_10rlz\tpa.out*) for step 1are as follows:

```
exec: calling uzft
layer #  1  is type  2
layer #  2  is type  1
layer #  3  is type  2
layer #  4  is type  2
layer #  5  is type  2
layer #  6  is type  2
layer #  7  is type  2
Layer #  1  matrix conductivity =  4.752038277000000E-04
```

```
Layer #  2  matrix conductivity =  14.93867831400000
Layer #  3  matrix conductivity =  3.994994745000000E-03
Layer #  4  matrix conductivity =  7.394766497999999E-03
Layer #  5  matrix conductivity =  1.435012015500000E-03
Highest matrix conductivity =  14.93867831400000  in layer  2
infil  1.730243823006714E-02  fracture fraction  0.000000000000000E+00
infil  1.741062950326815E-02  fracture fraction  0.000000000000000E+00
infil  1.752135368587037E-02  fracture fraction  0.000000000000000E+00
infil  1.763467007683429E-02  fracture fraction  0.000000000000000E+00
infil  1.775063936339220E-02  fracture fraction  0.000000000000000E+00
infil  1.786932365354961E-02  fracture fraction  0.000000000000000E+00
infil  1.799078650934749E-02  fracture fraction  0.000000000000000E+00
infil  1.811509298090333E-02  fracture fraction  0.000000000000000E+00
infil  1.824230964124907E-02  fracture fraction  0.000000000000000E+00
...
...
...
kept matrix layer # =  2
travel time =  9.411797158410465
reset leg length =  8.276062338465769
total travel time =  40.02000000000000
layer #  2  incl in NEFTRAN input with trav time =  20.02000000000000
```

Layer # 2 is the CHnv layer, and its matrix conductivity exceeds the "infil" values for the timesteps shown, so the fracture fraction is zero (indicating that all flux is conveyed through the matrix). The kept layer is also CHnv but its travel time less than 20, so the thickness (NEFTRAN leg length) is reset to give a travel time of at least 20 years.

Likewise, the relevant parts of the screenprint (*\run_tpa502r_10rlz_noCHnv\tpa.out*) for step 3are as follows (from realization #1, subarea #1):

```
exec: calling uzft
layer #  1  is type  2
layer #  2  is type  1
layer #  3  is type  2
layer #  4  is type  2
layer #  5  is type  2
layer #  6  is type  2
layer #  7  is type  2
Layer #  1  matrix conductivity =  1.626585987600000E-04
Layer #  3  matrix conductivity =  3.491468001000000E-03
Layer #  4  matrix conductivity =  1.894933958400000E-03
Layer #  5  matrix conductivity =  2.849716201500000E-03
Highest matrix conductivity =  3.491468001000000E-03  in layer  3
infil  8.897154360219622E-03  fracture fraction  0.6075747525960857
infil  8.937048189421204E-03  fracture fraction  0.6093264882321150
infil  8.977875989099751E-03  fracture fraction  0.6111031155655222
infil  9.019659624813653E-03  fracture fraction  0.6129046830775353
infil  9.062421474024680E-03  fracture fraction  0.6147312270779417
infil  9.106184438082360E-03  fracture fraction  0.6165827713308148
infil  9.150971954488921E-03  fracture fraction  0.6184593266852606
infil  9.196808009451381E-03  fracture fraction  0.6203608907120943
infil  9.243717150727493E-03  fracture fraction  0.6222874473473892
...
...
```

```
...
...
kept matrix layer # =  3
travel time =  7423.120197966256
total travel time =  7451.148548794754
layer #  3  incl in NEFTRAN input with trav time =  7423.120197966256
```

Layer # 3 is the CHnz layer. For the timesteps shown, the highest matrix conductivity is about 40% of the "infil" values, indicating that about 60% of the flux is conveyed through fractures). The kept layer is also CHnz. No leg length reset is required since its travel time exceeds 20 years.

Test Status: <u>PASS</u>

PL-2. Name: Colloid Filtration Factor

Path for run directory: d:\oosidele\run_tpa502q

Path for archive of results: \scr614_test\PC\Test2
(archived on CD named "Test Plan for SCR 614")

Environment variables: TPA_TEST=d:\oosidele\tpa502q
TPA_DATA=d:\oosidele\tpa502q

Special input files or modifications to input files required: None

Special diagnostic code modifications required :
Print statements added to *uzft.f* to display: (i) the list of colloid filtration factors for the UZ layers (read from *tpa.inp*); (ii) the list of existing (i.e., non-zero thickness) layers; and (iii) the highest colloid filtration factor determined from the code calculations.

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description:
Calculatation of the highest colloid filtration factor among the layers that exist in the UZ.

Objective:
Verify that (i) *tpa.inp* is updated with the new filtration factors; (ii) only the layers with non-zero thickness are used in determining the highest colloid filtration factor; and (iii) the calculation of the highest filtration factor is correct.

Assumptions: None

Constraints: None

Output files to compare or examine: Screen print (*tpa.out)*

Step by step test procedure to be used:
1. Execute one realization of the test code using the basecase *tpa.inp* file and capture the screenprint in the *tpa.out* file.
2. Extract the layer thicknesses and colloid filtration factors used in the simulation from *tpa.inp* and *samplpar.res* into a spreadsheet for calculating the highest colloid filtration factor.
3. Compare the screen print with the spreadsheet calculations.

Pass/Fail criteria:

1. The screen print of the list of UZ layers that exist in each subarea should correspond with the non-empty spreadsheet cells containing the filtration factors. The numbers in these cells are used to determine the highest filtration factor.
2. The colloid filtration factor calculated in the spreadsheet should be the same as that displayed in the screen print.

Test Results:

Files on the CD in the *\scr614_test\PC\Test2* subdirectory contain results for this test run. The relevant parts (from subarea #s 1, 4 and 7) of the screenprint (*\run_tpa502q\tpa.out*) for step 1are as follows:

```
-----------------------------------------------------------------------
    subarea   1 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzft
PermanentLossColloidFilterFactor_TSw_[] =  0.6500000000000000
PermanentLossColloidFilterFactor_CHnv[] =  0.5700000000000000
PermanentLossColloidFilterFactor_CHnz[] =  0.7500000000000000
PermanentLossColloidFilterFactor_PPw_[] =  0.4100000000000000
PermanentLossColloidFilterFactor_UCF_[] =  0.5100000000000000
PermanentLossColloidFilterFactor_BFw_[] =  0.6600000000000000
PermanentLossColloidFilterFactor_UFZ_[] =  0.000000000000000E+00
UZ layer #  1  exists
UZ layer #  2  exists
UZ layer #  3  exists
UZ layer #  4  exists
UZ layer #  5  exists
highest colloid filter factor =  0.7500000000000000

-----------------------------------------------------------------------
    subarea   4 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzft
PermanentLossColloidFilterFactor_TSw_[] =  0.6500000000000000
PermanentLossColloidFilterFactor_CHnv[] =  0.5700000000000000
PermanentLossColloidFilterFactor_CHnz[] =  0.7500000000000000
PermanentLossColloidFilterFactor_PPw_[] =  0.4100000000000000
PermanentLossColloidFilterFactor_UCF_[] =  0.5100000000000000
PermanentLossColloidFilterFactor_BFw_[] =  0.6600000000000000
PermanentLossColloidFilterFactor_UFZ_[] =  0.000000000000000E+00
UZ layer #  1  exists
UZ layer #  2  exists
UZ layer #  3  exists
UZ layer #  4  exists
highest colloid filter factor =  0.7500000000000000

-----------------------------------------------------------------------
    subarea   7 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzft
PermanentLossColloidFilterFactor_TSw_[] =  0.6500000000000000
PermanentLossColloidFilterFactor_CHnv[] =  0.5700000000000000
PermanentLossColloidFilterFactor_CHnz[] =  0.7500000000000000
PermanentLossColloidFilterFactor_PPw_[] =  0.4100000000000000
```

```
PermanentLossColloidFilterFactor_UCF_[] =  0.5100000000000000
PermanentLossColloidFilterFactor_BFw_[] =  0.6600000000000000
PermanentLossColloidFilterFactor_UFZ_[] =  0.000000000000000E+00
UZ layer #  1  exists
UZ layer #  2  exists
UZ layer #  3  exists
UZ layer #  4  exists
UZ layer #  5  exists
UZ layer #  6  exists
highest colloid filter factor =  0.7500000000000000
```

The corresponding parts of the spreadsheet calculations are as follows (see *\run_tpa502q\LayerThicknessColloidFilterFactor.xls*):

		1	4	7
Layer Thickness (from tpa.inp)	Layer #			
TSw_Thickness[m]	1	53.1	111.4	112.6
CHnvThickness[m] (sampled)	2	49.41	4.31	52.43
CHnzThickness[m] (calculated)	3	58.59	153.09	48.77
PPw_Thickness[m]	4	43.1	10	45.7
UCF_Thickness[m]	5	44.8	0	37.1
BFw_Thickness[m]	6	0	0	3
UFZ_Thickness[m]	7	0	0	0
CH_Total_Thickness[m]		108	157.4	101.2
PermanentLossColloidFilterFactor (from tpa.inp)				
TSw_Thickness[m]	1	0.65	0.65	0.65
CHnvThickness[m]	2	0.57	0.57	0.57
CHnzThickness[m]	3	0.75	0.75	0.75
PPw_Thickness[m]	4	0.41	0.41	0.41
UCF_Thickness[m]	5	0.51	0.51	0.51
BFw_Thickness[m]	6	0.66	0.66	0.66
UFZ_Thickness[m]	7	0	0	0
Filter factor for Layers with non-zero thickness				
	1	0.65	0.65	0.65
	2	0.57	0.57	0.57
	3	0.75	0.75	0.75
	4	0.41	0.41	0.41
	5	0.51		0.51
	6			0.66
	7			
Highest Colloid filter factor		0.75	0.75	0.75

In all subareas the highest colloid filtration factor is 0.75, which agrees with the screen print. Also, the non-zero highlighted filtration factors correspond to the existing layers listed in the screen print.

Test Status: PASS

PL-3. Name: Calico Hills Layer Thickness and NEFTRAN Output Precision

Path for run directory: d:\oosidele\run_tpa502m
d:\oosidele\run_tpa502q

Path for archive of results: \scr614_test\PC\Test3
(archived on CD named "Test Plan for SCR 614")

Environment variables: TPA_TEST=d:\oosidele\tpa502m
TPA_DATA=d:\oosidele\tpa502m
TPA_TEST=d:\oosidele\tpa502q
TPA_DATA=d:\oosidele\tpa502q

Special input files or modifications to input files required: None

Special diagnostic code modifications required :
In the baseline and test versions, CHnv thickness parameter set to constant 1.5 m in *tpa.inp*. Print statements added to *uzft.f* to display the thickness of each layer in the UZ.

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description:
Removal of code that sets CHnv thickness to zero if a value less than 2 m is sampled. Reformating of NEFTRAN output times.

Objective:
Verify that (i) the CHnv layer thickness is not reset to zero if a value less than 2 m is sampled; (ii) the precision of the NEFTRAN output times is increased from 4 to 6 decimal places.

Assumptions: None

Constraints: None

Output files to compare or examine: Screen print (*tpa.out*); NEFTRAN output (*nefii*.out*)

Step by step test procedure to be used:
1. Execute one realization of the test code with the specified modifications using the basecase *tpa.inp* file and capture the screenprint in the *tpa.out* file.
2. Execute one realization of the baseline code with the specified modifications using the basecase *tpa.inp* file and capture the screenprint in the *tpa.out* file.
3. Compare the screen prints and the NEFTRAN output files obtained in steps 1 and 2..

Pass/Fail criteria:

1. The screen print obtained from the test version (step 1) should list the CHnv thickness as 1.5, while the baseline version (step 2) should list it as 0.0. Also, since previous tests have shown that CHnv is the only layer selected by the baseline version, the baseline run should skip NEFTRAN, because the thickness of CHnv was reset to 0.0.
2. In the NEFTRAN output files (*nefiiuz.out* and *nefiisz.out*) obtained from the test version (step 1), the output times for radionuclide discharge rates should be written in 6 decimal places. Output times for the baseline version should be in 4 decimal places.

Test Results:

Files on the CD in the *\scr614_test\PC\Test3* subdirectory contain results for this test. The relevant parts of the screenprint for the test version (step 1) in *\run_tpa502q\tpa.out* are as follows:

```
exec: calling uzft
TSw_Thickness_1SubArea[m] = 53.10000000000000
CHnvThickness_1SubArea[m] = 1.500000000000000
CH_Total_Thickness_1SubArea[m] = 106.5000000000000
PPw_Thickness_1SubArea[m] = 43.10000000000000
UCF_Thickness_1SubArea[m] = 44.80000000000000
BFw_Thickness_1SubArea[m] = 0.000000000000000E+00
UFZ_Thickness_1SubArea[m] = 0.000000000000000E+00
                     Highest release rates from UZ
```

The relevant parts of the screenprint for the baseline version (step 2) in *\run_tpa502m\tpa.out* are as follows:

```
exec: calling uzft
TSw_Thickness_1SubArea[m] = 53.10000000000000
CHnvThickness_1SubArea[m] = 0.000000000000000E+00
CH_Total_Thickness_1SubArea[m] = 108.0000000000000
PPw_Thickness_1SubArea[m] = 43.10000000000000
UCF_Thickness_1SubArea[m] = 44.80000000000000
BFw_Thickness_1SubArea[m] = 0.000000000000000E+00
UFZ_Thickness_1SubArea[m] = 0.000000000000000E+00
      *** NEFTRAN is skipped for this UZ path since no layers have significant
ground water travel time. ***
                     Highest release rates from UZ
```

The constant value of 1.5 specified in *tpa.inp* was retained in the test version, but reset to zero in the baseline version. The relevant parts of the NEFTRAN output file (see *\run_tpa502q\nefiiuz.out*) for the test version are as follows:

```
 SETUP COMPLETE, TRANSPORT CHAIN 1

1

 RADIONUCLIDE DISCHARGE RATE (CI/Y)
      YEAR      CM246        U238
 0.000000E+00  0.000000E+00  0.000000E+00
 1.000000E+03  0.000000E+00  0.000000E+00
 3.000000E+03  0.000000E+00  0.000000E+00
 5.000000E+03  0.000000E+00  0.000000E+00
```

```
 7.000000E+03  0.000000E+00  0.000000E+00
 9.000000E+03  0.000000E+00  0.000000E+00
 1.100000E+04  0.000000E+00  1.264999E-12
```

The relevant parts of the NEFTRAN output file (see *\run_tpa502m\nefiisz.out*) for the baseline version are as follows:

```
 SETUP COMPLETE, TRANSPORT CHAIN 1

1

 RADIONUCLIDE DISCHARGE RATE (CI/Y)
      YEAR      CM246        U238
 0.0000E+00  0.0000E+00  0.0000E+00
 1.0309E+02  0.0000E+00  0.0000E+00
 3.0928E+02  0.0000E+00  0.0000E+00
 5.1546E+02  0.0000E+00  0.0000E+00
 7.2165E+02  0.0000E+00  0.0000E+00
```

Output times are written in 6 decimal places for the test version, and in 4 decimal places for the baseline version.

