SCIENTIFIC NOTEBOOK

612-3E

by

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INITIAL ENTRIES

Scientific Notebook: #612-3E

Issued to: R. Rice

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Title: TPA 5.0 Code Development

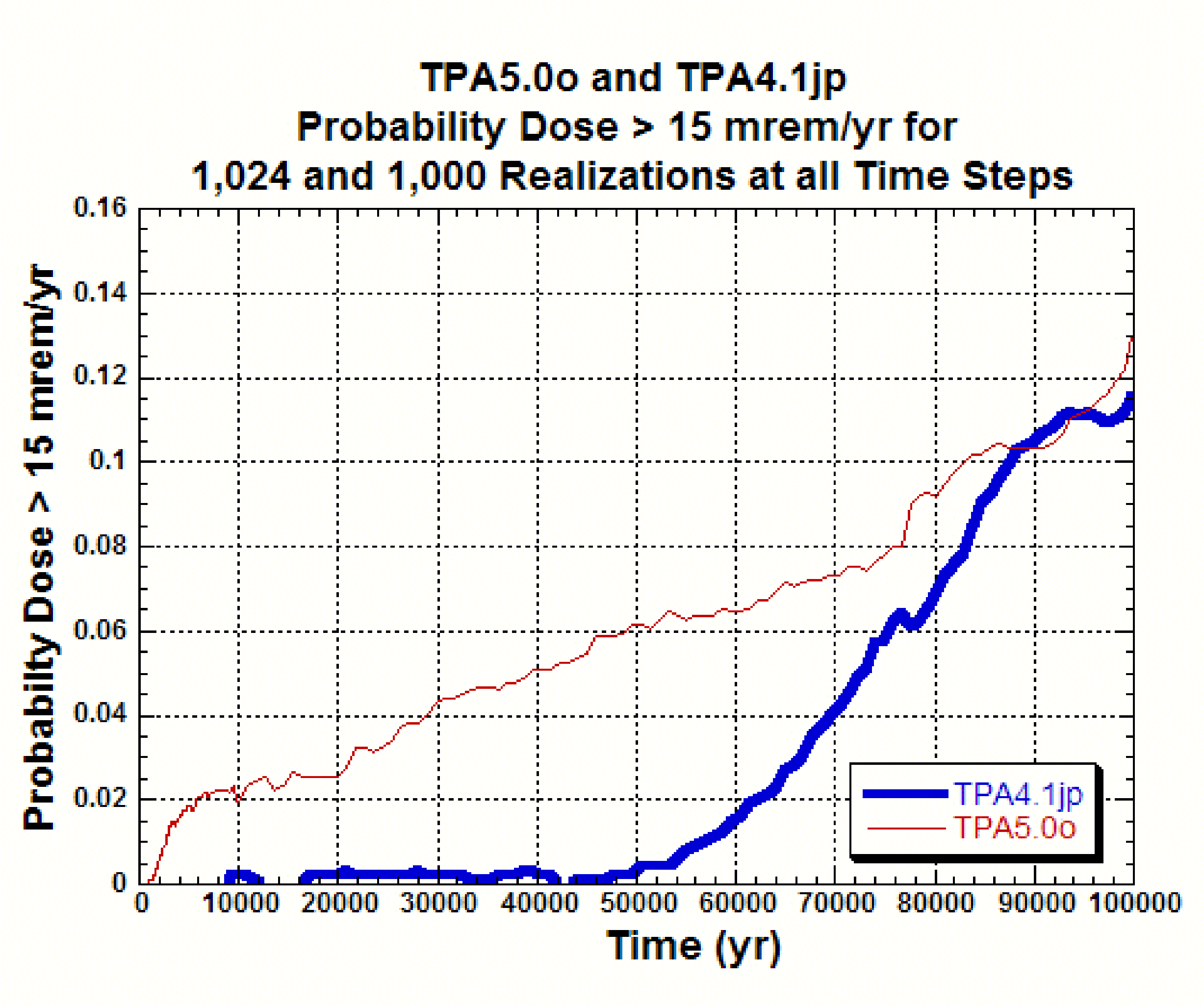
Participants: R. Rice

Objective:

This scientific notebook will document the work performed in the development of the TPA code.

09/05/03

At the request of G. Wittmeyer, a plot of TPA output was generated to examine dose above a threshold value of 15 mrem/yr. This plot was prepared from TPA 4.1j and TPA 5.0 runs. The following plot was transmitted in an email and presented to G. Wittmeyer.



Other work was conducted to compare TPA 4.1j and 5.0o output. This following email was prepared to document the differences in doses from basecase TPA 4.1 and 5.0 runs.

9/5/03

Gordon, Ron, Sitakanta,

Here are some plots that you've asked me about and some that I thoughnt might be useful in looking at some Version 4.1 and 5.0 differences. Below are my initial thoughts about this stuff.