Test Status: <u>PASS</u>

PL-4. Name: NEFTRAN Input File

Path for run directory: d:\oosidele\run_tpa502r

Path for archive of results: \scr614_test\PC\Test4
(archived on CD named "Test Plan for SCR 614")

Environment variables: TPA_TEST=d:\oosidele\tpa502r
TPA_DATA=d:\oosidele\tpa502r

Special input files or modifications to input files required: None

Special diagnostic code modifications required :
tpa.inp: set thickness of CHnv layer to zero

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description:
Implement a flag in *tpa.inp* to allow the user to select using either average or time-dependent velocities in a NEFTRAN run; use the velocity of the first kept layer for the repository leg velocity; ensure the length of the first kept layer from the tpa.inp file is equal to the sum of the repository layer length and the adjusted length of that kept layer; ensure the dispersivities of the repository leg and the first kept layer are consistent with their lengths

Objective:
Verify that the changes described in the Test Description are correctly implemented.

Assumptions: None

Constraints: None

Output files to compare or examine: NEFTRAN input *(nefiiuz.inp)*

Step by step test procedure to be used:
1. Execute one realization of the test code with the specified modifications using the basecase *tpa.inp* file.
2. Set thickness of CHnv layer to zero to force selection of other UZ layers.
3. Repeat step 1.
4. Examine the layer properties in *nefiiuz.inp* obtained in steps 1 and 2.

Pass/Fail criteria:
1. When the tpa.inp parameter **UZVelocity(0=average,1=time-dependent)** is set to 0 the

NEFTRAN input file for uz calculations will use an average velocity value and when the parameter is set to 1 the NEFTRAN input file will select a time dependent velocity field.

2. The length of the first kept layer from the tpa.inp file is equal to the sum of the repository layer length and the adjusted length of that kept layer, and that the dispersivities of the repository leg and the first kept layer are consistent with their lengths.

Test Results:

-criterion 1

In the tpa.inp file the **UZVelocity(0=average,1=time-dependent)** parameter was set to zero and the TPA code was run. The tpa.inp and results of the run were saved in the CD archived directory *scr614\PC\Test4\runtpa502r_sa3_uzflag0.*

In addition the **UZVelocity(0=average,1=time-dependent)** parameter was set to one and the TPA code was run. The tpa.inp and results of the run were saved in the CD archived directory *scr614\PC\Test4\runtpa502r_sa3_uzflag1.*

A comparison between the two NEFTRAN input files shows the following differences

```
Comparing files RUN_TPA502R_SA3_UZFLAG0\nefiiuz.inp and
RUN_TPA502R_SA3_UZFLAG1\NEFIIUZ.INP
***** RUN_TPA502R_SA3_UZFLAG0\nefiiuz.inp
    1      SAMP.DAT, SAMPLED DATA FOR REPEATED TRIALS - READ FROM UNIT 10
    0      NEFII.VEL, UNIT 11, TIME-DEPENDENT VELOCITIES READ FROM
    0      SFLOW.DAT, UNIT 12, TIME-DEPENDENT SOURCE FLOW RATES READ FROM
***** RUN_TPA502R_SA3_UZFLAG1\NEFIIUZ.INP
    1      SAMP.DAT, SAMPLED DATA FOR REPEATED TRIALS - READ FROM UNIT 10
    1      NEFII.VEL, UNIT 11, TIME-DEPENDENT VELOCITIES READ FROM
    0      SFLOW.DAT, UNIT 12, TIME-DEPENDENT SOURCE FLOW RATES READ FROM
*****

***** RUN_TPA502R_SA3_UZFLAG0\nefiiuz.inp
    0      LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
    0      VELOCITY FIELDS FROM UNIT 11
    0      THE ATOM COUNT SUMMARY
***** RUN_TPA502R_SA3_UZFLAG1\NEFIIUZ.INP
    0      LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
    1      VELOCITY FIELDS FROM UNIT 11
    0      THE ATOM COUNT SUMMARY
*****

***** RUN_TPA502R_SA3_UZFLAG0\nefiiuz.inp
 #      (M)          (M)      N/Y=0/1  POROS.   POROS.   COEF(1/Y)      (M/YR)
  1 0.6684E+01      0.0        0     0.800E-01   0.000E+00   0.000E+00   0.269E+00
  2 0.6624E+01      0.0        0     0.800E-01   0.000E+00   0.000E+00   0.269E+00
***** RUN_TPA502R_SA3_UZFLAG1\NEFIIUZ.INP
 #      (M)          (M)      N/Y=0/1  POROS.   POROS.   COEF(1/Y)      (M/YR)
  1 0.6000E-01      0.0        0     0.800E-01   0.000E+00   0.000E+00   0.269E+00
  2 0.6624E+01      0.0        0     0.800E-01   0.000E+00   0.000E+00   0.269E+00
*****
```

The velocity Field in *scr614\PC\Test4\runtpa502r_sa3_uzflag1\nefiiuz.inp* is set to 1 requiring the velocity will be read in from a data file. In *scr614\PC\Test4\runtpa502r_sa3_uzflag0\nefiiuz.inp* the velocity field flag is set to zero and a mean velocity value is used for transport calculations.

These results are presented as evidence that SCR614 has been properly implemented.

-criterion 2

The length of the first leg accepted should be equal to the sum of the legs of the layer kept.
And the porosity and dispersivities should been properly calculated or retained.

When time dependent field velocities are used the dispersivity of each leg should be calculated using its individual leg length.

The following excerpt from the NEFTRAN input file
scr614\PC\Test4\runtpa502r_sa3_uzflag1\nefiiuz.inp , show a combined length of the two legs equal to 111.4 m and a porosity of 0.08.

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
LEG  INLET  OUTLET    LENGTH    AREA    HYDRAULIC   BRINE
 #    JCT    JCT       (M)     (M**2)   K  (M/YR)   CONC.
 1      1      2       1.0       0.0       0.0       0.0
 2      2      3     110.4       0.0       0.0       0.0
                    MIGRATION PATH PROPERTIES ARRAY
LEG   DISPERS.    SPA. STEP  DIFFUS  MOBILE  IMMOB   MASS  XFER   VELOCITY
 #      (M)         (M)     N/Y=0/1  POROS.  POROS.  COEF(1/Y)     (M/YR)
  1 0.6000E-01     0.0       0     0.800E-01  0.000E+00  0.000E+00  0.269E+00
  2 0.6624E+01     0.0       0     0.800E-01  0.000E+00  0.000E+00  0.269E+00
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

These values correspond to the Tsw_Thickness and its porosity from the *tpa.inp* file

The following is an excerpt from the tpa.inp file
scr614\PC\Test4\runtpa502r_sa3_uzflag0\tpa.inp

```
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
constant
TSw_Thickness_3SubArea[m]
111.4

constant
MatrixPorosity_TSw_
0.08

constant
MatrixLongitudinalDispersivity[FractionOfLayer]
0.06
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
```

The dispersivity of the first leg is 0.06 and the second leg is 6.6242. These values correctly reflect the value of the **MatrixLongitudinalDispersivity***leg length=dispersivity
ie. 0.06*1.0=0.06

and 0.06*110.4=6.624

However when an average field velocity is used, the dispersivity of the first leg should be calculated using the length of the entire thickness of the first layer and the remaining leg should use the remaining length of the layer

The following excerpt is from *scr614\PC\Test4\runtpa502r_sa3_uzflag1\nefiiuz.inp*, this realization used a average field velocity and the dispersivities of the first and second leg are 6.684 and 6.624.

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
LEG  INLET  OUTLET    LENGTH    AREA    HYDRAULIC   BRINE
 #    JCT    JCT        (M)     (M**2)   K  (M/YR)   CONC.
 1     1      2        1.0       0.0       0.0        0.0
 2     2      3      110.4       0.0       0.0        0.0
                    MIGRATION PATH PROPERTIES ARRAY
LEG   DISPERS.    SPA. STEP  DIFFUS  MOBILE  IMMOB   MASS  XFER   VELOCITY
 #      (M)         (M)     N/Y=0/1  POROS.  POROS.  COEF(1/Y)      (M/YR)
  1 0.6684E+01     0.0       0    0.800E-01  0.000E+00  0.000E+00   0.269E+00
  2 0.6624E+01     0.0       0    0.800E-01  0.000E+00  0.000E+00   0.269E+00
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

The dispersivity of the first leg reflects the dispersivity through the entire length of the layer 0.06*111.4=6.684.

The dispersitivity of the second leg reflects the dispersivity through the remaining lenght of the layer 0.06*110.4=6.624.

These results are presented as evidence that SCR614 has been properly implemented.

Test Status: <u>PASS</u>

PL-5. Name: Minimum Layer Thickness

Path for run directory: d:\oosidele\run_tpa502m
d:\oosidele\run_tpa502q

Path for archive of results: \scr614_test\PC\Test5
(archived on CD named "Test Plan for SCR 614")

Environment variables: TPA_TEST=d:\oosidele\tpa502m
TPA_DATA=d:\oosidele\tpa502m
TPA_TEST=d:\oosidele\tpa502q
TPA_DATA=d:\oosidele\tpa502q

Special input files or modifications to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Test description:
Setting UZ layer minimum sampled thickness to 5 cm. The code currently samples the thickness of the CHnv layer from a triangular distribution.

Objective:
Verify that users cannot sample UZ layer thickness less than 5cm.

Assumptions: None

Constraints: None

Output files to compare or examine: *tpamin.out* (minimum values of the parameters in *tpa.inp*)

Step by step test procedure to be used:
1. Execute one realization of the test code using the basecase *tpa.inp* file.
2. Execute one realization of the baseline code using the basecase *tpa.inp* file.
3. Compare the minimum parameter values written to *tpamin.out* in steps 1 and 2.

Pass/Fail criteria:
The minimum sampled layer thickness obtained from the test version (step 1) should be greater than or equal to 5 cm (0.05 m) in any subarea, while that obtained from the baseline version should be greater than or equal to 0.0 m.

Test Results:

Files on the CD in the *\scr614_test\PC\Test5* subdirectory contain results for this test. The relevant parts of *tpamin.out* from the test version (step 1) in *\run_tpa502q\tpamin.out* are as follows:

```
constant
CHnvThickness_1SubArea[m]
 5.000000000000000E-02
**
constant
CHnvThickness_2SubArea[m]
 5.000000000000000E-02
**
constant
CHnvThickness_3SubArea[m]
 5.000000000000000E-02
**
constant
CHnvThickness_4SubArea[m]
 5.000000000000000E-02
**
constant
CHnvThickness_5SubArea[m]
 5.000000000000000E-02
**
constant
CHnvThickness_6SubArea[m]
 51.70000000000000
**
constant
CHnvThickness_7SubArea[m]
 3.200000000000000
**
constant
CHnvThickness_8SubArea[m]
 2.400000000000000
**
constant
CHnvThickness_9SubArea[m]
 2.400000000000000
**
constant
CHnvThickness_10SubArea[m]
 3.900000000000000
**
```

The relevant parts of *tpamin.out* from the test version (step 2) in *\run_tpa502m\tpamin.out* are as follows:

```
constant
CHnvThickness_1SubArea[m]
 0.000000000000000E+00
**
constant
CHnvThickness_2SubArea[m]
 0.000000000000000E+00
```

```
**
constant
CHnvThickness_3SubArea[m]
 0.000000000000000E+00
**
constant
CHnvThickness_4SubArea[m]
 0.000000000000000E+00
**
constant
CHnvThickness_5SubArea[m]
 0.000000000000000E+00
**
constant
CHnvThickness_6SubArea[m]
 51.70000000000000
**
constant
CHnvThickness_7SubArea[m]
 3.200000000000000
**
constant
CHnvThickness_8SubArea[m]
 2.400000000000000
**
constant
CHnvThickness_9SubArea[m]
 2.400000000000000
**
constant
CHnvThickness_10SubArea[m]
 3.900000000000000
**
```

The minimum sampled layer thicknesses occur in subareas 1 through 5, which is concictent with the changes made in the *tpa.inp* file (see the parameter revisions table on pages 4 and 5 above).

Test Status: <u>PASS</u>

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 618	**2. Software Title and Version:** TPA 5.0.2a	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *gnewdf.dat*

Dose conversion factors have been recommended by the ICRP for calculating effective dose from internal and external sources and the NRC has requested implementation of the capability to use these alternate dose conversion factors. In order to keep the code consistent with the newest ICRP recommendations, updated dose conversion factors must be implemented that are derived from either a non-copyrighted source, a source from which permission has been granted, or a table with numeric indices for conversion factors.

5. Change Requested by: J Durham Date: 11-7-05	**6. Change Authorized by** (*Software Developer*): Ron Janetzke Date: 11-7-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See Attachment A

8. Implemented by: J. Mancillas	**Date:** 11-23 -05

9. Description of Acceptance Tests:

See Attachment B

10. Tested by: J Durham	**Date:** 12-19-05

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 618

Status (*ADD, DELETE, MODIFY TO, MODIFY FROM)*	Module	Parameter Name	Description (*Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)*	Distribution	Range	Justification *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	Source

ATTACHMENT A

The data file *gnewdf.dat* contains dose coefficients for the radionuclides considered within the TPA for dose assessment for the following age groups; infant, toddler, preteen, teen and adult. The dose coefficients for both inhalation and ingestion pathways for each age group were obtained from a search of the ICRP Database of Dose Coefficients: Workers and Members of the Public Version 2.0.1.

The value of the dose coefficients are dependent on particle size and Clearance Class (fast [f], moderate [m], and slow [s]) and whose selection was made on the judgement of technical experts: Patrick LaPlante and Roland Benke. These evaluations are recorded in the scientific notebook of Patrick LaPlante (#612-07E).