I'll email you the color versions of these plots.

Please let me know if you have any questions.

Thanks,

Rob

Plot 1. Cumulative fraction of WPs failed by corrosion for TPA5.0o (blue), TPA4.1jp (red), and TPA5.0o with no local corrosion failures (green). Note that TPA4.1jp (red) and TPA5.0o with no local corrosion failures (green) coincide and indicate that TPA Versions 5.0o and 4.1jp will yield consistent WPs failed by corrosion if local corrosion is removed from TPA Version 5.0o. Local corrosion was removed by setting the chloride concentration at a high value (100) as per recommendation by Osvaldo.

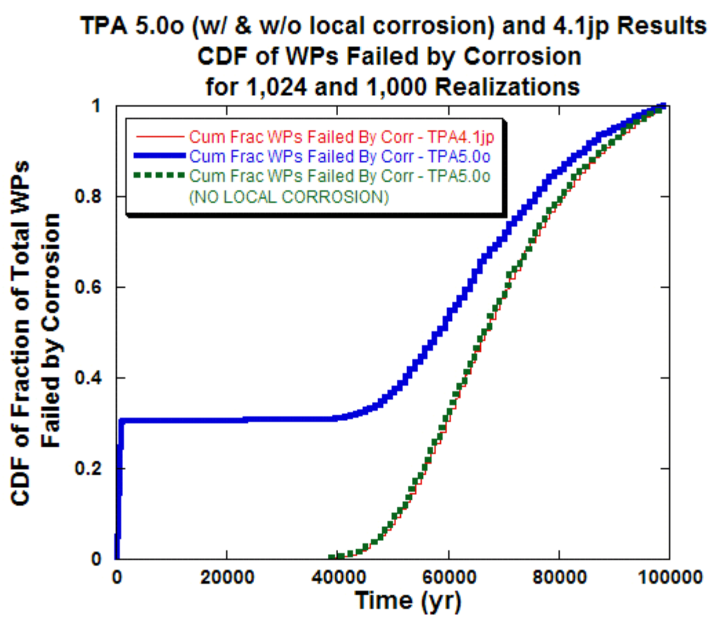
Plot 2. Same as Plot 1, except the time axis is from 0 to 10,000 yrs instead of from 0 to 100,000 yr. This shows local corrosion failures in TPA Version 5.0o are from about 250 to 1,000 yrs.

Plot 3. Average groundwater dose for TPA5.0o (blue), TPA4.1jp (red), and TPA5.0o with no local corrosion failures (green). Note that TPA5.0o (blue) and TPA5.0o with no local corrosion failures (green) coincide through about 300 yrs (caused by initial WP failures and possibly a different drip shield failure and/or release calculation maybe related to diffusion?). Then TPA5.0o with no local corrosion failures (green) transitions to be consistent with TPA4.1jp (red) at about 8,000 yrs. The removal of local corrosion failures and possibly a different drip shield failure and/or release calculation maybe related to diffusion(?) are probably causing this transition.

Plots 4, 5, and 6. Average groundwater doses by radionuclide for TPA Version 4.1jp (Plot 4), TPA Version 5.0o (Plot 5), and TPA Version 5.0o (Plot 6). Note that Pu240 and Pu239 doses increase by 3 or more orders of magnitude and become the leading contributors to groundwater dose at 10,000 yrs and 100,000 yrs. I129, Tc99, and Np237 behavior is similar in TPA Versions 4.1jp and 5.0o. Also, Am241 dose is increased from TPA Versions 4.1jp to 5.0o. This might is caused by different Rds (Kds) used in TPA Versions 4.1jp and 5.0o (possibly the fix that was needed because NEFTRAN was having long runs and array out-of-bounds situations and a limit on the delta Rd(Kd) was introduced into the TPA code?).

Plots of this results (Plots 1 - 6) follow.