A brief summary of the selection method is as follows: particle size of 10 microns; for the age group 'toddler' the average of the ICRP values for ages 1yr and 5yr were used; and coefficient values were formatted to be consistent with the previous *gnewdf.dat* data format (3 significant figures).
The following is a list of the clearance classes used for each radionuclide.

Nuclide	Clearance Class
C 14	m
CL36	m
NI59	m
NI63	m
SE79	f
SR90	m
Y 90	s
MO93	m
ZR93	m
NB93M	m
NB94	m
TC99	m
PD107	s
AG108M	m
SN121M	m
SN121	m
SN126	f
SB126M	m
SB126	m
I 129	f
CS135	f
CS137	f
SM151	m
TH230	s
RA226	m
RN222	m
PB210	m

BI210	m
PO210	m
U 232	m
TH232	s
RA228	m
AC228	f
TH228	s
RA224	m
PB212	m
BI212	m
U 234	m
U 236	m
U 235	m
TH231	s
PA231	m
AC227	f
TH227	s
FR223	f
RA223	m
NP237	m
PA233	s
U 233	m
TH229	s
RA225	m
AC225	f
U 238	m
TH234	s
PA234	s
AM242M	s
AM242	m
CM242	m
PU242	m
NP238	m
PU238	m
CM244	m
PU244	m
U 240	m
PU240	m
CM245	m
PU241	m
AM241	m
CM246	m
CM243	m
PU243	m
AM243	m
NP239	m
PU239	m

The dose coefficients updated into *gnewdf.dat* are contained in the following data table generated by Patrick LaPlante.

Intake-to-Dose Conversion Factors for Inhalation and Ingestion from ICRP72 and Federal Guidance 11 (Sv/Bq) PAL 1/24/00,(MAS 1-26-00 Ag108m added), (MAS 1-27-00 new FGR11 values for Bi210, Pb212, Bi212), (PAL 1-27-00 Np238 added),(PAL 5-17-05 all ICRP 72 values for all age groups updated, all ICRP72 inhalation values based on 10 micron AMAD)

ICRP values (first 10 columns in data file) were queried from ICRPDOSE2 v2.01 software. Licence agreement contains the following statements:

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Nuclide	Infant --ing---^	Infant ---inh---^	Toddler ---ing---^	Toddler ---inh---^	Pre-teen ---ing---^	Pre-teen ---inh---^	Teen ---ing---^	Teen ---inh---^	Adult72 ---ing---^	Adult72 ---inh---^	AdultFG11 ---ing---^	AdultFG11 ---inh---
start_data												
C 14	1.40E-09	3.00E-09	1.30E-09	2.10E-09	8.00E-10	1.30E-09	5.70E-10	1.30E-09	5.80E-10	9.50E-10	5.64E-10	5.64E-10
CL36	9.80E-09	1.10E-08	4.75E-09	6.80E-09	1.90E-09	3.80E-09	1.20E-09	4.30E-09	9.30E-10	3.10E-09	8.18E-10	5.93E-09
NI59	6.40E-10	3.90E-10	2.65E-10	2.15E-10	1.10E-10	1.00E-10	7.30E-11	8.10E-11	6.30E-11	6.90E-11	5.67E-11	7.31E-10
NI63	1.60E-09	1.10E-09	6.50E-10	6.50E-10	2.80E-10	3.40E-10	1.80E-10	2.70E-10	1.50E-10	2.20E-10	1.56E-10	1.70E-09
SE79	4.10E-08	1.70E-08	2.35E-08	1.10E-08	1.40E-08	6.60E-09	4.10E-09	2.10E-09	2.90E-09	1.40E-09	2.35E-09	2.66E-09
SR90	2.30E-07	6.10E-08	6.00E-08	2.65E-08	6.00E-08	2.10E-08	8.00E-08	2.80E-08	2.80E-08	1.60E-08	3.85E-08	3.51E-07
Y 90	3.10E-08	1.30E-08	1.50E-08	6.55E-09	5.90E-09	2.70E-09	3.30E-09	1.90E-09	2.70E-09	1.40E-09	2.91E-09	2.28E-09
MO93	7.90E-09	1.10E-09	5.95E-09	7.50E-10	4.00E-09	4.10E-10	3.40E-09	3.90E-10	3.10E-09	3.30E-10	3.64E-10	7.68E-09
ZR93	1.20E-09	1.10E-09	6.35E-10	1.05E-09	5.80E-10	1.70E-09	8.60E-10	3.70E-09	1.10E-09	4.70E-09	4.48E-10	8.67E-08
NB93M	1.50E-09	1.20E-09	6.85E-10	6.95E-10	2.70E-10	3.40E-10	1.50E-10	2.50E-10	1.20E-10	2.00E-10	1.41E-10	7.90E-09
NB94	1.50E-08	1.80E-08	7.50E-09	1.25E-08	3.40E-09	7.10E-09	2.10E-09	6.30E-09	1.70E-09	4.70E-09	1.93E-09	1.12E-07
TC99	1.00E-08	6.70E-09	3.55E-09	4.05E-09	1.30E-09	2.30E-09	8.20E-10	2.80E-09	6.40E-10	1.90E-09	3.95E-10	2.25E-09
PD107	4.40E-10	4.60E-10	2.10E-10	3.45E-10	8.10E-11	2.00E-10	4.60E-11	1.90E-10	3.70E-11	1.70E-10	4.04E-11	3.45E-09
AG108M	2.10E-08	1.70E-08	8.75E-09	1.02E-08	4.30E-09	5.50E-09	2.80E-09	4.60E-09	2.30E-09	3.70E-09	2.06E-09	7.66E-08
SN121M	4.60E-09	6.70E-09	2.05E-09	4.30E-09	8.20E-10	2.40E-09	4.70E-10	2.90E-09	3.80E-10	2.10E-09	4.19E-10	3.11E-09
SN121	2.60E-09	1.40E-09	1.27E-09	7.50E-10	5.00E-10	3.50E-10	2.80E-10	3.00E-10	2.30E-10	2.20E-10	2.44E-10	1.38E-10
SN126	5.00E-08	6.70E-08	2.30E-08	4.20E-08	9.80E-09	2.00E-08	5.90E-09	1.50E-08	4.70E-09	1.20E-08	5.27E-09	2.69E-08
SB126M	3.90E-10	2.30E-10	1.65E-10	1.23E-10	6.60E-11	5.20E-11	4.50E-11	3.90E-11	3.60E-11	3.10E-11	2.54E-11	9.17E-12
SB126	2.00E-08	1.40E-08	1.08E-08	8.75E-09	4.90E-09	4.20E-09	3.10E-09	3.40E-09	2.40E-09	2.50E-09	2.89E-09	3.17E-09
I 129	1.80E-07	7.60E-08	1.95E-07	8.15E-08	1.90E-07	8.00E-08	1.40E-07	6.30E-08	1.10E-07	4.60E-08	7.46E-08	4.69E-08
CS135	4.10E-09	1.90E-09	2.00E-09	9.35E-10	1.70E-09	7.50E-10	2.00E-09	9.40E-10	2.00E-09	8.90E-10	1.91E-09	1.23E-09
CS137	2.10E-08	9.80E-09	1.08E-08	5.30E-09	1.00E-08	4.60E-09	1.30E-08	6.20E-09	1.30E-08	6.00E-09	1.35E-08	8.63E-09
SM151	1.50E-09	4.10E-09	4.85E-10	3.15E-09	2.00E-10	2.00E-09	1.20E-10	2.00E-09	9.80E-11	1.80E-09	1.05E-10	8.10E-09

TH230	4.10E-06	1.50E-05	3.60E-07	1.07E-05	2.40E-07	6.70E-06	2.20E-07	5.10E-06	2.10E-07	4.40E-06	1.48E-07	8.80E-05
RA226	4.70E-06	4.80E-06	7.90E-07	3.05E-06	8.00E-07	2.00E-06	1.50E-06	2.10E-06	2.80E-07	1.60E-06	3.58E-07	2.32E-06
RN222	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
PB210	8.40E-06	2.60E-06	2.90E-06	1.35E-06	1.90E-06	8.30E-07	1.90E-06	7.00E-07	6.90E-07	5.20E-07	1.45E-06	3.67E-06
BI210	1.50E-08	1.10E-07	7.25E-09	7.70E-08	2.90E-09	5.00E-08	1.60E-09	5.20E-08	1.30E-09	3.70E-08	1.73E-09	5.29E-08
PO210	2.60E-05	5.40E-06	6.60E-06	3.10E-06	2.60E-06	1.60E-06	1.60E-06	1.90E-06	1.20E-06	1.40E-06	5.14E-07	2.54E-06
U 232	2.50E-06	9.08E-04	7.00E-07	6.65E-06	5.70E-07	3.70E-06	6.40E-07	4.70E-06	3.30E-07	3.10E-06	3.54E-07	1.78E-04
TH232	4.60E-06	1.80E-05	4.00E-07	1.40E-05	2.90E-07	9.60E-06	2.50E-07	1.00E-05	2.30E-07	9.60E-06	7.38E-07	4.43E-04
RA228	3.00E-05	6.50E-06	4.55E-06	2.30E-06	3.90E-06	1.80E-06	5.30E-06	2.40E-06	6.90E-07	9.90E-07	3.88E-07	1.29E-06
AC228	7.40E-09	1.60E-07	2.10E-09	1.17E-07	8.70E-10	5.50E-08	5.30E-10	3.20E-08	4.30E-10	2.60E-08	5.85E-10	8.33E-08
TH228	3.70E-06	5.30E-05	2.95E-07	3.95E-05	1.50E-07	2.40E-05	9.40E-08	2.70E-05	7.20E-08	2.00E-05	1.07E-07	9.23E-05
RA224	2.70E-06	3.70E-06	5.05E-07	2.30E-06	2.60E-07	1.50E-06	2.00E-07	2.10E-06	6.50E-08	1.40E-06	9.89E-08	8.53E-07
PB212	1.50E-07	3.80E-07	4.80E-08	2.35E-07	2.00E-08	1.50E-07	1.30E-08	1.40E-07	6.00E-09	1.20E-07	1.23E-08	4.56E-08
BI212	3.20E-09	1.40E-07	1.34E-09	8.00E-08	5.00E-10	4.30E-08	3.30E-10	4.50E-08	2.60E-10	3.40E-08	2.87E-10	5.83E-09
U 234	3.70E-07	4.30E-06	1.09E-07	3.00E-06	7.40E-08	1.90E-06	7.40E-08	1.80E-06	4.90E-08	1.60E-06	7.66E-08	3.58E-05
U 236	3.50E-07	4.00E-06	1.07E-07	2.80E-06	7.00E-08	1.80E-06	7.00E-08	1.70E-06	4.70E-08	1.50E-06	7.26E-08	3.39E-05
U 235	3.50E-07	3.80E-06	1.08E-07	2.70E-06	7.10E-08	1.70E-06	7.00E-08	1.60E-06	4.70E-08	1.40E-06	7.19E-08	3.32E-05
TH231	3.90E-09	2.20E-09	1.85E-09	1.18E-09	7.40E-10	5.40E-10	4.20E-10	4.30E-10	3.40E-10	3.20E-10	3.65E-10	2.37E-10
PA231	1.30E-05	8.40E-05	1.20E-06	7.90E-05	9.20E-07	6.80E-05	8.00E-07	7.30E-05	7.10E-07	6.30E-05	2.86E-06	3.47E-04
AC227	3.30E-05	1.50E-03	2.65E-06	1.15E-03	1.50E-06	7.00E-04	1.20E-06	6.10E-04	1.10E-06	5.50E-04	3.80E-06	1.81E-03
TH227	3.00E-07	9.80E-06	5.30E-08	7.15E-06	2.30E-08	4.90E-06	1.50E-08	6.80E-06	8.80E-09	4.70E-06	1.03E-08	4.37E-06
FR223	2.60E-08	1.20E-08	1.27E-08	6.05E-09	5.00E-09	2.40E-09	2.90E-09	1.50E-09	2.40E-09	1.20E-09	2.33E-09	1.68E-09
RA223	5.30E-06	8.60E-06	8.35E-07	5.50E-06	4.50E-07	3.70E-06	3.70E-07	5.10E-06	1.00E-07	3.50E-06	1.78E-07	2.12E-06
NP237	2.00E-06	1.40E-05	1.75E-07	1.20E-05	1.10E-07	8.90E-06	1.10E-07	1.10E-05	1.10E-07	1.00E-05	1.20E-06	1.46E-04
PA233	9.70E-09	8.10E-09	4.70E-09	5.05E-09	1.90E-09	2.60E-09	1.10E-09	3.00E-09	8.70E-10	2.10E-09	9.81E-10	2.58E-09
U 233	3.80E-07	4.40E-06	1.16E-07	3.05E-06	7.80E-08	2.00E-06	7.80E-08	1.90E-06	5.10E-08	1.70E-06	7.81E-08	3.66E-05
TH229	1.10E-05	7.70E-05	8.90E-07	5.80E-05	6.20E-07	3.60E-05	5.30E-07	3.80E-05	4.90E-07	3.20E-05	9.54E-07	5.80E-04
RA225	7.10E-06	5.80E-06	9.05E-07	4.10E-06	5.00E-07	3.10E-06	4.40E-07	4.30E-06	9.90E-08	2.90E-06	1.04E-07	2.10E-06
AC225	4.60E-07	9.20E-06	1.36E-07	5.20E-06	5.40E-08	2.60E-06	3.00E-08	1.20E-06	2.40E-08	8.80E-07	3.00E-08	2.92E-06
U 238	3.40E-07	3.60E-06	1.00E-07	2.45E-06	6.80E-08	1.60E-06	6.70E-08	1.40E-06	4.50E-08	1.30E-06	6.88E-08	3.20E-05
TH234	4.00E-08	2.10E-08	1.90E-08	1.14E-08	7.40E-09	5.90E-09	4.20E-09	5.30E-09	3.40E-09	4.00E-09	3.69E-09	9.47E-09
PA234	5.00E-09	3.40E-09	2.45E-09	1.95E-09	1.00E-09	8.90E-10	6.40E-10	6.80E-10	5.10E-10	5.10E-10	5.84E-10	2.20E-10
AM242M	3.10E-06	2.00E-05	2.65E-07	1.75E-05	2.00E-07	1.50E-05	1.90E-07	1.70E-05	1.90E-07	1.70E-05	9.50E-07	1.15E-04
AM242	5.00E-09	2.10E-08	1.65E-09	1.50E-08	6.40E-10	9.40E-09	3.70E-10	1.10E-08	3.00E-10	7.80E-09	3.81E-10	1.58E-08
CM242	5.90E-07	6.00E-06	5.75E-08	4.30E-06	2.40E-08	2.80E-06	1.50E-08	3.30E-06	1.20E-08	2.30E-06	3.10E-08	4.67E-06
PU242	4.00E-06	2.70E-05	3.60E-07	2.40E-05	2.60E-07	1.90E-05	2.30E-07	2.20E-05	2.40E-07	2.20E-05	9.08E-07	1.11E-04
NP238	9.50E-09	6.00E-09	4.70E-09	3.30E-09	1.90E-09	1.60E-09	1.10E-09	1.50E-09	9.10E-10	1.20E-09	1.08E-09	1.00E-08
PU238	4.00E-06	2.70E-05	3.55E-07	2.40E-05	2.40E-07	1.90E-05	2.20E-07	2.10E-05	2.30E-07	2.10E-05	8.65E-07	1.06E-04
CM244	2.90E-06	2.10E-05	2.40E-07	1.65E-05	1.40E-07	1.10E-05	1.20E-07	1.30E-05	1.20E-07	1.20E-05	5.45E-07	6.70E-05
PU244	4.00E-06	2.60E-05	3.65E-07	2.35E-05	2.60E-07	1.90E-05	2.30E-07	2.20E-05	2.40E-07	2.10E-05	8.97E-07	1.09E-04
U 240	1.30E-08	5.00E-09	6.10E-09	3.00E-09	2.40E-09	1.30E-09	1.40E-09	8.90E-10	1.10E-09	6.80E-10	1.20E-09	6.13E-10
PU240	4.20E-06	2.80E-05	3.75E-07	2.55E-05	2.70E-07	2.10E-05	2.40E-07	2.30E-05	2.50E-07	2.30E-05	9.56E-07	1.16E-04
CM245	3.70E-06	2.50E-05	3.25E-07	2.20E-05	2.30E-07	1.70E-05	2.10E-07	2.00E-05	2.10E-07	1.90E-05	1.01E-06	1.23E-04
PU241	5.60E-08	3.50E-07	5.60E-09	3.70E-07	5.10E-09	3.70E-07	4.80E-09	4.30E-07	4.80E-09	4.20E-07	1.85E-08	2.23E-06
AM241	3.70E-06	2.50E-05	3.20E-07	2.20E-05	2.20E-07	1.70E-05	2.00E-07	2.00E-05	2.00E-07	1.90E-05	9.84E-07	1.20E-04
CM246	3.70E-06	2.50E-05	3.25E-07	2.20E-05	2.20E-07	1.70E-05	2.10E-07	2.00E-05	2.10E-07	1.90E-05	1.00E-06	1.22E-04
CM243	3.20E-06	2.30E-05	2.75E-07	1.85E-05	1.60E-07	1.30E-05	1.40E-07	1.50E-05	1.50E-07	1.40E-05	6.79E-07	8.30E-05