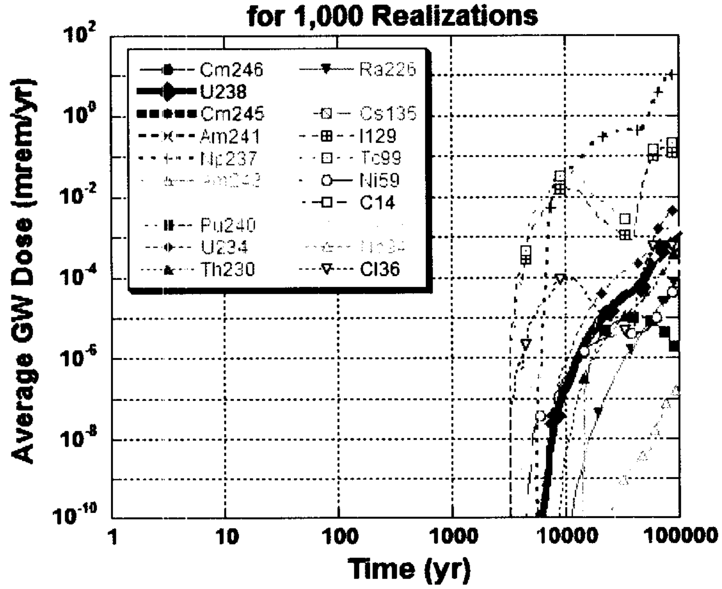
Plot 1



Plot 2

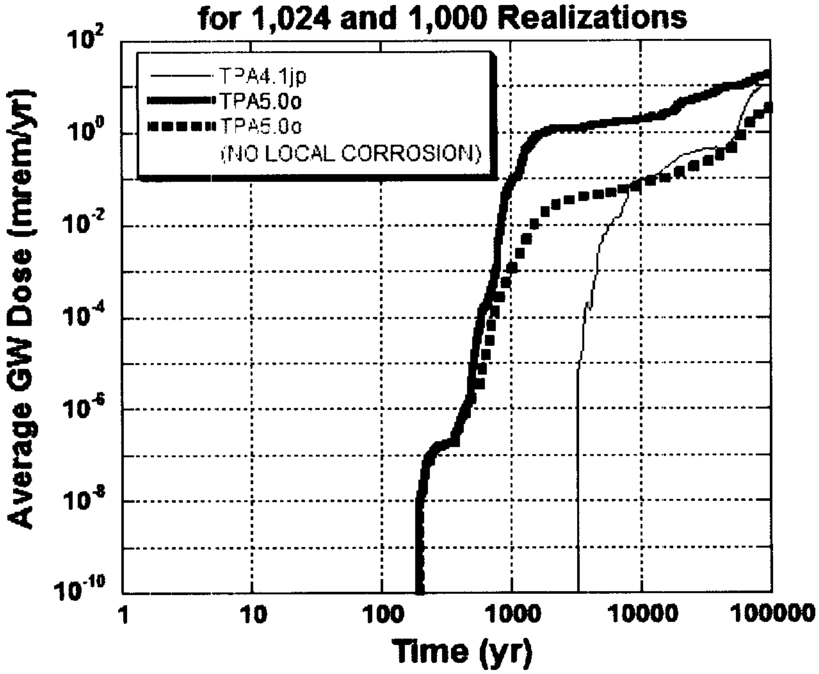
TPA 4.1jp Results
Average GW Dose (mrem/yr)
for 1,000 Realizations

Plot 3

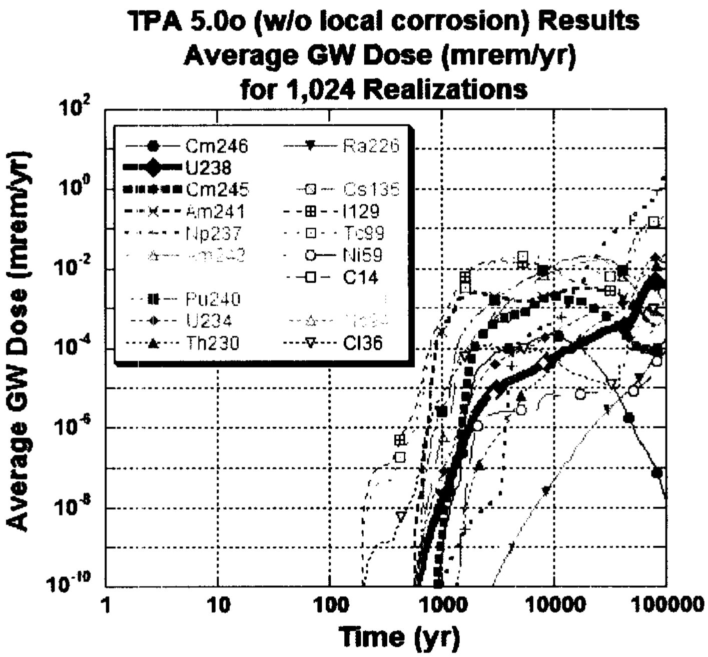


TPA 5.0o (w/ & w/o local corrosion) and 4.1jp Results
Average GW Dose (mrem/yr)
for 1,024 and 1,000 Realizations