PU243	1.00E-09	6.10E-10	4.65E-10	3.15E-10	1.80E-10	1.40E-10	1.10E-10	1.20E-10	8.50E-11	9.20E-11	9.02E-11	4.44E-11
AM243	3.60E-06	2.50E-05	3.20E-07	2.10E-05	2.20E-07	1.70E-05	2.00E-07	2.00E-05	2.00E-07	1.90E-05	9.79E-07	1.19E-04
NP239	8.90E-09	5.10E-09	4.30E-09	2.75E-09	1.70E-09	1.30E-09	1.00E-09	1.10E-09	8.00E-10	8.30E-10	8.82E-10	6.78E-10
PU239	4.20E-06	2.80E-05	3.75E-07	2.55E-05	2.70E-07	2.10E-05	2.40E-07	2.30E-05	2.50E-07	2.30E-05	9.56E-07	1.16E-04

Attachment B
Test Plan for TPA SCR#618

Test Plan Name:

Tested By: JS Durham | Date: 12/19/05

Host Machine: GoldSim, Spock | Host OS: Windows XP, UNIX

Baseline Version: TPA 5.02 | Test Version: TPA 5.02a

System Level (SL) Tests

PL-1. Name: Data Verification
Path for run directory: [GRYPHON]:ICRPDOSE2 Version 2.0.1
Path for archive of results: N/A
Environment variables: N/A
Special input files or modifications to input files required: N/A
Special diagnostic code modifications required: N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data: N/A

Test description:
- The objective of the test was to verify that the data in the table supplied by Pat LaPlante were consistent with the data generated using ICRPDOSE2 Version 2.0.1.
- The only assumption made was that the technical basis for selecting the clearance class for each radionuclide was correct

Procedure: 1) verify the data supplied by Pat LaPlante by reproducing each of the values and comparing them to the supplied data
- The data supplied by Pat LaPlante will pass if the values can be reproduced using ICRPDOSE2 Version 2.0.1

Test Results: - The following calculated data parameters did not match the data supplied by Pat LaPlante: U-232, Infant, Inhalation: LaPlante: 9.08E-04, Current Test: 9.08E-08
LaPlante: Th-228, Preteen, Ingestion:: LaPlante: 1.50E-07, Current Test: 1.40E-07

Evidence: See Attachment C for the ICRPDOSE2 data that did not match the LaPlante file.

- **Overall test status**: **FAIL** This item will be addressed in SCR621.

System Level Test SL-2. Name: Input File Data Verification
Path for run directory: N/A
Path for archive of results: N/A
Environment variables: N/A
Special input files or modifications to input files required: N/A
Special diagnostic code modifications required: N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data: N/A

Test description: - The objective of the test was to verify that the data in the table supplied by Pat LaPlante were correctly implemented into *gnewdf.dat*

Procedure: 1) verify the data in *gnewdf.dat* by comparing the data in the file with the data supplied by Pat LaPlante

- The datafile will pass if the values are identical to the data supplied by Pat LaPlante

Test Results: - All data matched the data supplied by Pat LaPlante.

- Overall test status: **PASS**

System Level Test SL-3. Name: Code Execution Test

Path for run directory: Windows Base case: [Goldsim]\SCR618PC\tpa502\
Windows Test case: [Goldsim]\SCR618PC\tpa502a\
UNIX Base case: [Spock]\SCR618UNIX\tpa502\
Unix Test case: [Spock]\SCR618UNIX\tpa502a\

Path for archive of results: Windows Base Case: \SCR618PC\tpa502\SCRBASE\
Windows Test Case: \SCR618PC\tpa502a\SCRTEST\
UNIX Base Case: \SCR618UNIX\tpa502\SCRBASE\
UNIX Test Case: \SCR618UNIX\tpa502a\SCRTEST\

All files are on CD Rom entitled "TPA SCR-618"

Environment variables: Windows Base Case: \SCR618PC\tpa502\
Windows Test Case: \SCR618PC\tpa502a\
UNIX Base Case: \SCR618PC\tpa502\
UNIX Test Case: \SCR618PC\tpa502a\

Special input files or modifications to input files required: Updated *gnewdf.dat* by replacing the existing file with a file containing two corrections. The new *gnewdf.dat* will be incorporated into the TPA code in the future.

Special diagnostic code modifications required: N/A

Program modes to be used (append flags, scenario/model switches, etc.): N/A

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data: N/A

Test description: - The objective of the test was to verify that the TPA code operated properly with the new version of *gnewdf*.dat for both Windows and UNIX operating systems and that comparable results using the two operating systems were identical

- **Procedure**:

1) run the TPA code under the Windows OS with the old data in *gnewdf.dat*
2) run the TPA code under the Windows OS with the updated data in *gnewdf.dat*
3) compare the two output files (*tpa.out*) using the FC command (*FC_TPA.OUT*)
4) run the TPA code under the UNIX OS with the old data in *gnewdf.dat*
5) run the TPA code under the UNIX OS with the updated data in *gnewdf.dat*
6) compare the two output files (*tpa.out*) using the DIFF command (*DIFF_TPA.OUT*)

The datafile will pass if the code executes properly and there are small but measurable differences between the two output files

Test Results: - **Code operated properly**
- **Differences between old and new values were small but measurable**
- **Comparable results from Windows and UNIX Operating Systems were identical**
- **Evidence**: See data files \SCR618UNIX\tpa502a\scrtest*DIFF_TPA.OUT* for UNIX results and \SCR618PC\tpa502a\scrtest*FC_TPA.OUT* for Windows results. . The files contain the lines that are different between the base case and the test case for each operating system.

- **Overall test status: PASS**

Notes: Results of calculations are on the attached disk entitled "TPA SCR-618".

Attachment C

Results of ICRPDOSE2 Calculations that Did Not Match the Tabulated Values

U-232, 3-month-old member of the public
Inhalation of particulate aerosol: AMAD =10.000 micron, absorption Type M, f1 = 0.04
Highest committed equivalent dose coefficient: ET Airways, 1.2E-04 Sv/Bq
Remainder formulation: split

Time after intake	69y 9m
Effective dose	9.80E-06

Th-228, 10-year-old member of the public
Ingestion: f1 = 0.0005
Highest committed equivalent dose coefficient: Bone Surface, 4.3E-06 Sv/Bq
Remainder formulation: default

Time after intake	60 years
Effective dose	1.40E-07

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 619	**2. Software Title and Version:** TPA 5.0.2i	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *ashremob.f, remob_lut.dat*

There is a disconnect between the source term used for ASHREMOB and that provided by VOLCANO. ASHREMOB uses a sampled number of waste packages for the source term and VOLCANO provides the number of waste packages ejected due to an extrusive event. These are inconsistent since they are not constrained to be the same value.

5. Change Requested by:	**6. Change Authorized by** (*Software Developer*):
R. Benke Date: 11/04/2005	R. Janetzke Date: 11/4/2005

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): The following changes will affect a solution:

1) Accept MTU ejected from the VOLCANO module as the only source term.
2) Recompute the *remob_lut.dat* file to generate high-level waste values based on a constant source term of 1 MTU.
3) Allow for data with values of zero in the *remob_lut.dat* file.
4) Account for both spent nuclear fuel and glass waste forms when determining inventory.

DETAILS:

1) & 2) In *ashremob.f*, comment out the line:

```
remperyrpernuclgs(j,k) = doseinh(j,ik)
```

Add the following new comment and code lines:

```
cc SCR619 (add initials & date)  Since the look-up table values are now based on 1 MTU of HLW,
cc the dose calculation must scale the results for the actual MTU of HLW entrained in the
eruption.
      remperyrpernuclgs(j,k) = doseinh(j,ik) * amtuejected
```

3) Modify concentration factor calculations in *ashremob.f* to accept ash mass values of zero for initial and fluvial conditions by inserting an "`if..then`" test before the calculation to avoid error conditions.

4) Modify the calculation of `ciperghlw(it,k)`, via subroutines **decay43mol()** and **decay43molglass()** in the ASHREMOB module, to use both inventory sets in *nuclides.dat* under the column headers CPMTU[Ci/MTU] for CSNF and CPMGLASS[Ci/MTU] for non-CSNF waste, where one gram of high-level waste, averaged over the entire repository, is calculated as:

1 gram of average HLW = $(1-f)$ grams of CSNF waste + f grams of non-CSNF waste

with f = **FractionOfRepositoryWasteInGlassForm[]** (TPA input parameter).

8. Implemented by:	**Date:**
Jose M. Menchaca	02/16/2006

9. Description of Acceptance Tests:

See Attachment A

10. Tested by:	**Date:**
Ali A. Simpkins	3/28/06

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 619

Status (*ADD, DELETE, MODIFY TO, MODIFY FROM)*	Module	Parameter Name	Description (*Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)*	Distribution	Range	Justification *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	Source

Attachment A

Test Plan Name: TPA SCR#619

Tested By: Ali A. Simpkins | Date: 3/31/06

Host Machine: TPA | Host OS: DOS

Baseline Version: TPA 5.0.2i | Test Version: TPA 5.0.2j and 5.0.2l

System Level Tests

SL-1 Name: ASHREMOB Change testing different diameter of volcano (Test A)
Path for run directory:[TPA]:asimpkins\tparun
Path for archive of results:CD: [SCR620]SCR620\TestA
Environment variables:[TPA Machine]: Set TPA_TEST=d:\ASimpkins\tpa502j
Set TPA_DATA=d:\ASimpkins\tpa502j
Special input files or modifications to input files required : A new lookup table (remob_lut.dat) based on a 500-m grid spacing should be obtained from D. Hooper and N. Franklin. The lookup table should be incorporated into the \Data directory prior to performing the acceptance testing.
Special diagnostic code modifications required :N/A
Program modes to be used (append flags, scenario/model switches, etc.):N/A
Utility scripts needed to perform the test:N/A
Utility codes needed in the analysis of the test data:N/A
Test description: The objective of the test is to ensure resulting doses scale directly with changes to the diameter of the volcano conduit.

Test performed using TPA 5.0.2j
Setup the TPA code with the following inputs:
SimulationTime set to 10,000 years (default for basecase)
Turn on Volcano flag for igneous activity
TimeOfNextVolcanicEvent set to a constant at 500 years
DirectReleaseOnly set to 1
NumberOfRealizations set to 1024
AshEvolutionMode set to 1 (default)

Run the TPA code three times by setting the DiameterOfVolcanicConduit to a constant at 10 m, 20 m, or 50 m. For each run, record the total inhalation dose at two times, the year of the event (~500 years) and ~1000 years. For each time, normalize the 20-m and 50-m results by the 10-m result.

The test is passed if the 20-m results are between 1.9 to 2.1 times greater than the 10-m results for both times and if the 50-m results are between 4.75 to 5.25 times greater than the 10-m results for both times.

Test Results:

Diameter of Conduit (m)	Total Inhalation Dose at 501 yrs	Normalized to 10-m result	Normalized result in desired range?	Total Inhalation Dose at 1022 yrs	Normalized to 10-m result	Normalized result in desired range?
10	1.02E-01			1.21E-02		
20	2.04E-01	2.00	**PASSED**	2.42E-02	2.00	**PASSED**
50	5.09E-01	5.00	**PASSED**	6.05E-02	5.00	**PASSED**

Evidence: See data files : [SCR619]: \SCR619\Test A\totdoseA10.res
[SCR619]: \SCR619\Test A\totdoseA20.res
[SCR619]: \SCR619\Test A\totdoseA50.res

Overall test status: **PASSED**

SL-2 Name: ASHREMOB Change testing different number of waste packages entrained (Test B)
Path for run directory:[TPA]:asimpkins\tparun
Path for archive of results:CD: [SCR620]SCR620\TestB
Environment variables:[TPA Machine]: Set TPA_TEST=d:\ASimpkins\tpa502j
Set TPA_DATA=d:\ASimpkins\tpa502j
Special input files or modifications to input files required : A new lookup table (remob_lut.dat) based on a 500-m grid spacing should be obtained from D. Hooper and N. Franklin. The lookup table should be incorporated into the \Data directory prior to performing the acceptance testing.
Special diagnostic code modifications required :N/A
Program modes to be used (append flags, scenario/model switches, etc.):N/A
Utility scripts needed to perform the test:N/A
Utility codes needed in the analysis of the test data:N/A
Test description: The objective of the test is ensure resulting doses scale directly with changes to the number of entrained waste packages.
Test performed using TPA 5.0.2j
Setup the TPA code with the following inputs:
SimulationTime set to 10,000 years
Turn on Volcano flag for igneous activity
TimeOfNextVolcanicEvent set to a constant at 500 years
DirectReleaseOnly set to 1
Select the VOLCANO Distribution Model (not the Geometric model)
NumberOfRealizations set to 1024
AshEvolutionMode set to 1

Run the TPA code two times by setting the NumberOfWP Entrained In Ejecta to a constant at 10 and 100 waste packages. For each run, record the total inhalation dose at two times, the year of the event (~500 years) and ~1000 years. For each time, divide the 100-WP results by the 10-WP results.

The test is passed if the 100-WP result is between 9.95 to 10.5 times greater than the 10-WP result for both times.

Test Results:

Number of WP	Total Inhalation Dose at 501 yrs	Normalized to 10 WP result	Normalized result in desired range?	Total Inhalation Dose at 1022 yrs	Normalized to 10 WP result	Normalized result in desired range?
10	9.47E-01			1.29E-01		
100	9.47E+00	10	**PASSED**	1.29E+00	10	**PASSED**

Evidence: See data files: [SCR619]: \SCR619\Test B\totdoseB10.res
[SCR619]: \SCR619\Test B\totdoseB100.res

Overall test status: **PASSED**

SL-3 Name: ASHREMOB Change testing different glass repository fractions (Test C)
Path for run directory:[TPA]:asimpkins\tparun
Path for archive of results:CD: [SCR620]SCR620\TestC
Environment variables:[TPA Machine]: Set TPA_TEST=d:\ASimpkins\tpa502j
Set TPA_DATA=d:\ASimpkins\tpa502j
Special input files or modifications to input files required : A new lookup table (remob_lut.dat) based on a 500-m grid spacing should be obtained from D. Hooper and N. Franklin. The lookup table should be incorporated into the \Data directory prior to performing the acceptance testing.
Special diagnostic code modifications required :N/A
Program modes to be used (append flags, scenario/model switches, etc.):N/A
Utility scripts needed to perform the test:N/A
Utility codes needed in the analysis of the test data:N/A
Test description: The objective of the test is ensure resultant doses are produced correctly with various fractions of repository glass.
Test performed using TPA 5.0.2j
Setup the TPA code with the following inputs:
SimulationTime set to 10,000 years
Turn on Volcano flag for igneous activity
TimeOfNextVolcanicEvent set to a constant at 500 years
DirectReleaseOnly set to 1
NumberOfRealizations set to 1024
AshEvolutionMode set to 1
Set SpentFuelWastePackagePayload[MTU] to a constant at 6.0
Set EquivalentMTUPayloadOfGlassPackage[MTU] to a constant at 6.0

Record total inhalation dose from at two times, the year of the event (~500 years) and ~1000 years. These results are denoted by d_base(500yr) and d_base(1000yr). Record the default value for the input parameter FractionOfRepositoryAsGlass (referred to as f_default).

Change the value of the input parameter FractionOfRepositoryAsGlass to zero and rerun. Record total inhalation dose at two times, the year of the event (~500 years) and ~1000 years. These results are denoted by d_zero(500yr) and d_zero(1000yr).

Change the value of the input parameter FractionOfRepositoryAsGlass to one and rerun. Record total inhalation dose from at two times, the year of the event (~500 years) and ~1000 years. These results are denoted by d_one(500yr) and d_one(1000yr).

The test is passed if the following two conditions are met:

$$0.99 <= X <= 1.01 \quad \text{and} \quad 0.99 <= Y <= 1.01$$

where

$$X = \{ [d\_zero(500yr) * (1 - f\_default)] + [d\_one(500yr) * f\_default] \} / d\_base(500yr)$$

and

$$Y = \{ [d\_zero(1000yr) * (1 - f\_default)] + [d\_one(1000yr) * f\_default] \} / d\_base(1000yr)$$

Test results:

	Fraction of Repository as Glass	Inhalation Dose at 501 yr	Inhalation Dose at 1022 yr	X	Y
f_default	0.0126	2.43E-03	2.23E-03	1.000028567	0.999997351
	0	2.45E-03	2.24E-03	**PASSED**	**PASSED**
	1	1.17E-03	1.49E-03		

Evidence: See data files: [SCR619]: \SCR619\Test C\totdoseC0.res
[SCR619]: \SCR619\Test C\totdoseC1.res
[SCR619]: \SCR619\Test C\totdoseCdefault.res

Overall test status: **PASSED**

SL-4 Name: ASHREMOB Change testing remob_lut file (Test D)
Path for run directory:[TPA]:asimpkins\tparun
Path for archive of results:CD: [SCR620]SCR620\TestD
Environment variables:[TPA Machine]: Set TPA_TEST=d:\ASimpkins\tpa502j
Set TPA_DATA=d:\ASimpkins\tpa502j
Special input files or modifications to input files required : Use old remob_lut file that corresponds to previous version of TPA code
Special diagnostic code modifications required :N/A
Program modes to be used (append flags, scenario/model switches, etc.):N/A
Utility scripts needed to perform the test:N/A
Utility codes needed in the analysis of the test data:N/A
Test description: The objective of the test is to configure the modified version of the code to behave like the previous unmodified verison and quantitatively compare results.

Select a recent version of the TPA code just prior to the version with incorporated changes from this SCR. The version without incorporated changes from this SCR and the old lookup table (not the updated lookup table) is referred to as the "prior version." The version of the TPA code with incorporated changes from this SCR and the old lookup table (not the updated lookup table) is referred to as the "test version." The old lookup table (3 significant digits) should be used for all Test D calculations. Test D does not use the new lookup table (4 significant digits).

Identify and record the lookup table index value, AshPlumeRealizationIndex[] (*i.e., row number* in remob_lut.dat), corresponding to the largest value of m_HLW_f.
Check: The maximum value of m_HLW_f should be within 5 percent of 78.9 metric tons. Notify the requestor of this SCR if this check is not passed.

Run Prior Version (Source Term ~ 78.9 MTU) with the following inputs:

- SimulationTime set to 10,000 years
- Set VolcanismDisruptiveScenarioFlag(yes=1,no=0) to a value of 1
- TimeOfNextVolcanicEvent set to a constant at 500 years
- DirectReleaseOnly flag set to 1
- NumberOfRealizations set to 1
- AshEvolutionMode set to 1
- Set AshPlumeRealizationIndex[] to an iconstant at the value recorded above
- Set all MassLoad parameters (found in MASS LOADING AND OCCUPANCY FACTORS block) to constants at the maximum value from their default distributions
- WeightingFactorInitialDeposit[] set to 0
- WeightingFactorEolian[] set to 0
- Set SpentFuelWastePackagePayload[MTU] to a constant at 6.0
- Set EquivalentMTUPayloadOfGlassPackage[MTU] to a constant at 6.0
- AmbientSedimentYieldVolumePerBasinAreaPerEvent[m/event] set to a constant at 0.00003
- PostEruptionFluvialAshYieldVolumePerAreaPerEvent[m/event] set to a constant at 0.00006

(Note: The coorelation between AmbientSedimentYieldVolumePerBasinAreaPerEvent[m/event] & PostEruptionFluvialAshYieldVolumePerAreaPerEvent[m/event], defined in the input file, may have to relaxed to avoid warnings or errors.)
Record total inhalation dose from prior version at ~1000 years and ~1500 years.

Run Test Version (Source Term ~ 60.0*78.9 MTU) with the same inputs above plus the following settings:

- (Same inputs as noted above)
- Change VolcanoModel(1=Geometric,2=Distribution) to a value of 2
- Change the NumberOfWPsEntrainedByEjecta[] from a Beta distribution to a constant at 10
- Modify the *nuclides.dat* auxiliary data file by overwriting the GlassWP inventory column [Ci/MTU] with the same values in the CSNF column.

Record total inhalation dose from test version at ~1000 years and ~1500 years.

The test is passed if both conditions below are met (note factor of 60 equates the source term):
0.9 <= [(Test Version result at 1000 years) / (60.0 * Prior Version result at 1000 years)] <= 1.10
0.9 <= [(Test Version result at 1500 years) / (60.0 * Prior Version result at 1500 years)] <= 1.10

Test results

Row number in remob_lut.dat corresponding to the largest value of m_HLW_f = row 826
The maximum value of m_HLW_f is 78.9 metric tons which is within 5 percent of 78.9 metric tons

Time (yr)	Inhalation Dose - Prior Version	Inhalation Dose - Test Version	Test	
1022	6.43E-01	3.86E+01	1.00E+00	**PASSED**
1524	4.73E-01	2.84E+01	1.00E+00	**PASSED**

Evidence: See data files: [SCR619]: \SCR619\Test D\totdoseprior.res
[SCR619]: \SCR619\Test D\totdosetest.res

Overall test status: **PASSED**

SL-5 Name: ASHREMOB Change testing different diameter of volcano (Test E) - Test performed on UNIX platform
Path for run directory:[spock]:home/asimpkins/tparun
Path for archive of results:CD: [SCR620]SCR620\TestE
Environment variables:[SPOCK Machine]: Setenv TPA_TEST /home/ASimpkins\tpa502j
Setenv TPA_DATA /home/ASimpkins\tpa502j
Special input files or modifications to input files required : A new lookup table (remob_lut.dat) based on a 500-m grid spacing should be obtained from D. Hooper and N. Franklin. The lookup table should be incorporated into the \Data directory prior to performing the acceptance testing.
Special diagnostic code modifications required :N/A
Program modes to be used (append flags, scenario/model switches, etc.):N/A
Utility scripts needed to perform the test:N/A
Utility codes needed in the analysis of the test data:N/A

Test description: The objective of the test is to demonstrate the model executes correctly on the UNIX platform.

Test performed using TPA 5.0.2j
Setup the TPA code with the following inputs:
SimulationTime set to 10,000 years (default for basecase)
Turn on Volcano flag for igneous activity
TimeOfNextVolcanicEvent set to a constant at 500 years
DirectReleaseOnly set to 1
NumberOfRealizations set to 1024
AshEvolutionMode set to 1 (default)
Diameter of Volanic Conduit = 10 m

Test passes if output is the same as the PC version output.

Evidence: See data files: [SCR619]: \SCR619\Test E\totdoseE10unix.res
[SCR619]: \SCR619\Test E\tpaE10unix.out

Test Results: **PASSED**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 620	**2. Software Title and Version:** TPA 5.0.2i	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *ashremob.f*

ASHREMOB module output file, named *ashremob.out*, needs descriptive column headers.

5. Change Requested by:	**6. Change Authorized by** (*Software Developer*):
R. Benke Date: 11/04/2005	R. Janetzke Date: 11-4-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

Add the descriptive file and column headers, as shown in Figure 1, below the general TPA code header information (code version, date, etc.) in the output file named *ashremob.out*.

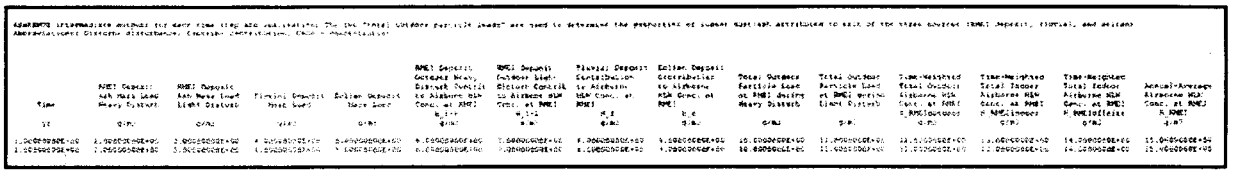

Figure 1. Descriptive header information for *ashremob.out*

Three sections of 5 columns each are provided in Attachment A, thus giving an enlargement of the 15 columns in Figure 1.

See Attachment B, for implementation **diff** file.