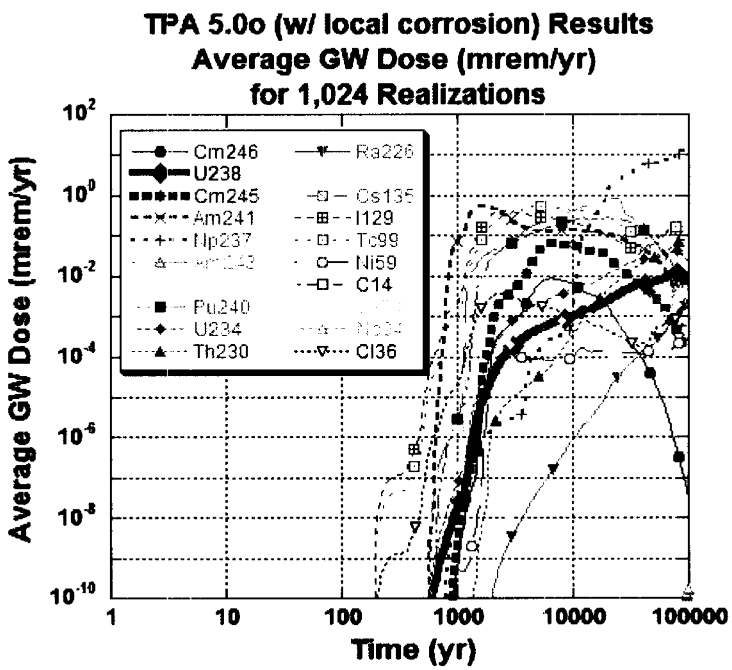
Plot 4



page # assigned by plot JRW 1/20/10



Plot 5



Plot 6

page # obscured by plot JRW 1/28/10

Working with Mike Smith, prepared a proposal using TPA5.0o for modifying DCAGS and ASHRMOVO to address the very high doses (millions and trillions of rem) when there are extremely thin ash blankets caused by pointing the wind direction opposite to the basecase (i.e., 90 instead of -90 degrees). This condition was undercovered by T. McCartin during his validation testing.

The proposal for the work, transmitted to M. Smith and R. Janetzke, follows.

TPA Version 5.0o

Proposed Changes to DCAGS/ASHRMOVO
(includes SCR 472 changes)

prepared by R.Rice 9/5/03 after consultation with M. Smith
and R. Janetzke

NOTE: The DCAGS and ASHRMOVO source code will be examined while accomplishing Changes 1 - 6 listed below and other changes may be identified.

Change 1. As listed in (i) of SCR 472, modify equations on lines 776, 838, 906, and 967 of DCAGS by replacing:

*& +dcfinh(k)/(gramsashpercm2*1.d+04)*

with:

& +dcfinh(k)/ amassash(it)

JUSTIFICATION: Allow for the time-varying redistribution of ash introduced in ASHRMOVO

Change 2. As listed in (ii) of SCR 472, modify equation on line 533 of DCAGS by replacing:

```
resuspendablefraction(it)=thickness*100
   &                  *dexp(-dlbr*(tim(it)-
tim(itoe)))/
   &                  resuspendabledepth
```

with:

```
   resuspendablefraction(it)=thickness*100/
   &                  resuspendabledepth
```

JUSTIFICATION: Allow for the time-varying redistribution of ash introduced in ASHRMOVO

Change 3. Delete on lines 1209-1211 of ASHRMOVO:

```
   if (amassasht(itoe+i).le.0.d0) then
     amassasht(itoe+i) = 1.d-99
   end if
```

Modify lines 1223 - 4 of ASHRMOVO:

```
dladd(itoe+i,m)=log(amassasht(itoe+i)/amassasht(itoe+i-1))
   &       /(time(itoe+i)-time(itoe+i-1))
```

This modification will set dladd(itoe+i,m) equal to zero, if amassasht() is zero (i.e., no ash).

Otherwise, the calculation in lines 1223-4 will be performed.

JUSTIFICATION: Eliminate problems caused by zero ash which can be introduced by a wind direction of 0 to 180 degrees (instead of the -90 degree value in the TPA default tpa.inp file that will not give zero ash)

Change 4. Modify lines 525-7 of DCAGS by replacing:

```
if (amassash(it).lt.amassash(it-1)) then
  ipeak = it
endif
```

with:

```
if (it .eq. 1) then
  ipeak = it
elseif (amassash(it).lt.amassash(it-1)) then
  ipeak = it
endif
```

JUSTIFICATION: Eliminate potential problems caused by array out-of-bounds

Change 5. Modify lines 844-5 of the function "dmyexp" in INVENT by replacing:

```
    if (x.le.-227.d0) then
      dmyexp = 0.d0
    else if (x.ge.227) then
      print *, ' dmyexp: WARNING: large exponential has
been'
      print *, '        truncated to 1.d+99'
      dmyexp = 1.d0 + 99
    else
      dmyexp = dexp(x)
    endif
```

with:

```
if (x.le.-227.d0) then
  dmyexp = 0.d0
 print *, ' dmyexp: ERROR: exponential .le. -227'
 print *, ' TPA Code execution has been stopped'
  STOP
else if (x.ge.227) then
  print *, ' dmyexp: ERROR: exponential .ge. 227'
 print *, ' TPA Code execution has been stopped'
  STOP
else
  dmyexp = dexp(x)
endif
```

JUSTIFICATION: Eliminate potential problems arising by the TPA code not stopping when there are "dexp()" arguments that are either very small or very large

Change 6. Copy lines 1189-1207 of ASHRMOVO, which are:

```
      bterm1 =(-erosratediswind-
erosratedisfl+erosrateund*areaasht*
    &         depfracairash/CGareainm2-
erosrateund*areaasht*
    &         depositfractionCG/CGareainm2)*(time(itoe+i)-
time(itoe))

      bterm2 =
(depositfractionCG*frashq*amassashred/CGareainm2 +
    &
erosrateund*areaasht*frashq*depositfractionCG/
    &          CGareainm2/rlq)*(1-exp(-rlq*(time(itoe+i)-
time(itoe))))

      bterm3 =
(depositfractionCG*frashm*amassashred/CGareainm2 +
    &
erosrateund*areaasht*frashm*depositfractionCG/
    &          CGareainm2/rlm)*(1-exp(-rlm*(time(itoe+i)-
time(itoe))))

      bterm4 =
(depositfractionCG*frashL*amassashred/CGareainm2 +
```

```
    &
erosrateund*areaasht*frashL*depositfractionCG/
    &         CGareainm2/rlL)*(1-exp(-rlL*(time(itoe+i)-
time(itoe))))

       bterm5 = amassash(itoe)

      amassasht(itoe+i) =
bterm1+bterm2+bterm3+bterm4+bterm5
```

and paste these lines just after line 1207. These lines will need to be modified slightly to accomplish the following. Place these lines inside of a "do-loop" that steps in time from "time(itoe)" to "time(nt)" using time steps of 1 year. Modify the last line in this section to compute "amassasht_new" and to save the largest value as "amassasht_largest" and the corresponding time as "amassasht_largest_time." Determine the "left-hand" TPA time that corresponds to "amassasht_largest_time" and then modify the "amassasht()" array at this time to be the value for "amassasht_largest".

JUSTIFICATION: Capture the peak amount of redistributed ash at a TPA time step (previously the amount of redistributed ash was determined only at TPA time steps and the peak was most often-times not captured)

A follow-up email from M. Smith discussing this proposal follows.

Subj: RE: DCAGS/ASHRMOVO changes
Date: 9/12/03 9:27:43 AM Mountain Daylight Time
From: masmith@cnwra.swri.edu
To: rwrice@aol.com
CC: rjanetzke@cnwra.swri.edu
Sent from the Internet (Details)

Rob,
Your proposal looks good to me. Please keep me informed about any additional problems/inconsistencies you may uncover when reviewing these modules.
Thanks for your help.
--Mike

10/03/03
The proposed work was completed and transmitted to M. Smith and R. Janetzke in the following email.

Subj: Re: DCAGS/ASHRMOVO changes
Date: 10/3/03
To: masmith@cnwra.swri.edu
CC: rjanetzke@cnwra.swri.edu
File: A:\scr472_rob.zip (207462 bytes) DL Time (32000 bps): < 2 minutes

Mike,

Attached please find the files that I've modified for SCR472 (exec.f, ashrmovo.f, and a), the original files (TPA Version 5.0o), and a "diff" file showing the differences between my modified files and the original files.

I'll be in touch. (I still have some questions/observations from my work.)

Please contact me if you have any questions.

Thanks and take care,

Rob
915 373 2472 (cell)
915 581 0853 (work)

As identified using a "fc" (file compare DOS command), the completed work contained the following changes. The unmodified files are named "*.F.ORIGINAL" and the modified files are named "*.f", where * = ASHRMOVO, EXEC, and DCAGS.