8. Implemented by:	**Date:**
Jose M. Menchaca	12/01/2005

9. Description of Acceptance Tests:

See Attachment C

10. Tested by:	**Date:**
Ali A. Simpkins	3/16/06

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 620

Status *(ADD, DELETE, MODIFY TO, MODIFY FROM)*	**Module**	**Parameter Name**	**Description** *(Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)*	**Distribution**	**Range**	**Justification** *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	**Source**

Attachment A

[Add General Header Info]

ASHREMOB intermediate outputs for each time step and realization; The two "total outdoor particle loads" are used to determine the
proportion of indoor dust/ash attributed to each of the three sources (initial deposit at receptor location, fluvial, and eolian)
Abbreviations: Disturb= disturbance; Contrib= contribution; Conc.= concentration; Dep= deposit

[See column headers below]

Time	RMEI Deposit Ash Mass Load Heavy Disturb	RMEI Deposit Ash Mass Load Light Disturb	Fluvial Deposit Mass Load	Eolian Deposit Mass Load
yr	g/m3	g/m3	g/m3	g/m3
1.00000000E+00	2.00000000E+00	3.00000000E+00	4.00000000E+00	5.00000000E+00
1.00000000E+00	2.00000000E+00	3.00000000E+00	4.00000000E+00	5.00000000E+00

RMEI Deposit Outdoor Heavy Disturb Contrib to Airbone HLW Conc. at RMEI H_i-H	RMEI Deposit Outdoor Light Disturb Contrib to Airbone HLW Conc. at RMEI H_i-L	Fluvial Deposit Contribution to Airborne HLW Conc. at RMEI H_f	Eolian Deposit Contribution to Airborne HLW Conc. at RMEI H_e	Total Outdoor Particle Load at RMEI during Heavy Disturb
g/m3	g/m3	g/m3	g/m3	g/m3
6.00000000E+00	7.00000000E+00	8.00000000E+00	9.00000000E+00	10.0000000E+00
6.00000000E+00	7.00000000E+00	8.00000000E+00	9.00000000E+00	10.0000000E+00

Total Outdoor Particle Load at RMEI during Light Disturb	Time-Weighted Total Outdoor Airborne HLW Conc. at RMEI H_RMEIoutdoor	Time-Weighted Total Indoor Airborne HLW Conc. at RMEI H_RMEIindoor	Time-Weighted Total Indoor Airborne HLW Conc. at RMEI H_RMEIoffsite	Annual-Average Airborne HLW Conc. at RMEI H_RMEI
g/m3	g/m3	g/m3	g/m3	g/m3
11.0000000E+00	12.0000000E+00	13.0000000E+00	14.0000000E+00	15.0000000E+00
11.0000000E+00	12.0000000E+00	13.0000000E+00	14.0000000E+00	15.0000000E+00

Attachment B

```
diff tpa501betaI/ashremob.f tpa501betaI/origs/ashremob.f
74,75d73
< c          12-01-05 jmm   SCR620; Add Headers to ashremob.out
< c
420,423d417
< c     --- LOGICAL DECLARATIONS ---
< cjmm 20051129 SCR620 for implementing ashremob.out headers.
<       logical firstcall
<
431,432d424
< cjmm 20051129 SCR620 for implementing ashremob.out headers.
<       save firstcall
434,437d425
< c     --- DATA STATEMENTS ---
< cjmm 20051129 SCR620 for implementing ashremob.out headers.
<       data firstcall /.true./
<
722,723d709
< cjmm
< cjmm
1441,1500c1427
< cjmm 20051129 SCR620 for implementing ashremob.out headers.
<       IF (firstcall) THEN
< cjmm+-^--1----+----2----+----3----+----4----+----5----+----6----+----7--!-+----8
< cjmm   Title line
<        write(ioutunit,'(A)')'ASHREMOB intermediate outputs for each ' //
<      & 'time step and realization; The two "total outdoor particle l' //
<      & 'oads" are used to determine the proportion of indoor dust/as' //
<      & 'h attributed to each of the three sources (initial deposit a' //
<      & 't receptor location, fluvial, and eolian)'
< cjmm   Abbreviation line
<        write(ioutunit,'(A)')'Abbreviations: Disturb= disturbance; Co' //
<      & 'ntrib= contribution; Conc.= concentration; Dep= deposit'
< cjmm   First skipped line
<        write(ioutunit,'(A)')' '
< cjmm   Second skipped line
<        write(ioutunit,'(A)')' '
< cjmm   line 1 of header column
<        write(ioutunit,'(85x,A)')'RMEI Deposit     RMEI Deposit     F' //
<      & 'luvial Deposit  Eolian Deposit'
< cjmm   line 2 of header column
<        write(ioutunit,'(85x,A)')'Outdoor Heavy    Outdoor Light    C' //
<      & 'ontribution     Contribution     Total Outdoor    Total Outd' //
<      & 'oor    Time-Weighted    Time-Weighted    Time-Weighted'
< cjmm   line 3 of header column
<        write(ioutunit,'(18x,A)')'RMEI Deposit     RMEI Deposit      ' //
<      & '                                Disturb Contrib  Disturb Con' //
<      & 'trib  to Airborne      to Airborne      Particle Load    Par' //
<      & 'ticle Load    Total Outdoor    Total Indoor     Total Indoor' //
<      & '     Annual-Average'
< cjmm   line 4 of header column
<        write(ioutunit,'(18x,A)')'Ash Mass Load    Ash Mass Load   Fl' //
<      & 'uvial Deposit  Eolian Deposit   to Airbone HLW   to Airbone ' //
<      & 'HLW   HLW Conc. at     HLW Conc. at     at RMEI during   at ' //
<      & 'RMEI during   Airborne HLW     Airborne HLW     Airborne HLW' //
<      & '     Airborne HLW'
< cjmm   line 5 of header column
<        write(ioutunit,'(5x,A)')'Time         Heavy Disturb    Light ' //
<      & 'Disturb      Mass Load        Mass Load     Conc. at RMEI   ' //
<      & ' Conc. at RMEI    RMEI             RMEI             Heavy Di' //
<      & 'sturb    Light Disturb    Conc. at RMEI    Conc. at RMEI    ' //
<      & 'Conc. at RMEI    Conc. at RMEI'
< cjmm   line 6 of header column
<        write(ioutunit,'(90x,A)')'H_i-H            H_i-L             ' //
<      & 'H_f              H_e                                        ' //
<      & '   H_RMEIoutdoor    H_RMEIindoor     H_RMEIoffsite      H_RM' //
<      & 'EI'
< cjmm   line 7 of header column
<        write(ioutunit,'(6x,A)')'yr              g/m3             g/m' //
<      & '3             g/m3             g/m3             g/m3        ' //
<      & '     g/m3             g/m3             g/m3             g/m3' //
<      & '             g/m3             g/m3             g/m3         ' //
<      & '    g/m3             g/m3'
< cjmm+-^--1----+----2----+----3----+----4----+----5----+----6----+----7--!-+----8
```

```
< cjmm   blank line after headers
<        write(ioutunit,'(A)')' '
<        firstcall = .false.
<       END IF
<
<
<       write( ioutunit, '(15(1pe14.8,3x))')
---
>       write( ioutunit, '(15(1x,'',',1pe14.6))')
```

Attachment C

Test Plan Name: Test Plan for TPA SCR#620

Tested By: Ali A. Simpkins Date: 3/16/06

Host Machine: TPA/SPOCK Host OS: DOS/UNIX

Baseline Version: TPA 5.0.2i Test Version: TPA 5.0.2j

System Level Tests

SL-1 Name: ASHREMOB output file changes - heading check
Path for run directory:[TPA]:asimpkins\tparun, [SPOCK]:home/asimpkins/tparun
Path for archive of results:CD: [SCR620]SCR620
Environment variables:[TPA Machine]: Set TPA_TEST=d:\ASimpkins\tpa502j
Set TPA_DATA=d:\ASimpkins\tpa502j
[SPOCK Machine] Setenv TPA_TEST /home/asimpkins/tpa502j
Setenv TPA_DATA /home/asimpkins/tpa502j
Special input files or modifications to input files required :N/A
Special diagnostic code modifications required :N/A
Program modes to be used (append flags, scenario/model switches, etc.):N/A
Utility scripts needed to perform the test:N/A
Utility codes needed in the analysis of the test data:N/A
Test description: - The objective of the test was to verify that the *ashremob.out* file is generated with the desired format.
-Run the TPA code with the following inputs:
SimulationTime set to 100,000 years
Turn on Disruptive Scenario flag for igneous activity
DirectReleaseOnly set to 1
NumberOfRealizations set to 1024
AshEvolutionMode set to 1 (default)
-Test is passed if *ashremob.out* is generated with the desired header format.
Evidence: See "ashremob.out" & "ashremobunix.out" in /SCR620/ AAS 3-30-06
Test Results: - **PASSED** on both platforms

SL-2 Name: Verification of File Removal
Path for run directory:[TPA]:asimpkins\tparun
Path for archive of results:CD: [SCR620]SCR620
Environment variables:[TPA Machine]: Set TPA_TEST=d:\ASimpkins\tpa502j
Set TPA_DATA=d:\ASimpkins\tpa502j
Special input files or modifications to input files required :N/A
Special diagnostic code modifications required :N/A
Program modes to be used (append flags, scenario/model switches, etc.):N/A
Utility scripts needed to perform the test:N/A
Utility codes needed in the analysis of the test data:N/A
Test description: - The objective of the test was to verify that the *ashremob.out* file is cleared and not included as an output file
-Run the TPA code with the following inputs:
SimulationTime set to 100,000 years
Turn on Disruptive Scenario flag for igneous activity
DirectReleaseOnly set to 1
NumberOfRealizations set to 1024
AshEvolutionMode set to 0

-Test is passed if *ashremob.out* is cleared and not included as an output file.

Test Results: - **FAILED** This item will be addressed in SCR599 .

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 621	**2. Software Title and Version:** TPA 5.0.2d	**3. Project No:** 20.06002.01.354
4. Affected Software Module(s), Description of Problem(s): *gnewdf.dat* The data updates for *genwdf.dat* presented in SCR618 contained some errors that caused a failed test. Corrections to the data are required.		
5. Change Requested by: J. Durham Date: 12-20-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 12-22-05	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment A		
8. Implemented by: J. Mancillas	**Date:** 12-27-05	
9. Description of Acceptance Tests: See Attachment B		
10. Tested by: J. Durham	**Date:** 1-26-06	

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 621

Status (*ADD, DELETE, MODIFY TO, MODIFY FROM)*	Module	Parameter Name	Description (*Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)*	Distribution	Range	Justification *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	Source

ATTACHMENT A

This SCR is a corrective action to a previous SCR, SCR618. SCR618 requested the update of values for effective dose conversion factors based on ICRP72 recommendations. The TPA code implements these values from the data file *gnewdf.dat*. During the implementation of SCR618, two values contained within the data file *gnewdf.dat* were entered incorrectly. The effective dose conversion factor for U232 infant inhalation was entered as 9.08×10^{-4}, but should have been entered as 9.80×10^{-6}. In addition the effective dose conversion factor for Th228 pre-teen ingestion was entered as 1.50×10^{-7}, but should have been entered as 1.40×10^{-7}. These two effective dose conversion factors were changed to their proper values in the data file *gnewdf.dat*.

In addition to the data corrections, the datafile *gnewdf.dat* was modified to include a more descriptive file header.

ATTACHMENT B

Test Plan for TPA SCR#621

System Level Test SL-1. Name: Input File Data Verification
Path for run directory: N/A
Path for archive of results: N/A
Environment variables: N/A
Special input files or modifications to input files required: N/A
Special diagnostic code modifications required: N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data: N/A

Test description:
- The objective of the test is to verify that the data in the table *gnewdf.dat* were the same as those described in this SCR.

Procedure: 1) verify the data in *gnewdf.dat* by comparing the data in the file with the data described in this SCR using the FC command

- The datafile will pass if the new values are identical to the data described in this SCR.

Test Results: - All data matched the data described in this SCR.

UNIX 9/3/20-04

Evidence: - See "FC.OUT" in \SCR621UNIX\ and \SCR621PC\.

- Overall test status: **PASS**

System Level Test SL-2. Name: Code Execution Test
Path for run directory: Windows Test case: [Goldsim]\SCR621PC\tpa502e\
Unix Test case: [Spock]\SCR621UNIX\tpa502e\

Path for archive of results: Windows Test Case: \SCR621PC\tpa502e\SCRTEST\
UNIX Test Case: \SCR621UNIX\tpa502e\SCRTEST\

All files are on the CD Rom entitled "TPA SCR-621"

Environment variables: Windows Test Case: \SCR621PC\tpa502~~a~~e\ JD 3-30-06
UNIX Test Case: \SCR621PC\tpa502~~a~~e\ JD 3-30-06
Special input files or modifications to input files required: N/A
Special diagnostic code modifications required: N/A
Program modes to be used (append flags, scenario/model switches, etc.): N/A
Utility scripts needed to perform the test: N/A
Utility codes needed in the analysis of the test data: N/A
Test description: - The objective of the test is to verify that the TPA code operated properly with the new version of *gnewdf*.dat for both Windows and UNIX operating systems

- **Procedure**:

1) run the TPA code under the Windows OS with the updated data in *gnewdf.dat*
2) run the TPA code under the UNIX OS with the updated data in *gnewdf.dat*

The datafile will pass if the code executes properly.

Test Results: - **Code operated properly**
- **Evidence**: See data files \SCR621UNIX\tpa502e\ for UNIX results and \SCR621PC\tpa502e\ for Windows results. Files are named OUT in both directories. JD 3-30-06

- **Overall test status**: **PASS**

Notes: Results of calculations are on the attached disk entitled "TPA SCR-621".

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 622	**2. Software Title and Version:** TPA 5.0.2j	**3. Project No::**q 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *ebsrel.f, nfenv.f*

The *ebsrel.inp* file is not saved in a separate file for the glass run of *releaset.e.* This file should be saved in a file called *ebsrelglass.inp* every time the glass waste form is analysed.

The *nfenv.f* file is difficult to read since it was divided into two sections. Many variables ending in "_DRY" are commented out in one section and used in the other section. The code should be cleaned up so that unused "_DRY" variable names do not appear in comment lines.

5. Change Requested by: R. Rice Date: 1/16/2006	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 3-3-06

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): The file nfenv.f was cleaned up by removing old comments, including commented out code, that were no longer relevant. In ebsrel.f, around line 1411 where ebsrelsf.inp was saved, new code was added to save ebsrelglass.inp also.

8. Implemented by: C. Scherer	**Date:** 3/10/2006

9. Description of Acceptance Tests:
See Attachments A for the PC platform test plan and
Attachment B for the Unix platform test plan.

10. Tested by: Jose M. Menchaca	**Date:** 03/28/2006

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 620

Status (*ADD, DELETE, MODIFY TO, MODIFY FROM*)	Module	Parameter Name	Description (*Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.*)	Distribution	Range	Justification *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	Source

Attachment A

PC Platform Test Plan for TPA SCR#622

Test Plan Name: ebsrelfail.inp test

Tested By: Jose M. Menchaca

Date: March 28, 2006

Host Machine: AMD Opteron PC

Host OS: MS Windows Server 2003 Version 5.2

Baseline Version: TPA 5.0.2j

Test Version: TPA 5.0.2k/l

Process Level (PL) Tests

PL-1. Name: Test of infilper.res results

Path for run directory: D:\JMenchaca\tpa502k\SCR622

Path for archive of results: R:\pc_tpa502k\SCR622 (for Test 1)
Note: The R: drive is the designated CD drive for stu2560.

Environment variables: set TPA_TEST=L:\tpa502k
set TPA_DATA=L:\tpa502k
Note: The L: drive is mapped to "ladybug:\public\jmenchaca"

Special input files or modifications to input files required : N/A

Pertinent Lines in the tpa.inp file: N/A

Special diagnostic code modifications required: N/A

Program modes to be used (append flags, scenario/model switches, etc.): N/A

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data: N/A

Test 1 description:

- objective:
The objective of this test is to verify that the ebsrelglass.inp is saved and not written over by the spent nuclear fuel ebsrel.inp data file.