For ASHRMOVO.F:

```
Comparing files ashrmovo.f and ASHRMOVO.F.ORIGINAL
***** ashrmovo.f

      double precision amassashred
***** ASHRMOVO.F.ORIGINAL



      double precision amassashred
*****

***** ashrmovo.f

cc SCR472 rwr 9/26/03 determine the time of peak
cc              ash - "amassash()" using the
cc              variable "amassashpeak()"
cc
cc new variables
```

```
      integer ipeak
      integer istore
      integer maxsimulationtime

      parameter ( maxsimulationtime=100000 )
      double precision ashthickventpeak(maxsimulationtime)
      double precision thicknessashpeak(maxsimulationtime)
      double precision dnpeak(maxsimulationtime,maxnnucsvol)
      double precision amassashpeak(maxsimulationtime)
      double precision amassashtpeak(maxsimulationtime)
      double precision dladdpeak(maxsimulationtime,maxnnucsvol)

      double precision peakash
      double precision peakashtime
cc end of new variables

      save ikey
***** ASHRMOVO.F.ORIGINAL

      save ikey
*****

***** ashrmovo.f
      it=1

cc SCR472 rwr 9/26/03 avoid potential array out of bounds
cc                for the "time()" array at "time(nt)"
      if (toe .ge. time(nt)) then
        iflag = 1
        itoe = nt
      endif

      do 10 while (iflag.eq.0)
***** ASHRMOVO.F.ORIGINAL
      it=1
      do 10 while (iflag.eq.0)
*****

***** ashrmovo.f
      tempnt=nt-itoe

cc SCR472 rwr 9/26/03 avoid potential array out of bounds
cc                for the "time()" array at "time(nt)"
     if (itoe .lt. nt) then

      do i=1,tempnt
***** ASHRMOVO.F.ORIGINAL
      tempnt=nt-itoe

      do i=1,tempnt
*****

***** ashrmovo.f

cc SCR472 rwr 9/26/03  comments out the next 3 lines - part
cc                of a change (see below) to examine
cc                "dladd(itoe+i,m)" and set it equal to zero
cc                whenever "amassasht()" is zero
cc       if (amassasht(itoe+i).le.0.d0) then
cc         amassasht(itoe+i) = 1.d-99
cc       end if
      if (amassasht(itoe+i).le.0.d0) then
        amassasht(itoe+i) = 0.0d0
```

```
      end if
***** ASHRMOVO.F.ORIGINAL

      if (amassasht(itoe+i).le.0.d0) then
       amassasht(itoe+i) = 1.d-99
      end if
*****

***** ashrmovo.f

cc SCR472 rwr 9/26/03  modified 2 lines - part
cc                  of a change (see above) to examine
cc                  "dladd(itoe+i,m)" and set it equal to zero
cc                  whenever "amassasht()" is zero
cc         dladd(itoe+i,m)=log(amassasht(itoe+i)/amassasht(itoe+i-1))
cc     &        /(time(itoe+i)-time(itoe+i-1))
       if (amassasht(itoe+i) .eq. 0.0d0 .or.
     &                       amassasht(itoe+i-1) .eq. 0.0d0) then
         dladd(itoe+i,m) = 0.0d0
       else
         dladd(itoe+i,m)=dlog(amassasht(itoe+i)/amassasht(itoe+i-1))
     &                  /(time(itoe+i)-time(itoe+i-1))
       endif

c mas 9/10/02
***** ASHRMOVO.F.ORIGINAL


      dladd(itoe+i,m)=log(amassasht(itoe+i)/amassasht(itoe+i-1))
     &        /(time(itoe+i)-time(itoe+i-1))
c mas 9/10/02
*****

***** ashrmovo.f
cc

         if(dll(m)*tempdnt1(m)*gramsfpercm2/100.d0.le.decision) then
***** ASHRMOVO.F.ORIGINAL
cc
         if(dll(m)*tempdnt1(m)*gramsfpercm2/100.d0.le.decision) then
*****

***** ashrmovo.f
c           dlt(m)=dlbr+dll(m)

          dlt(m)=dll(m)-dladd(itoe+i,m)
***** ASHRMOVO.F.ORIGINAL
c           dlt(m)=dlbr+dll(m)
          dlt(m)=dll(m)-dladd(itoe+i,m)
*****

***** ashrmovo.f
c     &            gramsfpercm2/100.d0)
cc SCR472 rwr 9/26/03  modified 2 lines to avoid division by zero
cc                  when gramsfpercm2 = 0.0d0
cc             dlt(m)=decision/(tempdnt1(m)*
cc     &             gramsfpercm2/100.d0)-dladd(itoe+i,m)
          if (gramsfpercm2 .eq. 0.0d0 .or.
     &                    tempdnt1(m) .eq. 0.0d0) then

           dlt(m) = -dladd(itoe+i,m)
          else
           dlt(m)=decision/(tempdnt1(m)*
```

```
    &            gramsfpercm2/100.d0)-dladd(itoe+i,m)
          endif

         end if
***** ASHRMOVO.F.ORIGINAL
c     &           gramsfpercm2/100.d0)
          dlt(m)=decision/(tempdnt1(m)*
    &            gramsfpercm2/100.d0)-dladd(itoe+i,m)
         end if
*****

***** ashrmovo.f
c Based on notes and initial programming by J.Weldy.

        call decayremove43mol( dt, dlt, tempdnt1, tempdn )
***** ASHRMOVO.F.ORIGINAL
c Based on notes and initial programming by J.Weldy.
        call decayremove43mol( dt, dlt, tempdnt1, tempdn )
*****

Resync Failed.  Files are too different.
***** ashrmovo.f

cc SCR472 rwr 9/26/03 determine the time of peak
cc                ash - "amassash()" using the
cc                variable "amassashpeak()"
cc
cc new variables
cc      parameter ( maxsimulationtime=100000 )
cc      double precision ashthickventpeak(maxsimulationtime)
cc      double precision thicknessashpeak(maxsimulationtime)
cc      double precision dnpeak(maxsimulationtime,maxnnucsvol)
cc      double precision amassashpeak(maxsimulationtime)
cc      double precision amassashtpeak(maxsimulationtime)
cc      double precision dladdpeak(maxsimulationtime,maxnnucsvol)
cc
cc      double precision peakash
cc      double precision peakashtime
cc
cc      integer ipeak
cc      integer istore
cc      integer maxsimulationtime
cc
cc
cc set a time step for these calculations
      dt = 1.0d0

cc determine number of time steps, assuming a time step of "dt"
cc and the first position in the array is at "itoe" - the time
cc of the event (thus, add 1)
      tempnt=dint( (time(nt) - time(itoe)) / dt) + 1

cc do an error check on the number of time steps calculated in "tempnt"
      if (tempnt .gt. maxsimulationtime) then
       print *, ' '
       print *, ' ***>>> Error in ashrmovo <<<*** '
       print *, ' problem with : '
       print *, '     tempnt .gt. maxsimulationtime'
       print *, ' The value "dt" set to compute the number'
       print *, ' of time steps in the calculations for'
       print *, ' determining peak ash yields more time steps'
       print *, ' than allowed by "maxsimulationtime"'
       print *, ' maxsimulationtime =',maxsimulationtime
```

```
      print *, ' time steps using "dt" = tempnt =',tempnt
      print *, ' dt =',dt
      print *, ' end of simulation time = time(nt) =',time(nt)
      print *, ' time of event = time(itoe) = ',time(itoe)
      print *, ' '
      STOP
     end if

cc initialize arrays
     do j=1,43
      do k=1,tempnt
        dnpeak(k,j)=0.d0
        amassashpeak(k)=0.d0
        amassashtpeak(k)=0.d0
        thicknessashpeak(k)=0.d0
        ashthickventpeak(k)=0.d0
        dladdpeak(k,j)=0.d0
      enddo
     enddo

cc set values for the "peak" arrays initialized above
cc equal to values at "time(itoe)" for (1)
     do n=1,43
      dnpeak(1,n) = dn(itoe,n)
      tempdnt1(n) = dn(itoe,n)
     enddo
     amassashpeak(1) = amassash(itoe)
     amassashtpeak(1) = amassasht(itoe)
     thicknessashpeak(1) = thicknessash(itoe)
     ashthickventpeak(1) = ashthickvent(itoe)

cc perform ash calculations starting at time step = 1 (time of event)
cc for every uniform "dt" through the maximum time "time(nt)"
cc (note that these are the same calculations as those conducted
cc  at TPA times specified in the "time()" array
     do i=1,tempnt
      if (ashthickventpeak(i).lt.depthfleros) then
        dilfl = ashthickventpeak(i)/depthfleros
      else
        dilfl=1
      endif

      if (ashthickventpeak(i).lt.depthwinderosund) then
        dilwindund = ashthickventpeak(i)/depthwinderosund
      else
        dilwindund=1
      endif

      if (thicknessashpeak(i).lt.depthwinderosdis) then
        dilwinddis = thicknessashpeak(i)/depthwinderosdis
      else
        dilwinddis=1
      endif

      if (thicknessashpeak(i).lt.depthfleros) then
        dilfldis = thicknessashpeak(i)/depthfleros
      else
        dilfldis=1
      endif
***** ASHRMOVO.F.ORIGINAL

cc
cc      dn numbers are in moles/MTU, must convert them to number/g of sf
```

```
cc
      do i=1,nt
        do j=1,43
          dn(i,j)=dn(i,j)*6.023d23/1.d6
        end do
      end do

cc
cc      Must tranform grams of sf per cm2 to Ci of radionuclide per m^2
cc
      do it=1,nt
        do inuc=1,43
cc mas 9-12-02  SCR384

c mas 9/10/02 new algorithm created to set activity to zero if mass of
c contaminated ash is <= 1e-99.
c Based on notes and initial programming by J.Weldy.
c          ciperm2(it,inuc)=(dlr(inuc)/365.d0/24.d0/3600.d0)*
c     &            dn(it,inuc)/3.7d10*gramsfpercm2*(1.0d+4)
c           if (ciperm2(it,inuc).lt.0.99d-99) then
c             ciperm2(it,inuc)=0.d0
c           end if

          if (amassasht(it).le.1.d-99) then
            ciperm2(it,inuc)=0.d0
          else
            ciperm2(it,inuc)=(dlr(inuc)/365.d0/24.d0/3600.d0)*
     &              dn(it,inuc)/3.7d10*gramsfpercm2*(1.d+4)
          end if

          if (ciperm2(it,inuc).lt.0.99d-99) then
            ciperm2(it,inuc)=0.d0
          end if
c mas 9/10/02

        end do
      end do
      return
      end
c=====================================================================
======
      subroutine leachrate(dkd,fpe,fpsat,fie,fisat,precip,dirr,
     &                  depthsoil,rhosoil,theta,dll)
c=====================================================================
======
c
c    NAME: leachrate -
c
c    PURPOSE:
c
c    METHOD:
c
c    INPUT:
c          dkd(maxn) = double precision, Array of soil kd values in cm3/g
c          fpe       = double precision, fraction of precipitation lost to
c                      evapotranspiration
c          fpsat     = double precision, Fraction of year soil is saturated
c                      due to precipitation
c          fie       = double precision, Fraction of irrigation lost to
c                      evapotranspiration
c          fisat     = double precision, Fraction of year soil is saturated
c                      due to irrigation
c          precip    = double precision, Annual precipitation in m/yr
```

```
c          dirr      = double precision, Annual irrigation in m/yr
c          depthsoil = double precision, Depth of the rooting zone in m
c          rhosoil   = double precision, Bulk density of the soil in g/cm3
c          theta     = double precision, Saturation fraction of soil
c
c     OUTPUT:
c           dll(maxn) = double precision, Array of leach rates for nuclides in the
c                blanket (1/yr)
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     --- TEST DRIVER ---
      include 'leachrate.t'

c     --- HEADER ---
      include 'leachrate.h'
c
cccccc
c
c     GLOSSARY:
c
c     depthsoil = Depth of the rooting zone in m
c     dirr = Annual irrigation in m/yr
c     dkd = Array of soil kd values in cm3/g
c     dll = Array of leach rates for nuclides in the blanket (1/yr)
c     fie = Fraction of irrigation lost to evapotranspiration
c     fisat = Fraction of year soil is saturated due to irrigation
c     fpe = fraction of precipitation lost to evapotranspiration
c     fpsat = Fraction of year soil is saturated due to precipitation
c     i =
c     maxn =
c     precip = Annual precipitation in m/yr
c     rhosoil = Bulk density of the soil in g/cm3
c     theta = Saturation fraction of soil
c
cccccc

      integer i
*****
```

For EXEC.F:

```
Comparing files exec.f and EXEC.F.ORIGINAL
***** exec.f
        endif
cc SCR472 rwr 9/26/03  removed "gramsashpercm2" from DCAGS argument list
cc                  ("amassash()" is used instead)
cc          write( iunitechodcags, fmt='(/,"gramsashpercm2 = ",1pe12.4)')
cc     &      gramsashpercm2
        write( iunitechodcags,
***** EXEC.F.ORIGINAL
        endif
        write( iunitechodcags, fmt='(/,"gramsashpercm2 = ",1pe12.4)')
     &      gramsashpercm2
        write( iunitechodcags,
*****

***** exec.f
cc     &       AAT, AAP, ciperm2gsatCP,gramsashpercm2,
cc SCR472 rwr 9/26/03  removed "gramsashpercm2" from DCAGS argument list
cc                  ("amassash()" is used instead)
cc     &       AAT, AAP, ciperm2gsatCP,gramsashpercm2,amassash,
     &       AAT, AAP, ciperm2gsatCP,amassash,
```

```
    &       remperyrgsnr  )
***** EXEC.F.ORIGINAL
cc    &       AAT, AAP, ciperm2gsatCP,gramsashpercm2,
    &       AAT, AAP, ciperm2gsatCP,gramsashpercm2,amassash,
    &       remperyrgsnr  )
*****
```