- assumptions: N/A

- constraints: N/A

- output files to compare or examine: ebsrelglass.inp

- step by step test procedure to be used:
Execute a single realization run of the standard tpa.inp file. Verify that the ebsrelglass.inp file is among the remaining data files after execution.

- pass fail criteria
The pass criteria is achieved if the ebsrelglass.inp file exists after completion of the run.

Test Results:

- disposition of output and supporting files:
Here is a portion of the list of files produced during the execution of a basecase run. The files were listed in date order and saved to a file named SCR622DirList.txt.

```
 Volume in drive P is Data
 Volume Serial Number is E88F-D312

 Directory of P:\pc_tpa502k\SCR622

03/18/2006  03:14 PM           125,669 tpa.inp
03/18/2006  03:14 PM             2,767 wpflow.def
        .
        .
        .
03/28/2006  02:55 PM            10,608 ebsrel.inp
03/28/2006  02:55 PM            10,608 ebsrelglass.inp
03/28/2006  02:55 PM            27,906 ebsflo.dat
        .
        .
        .
03/28/2006  02:55 PM            52,210 rgwnr.tpa
03/28/2006  02:55 PM            23,289 tpa.out
03/28/2006  02:55 PM            52,210 rgwnappla.tpa
        .
        .
        .
             184 File(s)     16,109,598 bytes
               2 Dir(s)  27,386,626,048 bytes free
```

The ebsrelglass.inp file does indeed exist.

- overall test status (PASS/FAIL): **PASS**

Test 2 description:

- objective
The objective of this test is to verify that old comments in the nfenv.f file have been removed, in particular those lines having to do with _DRY parameters that are no longer being used.

- assumptions: N/A

- constraints: N/A

- output files to compare or examine: N/A

- step by step test procedure to be used
A visual inspection of the nfenv.f file will verify that the obsolete comments have been removed.

- pass fail criteria
The test passes if the obsolete comments have been removed.

Test Results:
The transition from tpa502k/nfenv.f to tpa502l/nfenv.f includes a reduction of over 2400 lines of code, mainly comment lines that include the unused _DRY parameters.

- overall test status (PASS/FAIL): **PASS**

Attachment B

Unix Platform Test Plan for TPA SCR#622

Test Plan Name: ebsrelglass.inp test

Tested By: Jose M. Menchaca

Date: March 28, 2006

Host Machine: SUN Ultra-4 server: Spock

Host OS: Sun Solaris 5.8

Baseline Version: TPA 5.0.2j

Test Version: TPA 5.0.2k/l

Process Level (PL) Tests

PL-1. Name: Test of existence of ebsrelglass.inp

Path for run directory: ~jmench/tpa502k/basecaseRuns/singleVector

Path for archive of results: R:\unix_tpa502k\basecaseRuns\singleVector
Note: The R: drive is the designated CD drive for stu2560.

Environment variables: setenv TPA_TEST ~/tpa502k
setenv TPA_DATA ~/tpa502k

Special input files or modifications to input files required : N/A

Pertinent Lines in the tpa.inp file: N/A

Special diagnostic code modifications required: N/A

Program modes to be used (append flags, scenario/model switches, etc.): N/A

Utility scripts needed to perform the test: N/A

Utility codes needed in the analysis of the test data: N/A

Test 1 description:

- objective:
The objective of this test is to verify that the ebsrelglass.inp is saved and not written over by the spent nuclear fuel ebsrel.inp data file.

- assumptions: N/A

- constraints: N/A

- output files to compare or examine: ebsrelglass.inp

- step by step test procedure to be used:
Execute a single realization run of the standard tpa.inp file. Verify that the ebsrelglass.inp file is among the remaining data files after execution.

- pass fail criteria
The pass criteria is achieved if the ebsrelglass.inp file exists after completion of the run.

Test Results:

- disposition of output and supporting files:
Here is a portion of the list of files produced during the execution of a basecase run. The list is ordered by the date and time it was produced

```
>ls -ltr
-rw-r--r--    1 jmench   sunuser    117393 Mar 18 13:29 tpa.inp
-rw-r--r--    1 jmench   sunuser      2913 Mar 24 11:39 tpa_include.inp
-rw-r--r--    1 jmench   sunuser      1086 Mar 24 11:39 repdes.dat
        .
        .
        .
-rw-r--r--    1 jmench   sunuser    193817 Mar 24 11:45 ebssf.dat
-rw-r--r--    1 jmench   sunuser     10504 Mar 24 11:45 ebsrelglass.inp
-rw-r--r--    1 jmench   sunuser     10504 Mar 24 11:45 ebsrel.inp
        .
        .
        .
-rw-r--r--    1 jmench   sunuser      1191 Mar 24 11:45 wpfillstats.out
-rw-r--r--    1 jmench   sunuser     23323 Mar 24 11:45 tpa.out
-rw-r--r--    1 jmench   sunuser       570 Mar 24 11:45 rlccdf_c.res
        .
        .
        .
```

The ebsrelglass file does indeed exist.

- overall test status (PASS/FAIL): **PASS**

Test 2 description:

- objective
The objective of this test is to verify that old comments in the nfenv.f file have been removed, in particular those lines having to do with _DRY parameters that are no longer being used.

- assumptions: N/A

- constraints: N/A

- output files to compare or examine: N/A

- step by step test procedure to be used
A visual inspection of the nfenv.f file will verify that the obsolete comments have been removed.

- pass fail criteria
The test passes if the obsolete comments have been removed.

Test Results:
The transition from tpa502k/nfenv.f to tpa502l/nfenv.f includes a reduction of over 2400 lines of code, mainly comment lines that include the unused _DRY parameters.

- overall test status (PASS/FAIL): **PASS**

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 626	**2. Software Title and Version:** TPA _5.0.2p	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *tpa.inp, tpa_include.inp*

Based on additional tests and calculations, some values and PDFs for sampled parameters need to be updated. Removed C14 for groundwater calculations. Removed parameters that are not used.

5. Change Requested by:	**6. Change Authorized by** (*Software Developer*):
J. Winterle, O. Pensado	R. Janetzke
Date: 4-7-06	Date: 4-11-06

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See the attached table for *tpa.inp* file changes.

Note that parameter deletions and data/distribution changes for two parameters were implemented post-TPA Version 5.0.2t (i.e., the *tpa.inp* parameters "WPSeepageProtectionDegradationRate[1/yr]" and "WeldAdvectiveFraction[] "). Additionally, the comments in Attachment A and modifications to the distributions for the CHnv thicknesses for all subareas except Subarea 6 were also implemented post-TPA Version 5.0.2t.

8. Implemented by:	**Date:**
R. Rice	4-11-06

9. Description of Acceptance Tests:

Tests were carried out in accordance with the test plan tp_scr626.wpd (see Attachment B), which also includes the test report. All tests passed. Test directories are archived on the CD entitled "TPA SCR #626 - Test Directories".

10. Tested by:	**Date:**
C. Scherer	5-19-06

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 626

Status (***ADD, DELETE, MODIFY TO, MODIFY FROM***)	**Module**	**Parameter Name**	**Description** (***Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.***)	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
Modify From	EBSFAIL	WPWeldThickness[m]		constant	2.03e-2		OPR
Modify To	EBSFAIL	WPWeldThickness[m]	Self explanatory	constant	2.0e-2	Typographical error	OPR
Modify From	EBSREL	Preexponential_SF DissolutionModel2		lognormal	561.4, 1.54e6		OPR

Modify To	EBSREL	Preexponential_SF DissolutionModel2	Constant factor in an Arrhenius expression to derive the spent fuel dissolution rate as a function of the temperature. beta	logbeta	1.022e4, 1.022e7, 3.145, 2.072	Initial revision, further refinement is needed. The distribution is restricted to range from 0.01 to 10 mg/(m^2 d) at 25 °C, which is consistent with experimental data. The distribution was constructed so that the probability that the dissolution rate exceeds 5 mg/(m^2 d) at 25 °C is 5% and the 25 °C median is 0.7 mg/(m^2 d). Note that the activation energy is hard-wired inside releaset equal to 34.3 kJ/mol.	OPR
Modify From	EBSREL	InitialRadiusOfSFP article[m]		normal	7.0e-3, 3.0e-3		OPR

Modify To	EBSREL	InitialRadiusOfSFParticle[m]	Radius used to derive the specific area (in units of m^2/mg). The specific area is computed as 3/(radius × spent fuel density). The specific area is a factor used to determine the waste form dissolution rate.	logbeta	4.42e-4, 4.72e-3, 3.549, 9.664	Distribution selected to force the specific area (m^2/mg) approximately follow a normal distribution with mean equal to 3.5×10^{-7} m^2/mg and 0.001 and 0.999 quantile extremes at 6×10^{-8} m^2/mg and 6.4×10^{-7} m^2/mg, respectively. The mean and the low 0.001 low bound quantile are consistent with the observed fractures in spent nuclear fuel pellets (Poinsett, 2001) and flow though partially clad spent nuclear fuel, respectively (DOE, 2004).	OPR
Modify From	EBSFILT	InvertBypass(0=ebsfilt,1=bypass-ebsfilt)		iflag	0		OPR

Modify To	EBSFILT	InvertBypass(0=ebsfilt,1=bypass-ebsfilt)	Flag to enable or disable transport through the invert	iflag	1	The invert model does not account for ingrowth. Release rate of daughter radionuclides can be greatly underestimated. It is preferred to always bypass the invert to avoid underestimating release rates.	OPR
Modify From	SEEPAGE	DSSeepageProtectionDegradationRate[1/yr]		constant	0.0		OPR
Modify To	SEEPAGE	DSSeepageProtectionDegradationRate[1/yr]	Slope to linearly degrade the extent of the DS protection against seepage as a function of time	constant	1.0e-5	Guess. After 100,000 years it is likely the drip shield will be fully corroded, beyond which time it may not be appropriate to assume the DS provides protection against seepage.	OPR
Modify From	SEEPAGE	InitialSeepageReductionFractionByMechFailedDS		constant	1.0		OPR

Modify To	SEEPAGE	InitialSeepageReductionFractionByMechFailedDS	Initial factor to account for seepage protection (0 = full protection; 1 = no protection) in case of mechanical failure of the DS.	uniform	1.0e-3, 2.0e-1	Guess. Overlapping drip shields will open and allow water to contact the WP. The extent of the opening is uncertain. The extent of the waste package exposed to seepage may be of the order of 10%. The distribution was selected to have a mean value of 0.1. Further refinement on this distribution is necessary.	OPR
Modify From	SEEPAGE	WPSeepageProtectionDegradationRate[1/yr]		constant	0.0		OPR

Modify To	SEEPAGE	WPSeepageProtectionDegradationRate[1/yr]	Slope to linearly degrade the extent of the WP protection against seepage as a function of time. This slope is applied for corrosion of mechanically failed WPs.	constant	1.0e-6	Guess. The WP may fail by general corrosion until after one-million years. This factor suggests that after one-million years, the WP may not offer protection against seepage, provided that it has exhibited weld-corrosion or mechanical degradation. Note that the same slope is applied to WPs affected by weld corrosion or mechanical degradation. Sensitivity analyses are recommended to assess the relevance of this parameter. For the final version of the TPA code ilt will be considered 1) to assign different degradation rates to corrosion or	OPR

Modify From	SEEPAGE	InitialSeepageReductionFractionByMechFailedWP		constant	0.0		OPR
Modify To	SEEPAGE	InitialSeepageReductionFractionByMechFailedWP	Initial factor to account for seepage protection (0 = full protection; 1 = no protection) in case of mechanical failure of the waste package.	uniform	1.0e-5, 2.0e-3	Guess. The contact area between the waste package and drip shield may be of the order of 10^{-3} of the upper waste package surface. Of this fraction, only a smaller fraction may be initially breached. Assuming a distribution centered around 10^{-3} for this parameter is a conservative approach.	OPR
Modify From	SEEPAGE	X0FmultCoefficient		normal	0.45004, 2.25004		OPR
Modify To	SEEPAGE	X0FmultCoefficient	Displacement factor for the f-mult sigmoidal equation	triangular	1.0, 1.47, 2.0	Revised estimates by R. Fedors assuming constant values of AfmultCoefficient and BFmultCoefficient	OPR

Modify From	SEEPAGE	AFmultCoefficient		constant	0.910758		OPR
Modify To	SEEPAGE	AFmultCoefficient	Numerator for the f-mult sigmoidal equation	constant	0.9	Best estimate of most likely value by R. Fedors.	OPR
Modify From	SEEPAGE	BFmultCoefficient		constant	0.210994		OPR
Modify To	SEEPAGE	BFmultCoefficient	Shape factor for the f-mult sigmoidal equation	constant	0.22	Best estimate of most likely value by R. Fedors.	OPR
Modify From	SEEPAGE	WeldAdvectiveFraction[]		constant	0.03		OPR

Modify To	SEEPAGE	WeldAdvectiveFraction[]	Initial factor to account for seepage protection (0 = full protection; 1 = no protection) in case of failure of the waste package welds by corrosion. Note that the protection extent degrades with time according to the factor WPSeepageProtectionDegradationRate[1/yr].	loguniform	1.0e-4, 1.0e-2	The fraction of the WP surface covered by welds is of the order of 0.01. The most likely mechanism for weld failure during the simulation time is localized corrosion, which will affect only a small fraction of the weld. The distribution is intended to span a reasonable range of exposed weld surfaces.	OPR
Modify From	DSFAIL	DripShieldCorrosionRate[m/yr]		triangular	8.6e-8, 1.72e-7, 3.4e-6		OPR

Modify To	DSFAIL	DripShieldCorrosionRate[m/yr]		triangular	8.6e-8, 1.72e-7, 2.6e-7	Initial revision. Additional discussions with ENG1 are needed. Upper value was selected to define a symmetric distribution	OPR
Modify From	UZFT	UZInitialCourantNumber[]		constant	1.50		RWR
Modify To	UZFT	UZInitialCourantNumber[]		constant	0.15		RWR
Modify From	Nuclides and Chains	aqueousnuclides	number of nuclides; number of chains		22 13		RWR
Modify To	Nuclides and Chains	aqueousnuclides	number of nuclides; number of chains		21 12		RWR
Delete	Nuclides and Chains	chain 10	number of nuclides in chain; nuclide		1 C14		RWR
Delete	EBSREL	GapFractionForC14		constant	0.1		RWR