For DCAGS.F:

```
Comparing files dcags.f and DCAGS.F.ORIGINAL
***** dcags.f
    &       ntim, tim, nnucldr, namesdr,
cc SCR472 rwr 9/26/03  removed "gramsashpercm2" from DCAGS argument list
cc                  ("amassash()" is used instead)
cc    &       dMAT,dMAP,ciperm2gsatCP,gramsashpercm2,amassash,
    &       dMAT,dMAP,ciperm2gsatCP,amassash,
    &       remperyrpernuclgs )
***** DCAGS.F.ORIGINAL
    &       ntim, tim, nnucldr, namesdr,
    &       dMAT,dMAP,ciperm2gsatCP,gramsashpercm2,amassash,
    &       remperyrpernuclgs )
*****

***** dcags.f
      it=1

cc SCR472 rwr 9/26/03 avoid potential array out of bounds
cc                 for the "tim()" array at "tim(ntim)"
      if (toe .ge. tim(ntim)) then
        iflag = 1
        itoe = ntim
      endif

      do 10 while (iflag.eq.0)
***** DCAGS.F.ORIGINAL
      it=1
      do 10 while (iflag.eq.0)
*****

***** dcags.f
        thickness = amassash(it)/(rhoash*1e6)

cc SCR472 rwr 9/26/03  commented out "ipeak" determination and
cc                  assignment since "ipeak" is not currently used
cc        if (amassash(it).lt.amassash(it-1)) then
cc          ipeak = it
cc        endif

c mas 9/10/02
***** DCAGS.F.ORIGINAL
        thickness = amassash(it)/(rhoash*1e6)
          if (amassash(it