Add	EBSREL	GapFractionForPU 242		constant	0.0	Included in short list of nuclides for long simulations.	RWR
Delete	EBSREL	RD_Invert_C		constant	1.0		RWR
Delete	EBSREL	Solubility_C[kg/m3]		constant	1.4e1		RWR
Delete	EBSREL	DiffusionCorrection Factor_C[]		constant	0.59		RWR
Delete	UZFT	MatrixKD_TSw_C[m3/kg]		constant	0.0		RWR
Delete	UZFT	MaxtrixKD_CHnvC[m3/kg]		constant	0.0		RWR
Delete	UZFT	MaxtrixKD_CHnzC[m3/kg]		constant	0.0		RWR
Delete	UZFT	MaxtrixKD_PPw_C [m3/kg]		constant	0.0		RWR
Delete	UZFT	MaxtrixKD_UCF_C [m3/kg]		constant	0.0		RWR
Delete	UZFT	MaxtrixKD_BFw_C [m3/kg]		constant	0.0		RWR
Delete	UZFT	MaxtrixKD_UFZ_C[m3/kg]		constant	0.0		RWR
Delete	UZFT	FractureRD_TSw_ C		constant	1.0		RWR

Delete	UZFT	FractureRD_CHnv C		constant	1.0		RWR
Delete	UZFT	FractureRD_CHnz C		constant	1.0		RWR
Delete	UZFT	FractureRD_PPw_ C		constant	1.0		RWR
Delete	UZFT	FractureRD_UCF_ C		constant	1.0		RWR
Delete	UZFT	FractureRD_BFw_ C		constant	1.0		RWR
Delete	UZFT	FractureRD_UFZ_ C		constant	1.0		RWR
Delete	SZFT	FractureRD_STFF _C		constant	1.0		RWR
Delete	SZFT	AlluviumMatrixRD_ SAV_C		constant	1.0		RWR
Delete	SZFT	ImmobileRD_STFF _C		constant	1.0		RWR

Modify From	tpa_include.inp Subarea Size	subarea 5	coordinates		548690., 4080586., 549471.76, 4080815.13, 549068., 4079692., 548638., 4079555., 548689., 4080569.56		RWR
Modify To	tpa_include.inp Subarea Size	subarea 5	coordinates		548689., 4080569.56, 549471.76, 4080815.13, 549070., 4079692., 548638., 4079555., 548689., 4080569.56		RWR

Modify From	UZFT	CHnvThickness_1SubArea[m]	Thickness of the UZ CHnv unit for a subarea	triangular	0.05, 27.7, 66.9	Range modified to reflect subarea average thicknesses instead of the spatial variability of a layer thickness for the subarea; use a triangular distribution with a mean equal to the mean of the spatial variability distribution plus/minus 50% of that mean (except when this range exceeds the spatial variability distribution, in which case the original distribution is preserved; this is the case for Subarea 6)	RWR
Modify To	UZFT	CHnvThickness_1SubArea[m]	same as above	triangular	15.8, 31.6, 47.4	same as above	RWR
Modify From	UZFT	CHnvThickness_2SubArea[m]	same as above	triangular	0.05, 16.4, 77.8	same as above	RWR

Modify To	UZFT	CHnvThickness_2SubArea[m]	same as above	triangular	15.7, 31.4, 47.1	same as above	RWR
Modify From	UZFT	CHnvThickness_3SubArea[m]	same as above	triangular	0.05, 4.2, 9.1	same as above	RWR
Modify To	UZFT	CHnvThickness_3SubArea[m]	same as above	triangular	2.3, 4.5, 6.8	same as above	RWR
Modify From	UZFT	CHnvThickness_4SubArea[m]	same as above	triangular	0.05, 4.2, 9.1	same as above	RWR
Modify To	UZFT	CHnvThickness_4SubArea[m]	same as above	triangular	2.3, 4.5, 6.8	same as above	RWR
Modify From	UZFT	CHnvThickness_5SubArea[m]	same as above	triangular	0.05, 4.2, 9.1	same as above	RWR
Modify To	UZFT	CHnvThickness_5SubArea[m]	same as above	triangular	2.3, 4.5, 6.8	same as above	RWR
Modify From	UZFT	CHnvThickness_7SubArea[m]	same as above	triangular	3.2, 49.5, 62.7	same as above	RWR
Modify To	UZFT	CHnvThickness_7SubArea[m]	same as above	triangular	19.3, 38.5, 57.8	same as above	RWR
Modify From	UZFT	CHnvThickness_8SubArea[m]	same as above	triangular	2.4, 16.7, 71.2	same as above	RWR
Modify To	UZFT	CHnvThickness_8SubArea[m]	same as above	triangular	15.1, 30.1, 45.2	same as above	RWR

Modify From	UZFT	CHnvThickness_9SubArea[m]	same as above	triangular	2.4, 38.5, 104.0	same as above	RWR
Modify To	UZFT	CHnvThickness_9SubArea[m]	same as above	triangular	24.2, 48.3, 72.5	same as above	RWR
Modify From	UZFT	CHnvThickness_10SubArea[m]	same as above	triangular	3.9, 65.0, 96.0	same as above	RWR
Modify To	UZFT	CHnvThickness_10SubArea[m]	same as above	triangular	27.5, 55.0, 82.5	same as above	RWR
Delete	NFENV	LengthOfRefluxZone[m]		constant	20.0	unused parameter	RWR
Delete	NFENV	MaximumFluxInRefluxZone[m/s]		constant	1.0e-9	unused parameter	RWR
Delete	NFENV	PerchedBucketVolumePerSAarea[m3/m2]		constant	0.5	unused parameter	RWR
Delete	ASHRMOVO	ReceptorGroupArea[m2]		constant	1.5d+07	unused parameter	RWR
Delete	EBSFAIL	DripShieldTimeMark[yr]		constant	10000.0	unused parameter	RWR
Delete	EBSFAIL	ChlorideMultFactor		constant	1.0	unused parameter	RWR
Delete	EBSFAIL	ChlorideMultFactorIntactDripShield		constant	1.0	unused parameter	RWR

Delete	DRIFTFAIL	DriftDegradation MethodSelection Value		uniform	0.0,1.0	unused parameter (name changed)	RWR

ATTACHMENT A

Comments added to *tpa.inp* file for long simulations

The following comment lines were added just before the parameter named "MaximumTime[yr]."

```
** In long simulations (greater than 100,000 yr)
** for performance reasons, a modified nuclide list and an average
** velocity used in UZ NEFTRAN is recommended when the parameter
** below for "Simulation Time" is set at a times beyond 100,000 yrs:
** 1) un-comment the lists of 9 aqueousnuclides and 3 colloidalnuclides
**    provided in this file (currently commented-out) and comment-out
**    the existing lists of aqueousnuclides and colloidalnuclides
** 2) set parameter "UZVelocity(0=average,1=time-dependent)" equal to 0
**
** (Note: the recommended approach to accomplish the nuclide list changes are
** provided in comments.  To locate these comments, search the file
** for "aqueousnuclides" and "colloidalnuclides")
```

The two sets of comment lines referred to above are:

```
** In long simulations (greater than 100,000 yr)
** for performance reasons, it is recommended the following
** section be un-commented (lines from "aqueousnuclides" through
** "endofnuclides") by removing "**" from the lines.
** Also, the above section (lines from "aqueousnuclides" through
** "endofnuclides")  should be commented out by inserting "**" at the
** beginning of the line.
**
**aqueousnuclides
**9
**9
****  chain 1
**1
**Np237
****  chain 2
**1
**U238
****  chain 3
**1
**Pu239
****  chain 4
**1
**Th230
****  chain 5
**1
```

```
**Pu240
****  chain 6
**1
**I129
****  chain 7
**1
**Tc99
****  chain 8
**1
**Cs135
****  chain 9
**1
**Pu242
****
**endofnuclides
```

and

```
** In long simulations (greater than 100,000 yr)
** for performance reasons, it is recommended the following
** section be un-commented (lines from "colloidalnuclides" through
** "endofcolloidalnuclides") by removing "**" from the lines.
** Also, the above section (lines from "colloidalnuclides" through
** "endofcolloidalnuclides")  should be commented out by inserting "**" at the
** beginning of the line.
**
**colloidalnuclides
****  Enter colloid names in the same order as their source names are listed in the
****  regular solute radionuclide section.
****  number of colloidal nuclides (14 max)
**4
****  number of colloidal chains
**4
****  colloidal chain 1
**1
**Jp239
****  colloidal chain 2
**1
**Jp240
****  colloidal chain 3
**1
**Jt230
****  colloidal chain 4
**1
**Jp242
****
**endofcolloidalnuclides
```

ATTACHMENT B

Test Plan/Report for TPA SCR #626

Test Plan Name: Test Changes to *tpa.inp*

Tested By: Carol S. Scherer

Date: May 19, 2006

Host Machine: AMD Opteron PC: TPA

Host OS: MS Windows Server 2003 Version 5.2

Baseline Version: TPA 5.0.2 u

Test Version: TPA 5.1betaA

Testing Setup:

Directories\paths used for testing:
$HOME: Guardian = d:\css\scrs
Path for run directory: **TPA computer = d:**\public\cscherer\scr626-pc

Environment variables:

TPA_TEST = $HOME*SCR626*
TPA_DATA = $HOME*SCR626*

Disposition of documentation of results: All modified\new source code files, all executables used in testing, and all input\output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 626 - Test Directories*" (attached). PC versions of the test directories will follow the paths indicated under a root directory called scr626-pc.

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***SCR626*** and **SCR626\tpa502u**.

2. Copy **TPA** version 5.1betaA to ***$HOME\SCR626***. Compile *tpa.exe*.

3. Copy **TPA** version 5.0.2u to ***$HOME\SCR626\tpa502u***. Compile *tpa.exe*.

Process Level Tests:

These tests are designed to demonstrate the functionality of the specified module.

1. Name: Visual Inspection of tpa.inp version **TPA5.1betaA.**

   Path for archives of results: ***$HOME \SCR626***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use basecase *tpa.inp*

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that specified changes have been made to **tpa.inp**
   - assumptions: all setup instructions have been carried out.
   - constraints: none.
   - output files to compare or examine: none.
   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>**\tpa51betaA**
     2. visually compare the contents of *tpa.inp* with the "Update Requirements for TPA.INP" table contained in *scr_626.wpd.*
   - pass\fail criteria: the test passes if:
     1. All the changes specified for *tpa.inp* in the *scr_626.wpd* have been made.

   Results of running test:

   PASSED.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

1. Name: Verify that **TPA** will run using the modified *tpa.inp*.

   Paths for archives of results: ***$HOME \SCR626***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use basecase *tpa.inp*.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that **TPA** still runs with the changes made to **tpa.inp**.
   - assumptions: all setup instructions have been carried out.
   - constraints: none.
   - output files to compare or examine:
   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>**\tpa51betaA**
     2. run tpa.exe using command "***%TPA_TEST%tpa.exe > tpa_basecase.out***".
   - pass\fail criteria: the test passes if:
     1. **TPA** successfully runs to completion.

   Results of running test:

   PASSED.

NOTES:

ATTACHMENT C

Test Plan/Report for TPA SCR #626

Test Plan Name: Test Changes tpa.inp

Tested By: Carol S. Scherer **Date:** May 5, 2006

Host Machine: SUN Ultra-4 server: Spock **Host OS:** Sun Solaris 5.8

Baseline Version: TPA 5.0.2u **Test Version: TPA** 5.1betaA

Testing Setup:

Directories/paths used for testing:
$HOME = spock/home/cscherer
Path for run directory: ***$HOME/scr626***

Environment variables:

TPA_TEST = **$HOME/*SCR626***
TPA_DATA = **$HOME/*SCR626***

Disposition of documentation of results: All modified/new source code files, all executables used in testing, and all input/output files will be kept in the archive directories. The contents of the archive directories will be written out to a CD titled "*TPA SCR # 626 - Test Directories*" (attached). UNIX versions of the test directories will follow the paths indicated under a root directory called scr626-unix.

Test preparation instructions:

1. In the directory **$HOME**, create the following subdirectories: ***SCR626*** and **SCR626/tpa502u**.

2. Copy **TPA** version 5.1betaA to ***$HOME/SCR626***. Compile *tpa.exe*.

3. Copy **TPA** version 5.0.2u to ***$HOME/SCR626/tpa502u***. Compile *tpa.e*.

Process Level Tests:

These tests are designed to demonstrate the functionality of the specified module.

1. Name: Visual Inspection of tpa.inp version **TPA5.1betaA.**

   Path for archives of results: ***$HOME \SCR626***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use basecase *tpa.inp*

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that specified changes have been made to **tpa.inp**
   - assumptions: all setup instructions have been carried out.
   - constraints: none.
   - output files to compare or examine: none.
   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>**\tpa51betaA**
     2. visually compare the contents of *tpa.inp* with the "Update Requirements for TPA.INP" table contained in *scr_626.wpd.*
   - pass\fail criteria: the test passes if:
     1. All the changes specified for *tpa.inp* in the *scr_626.wpd* have been made.

   Results of running test:

   PASSED.

System Level Tests:

These tests are designed to demonstrate that the modified code affects overall **TPA** processing and output as planned with no unwanted side effects.

1. Name: Verify that **TPA** will run using the modified *tpa.inp*.

   Paths for archives of results: ***$HOME /SCR626***

   Special input files or modifications to input files required: none.

   Special diagnostic code modifications required: none.

   Program modes to be used: use basecase *tpa.inp*.

   Utility scripts needed to perform the test: none.

   Utility codes needed in the analysis of the test data: none.

   Test description:
   - objective: to verify that **TPA** still runs with the changes made to **tpa.inp**.
   - assumptions: all setup instructions have been carried out.
   - constraints: none.
   - output files to compare or examine:
   - step by step test procedure to be used:
     1. —> change directory to <<run directory>>**/tpa51betaA**
     2. run tpa.e using command "***tpa.e > tpa_basecase.out***".
     3. compare the output file with the output file from Appendix A - the PC version.
   - pass/fail criteria: the test passes if:
     1. **TPA** successfully runs to completion.
     2. Peak Mean Dose is the same for the PC and Unix versions of the code.

   Results of running test:

   PASSED.

NOTES: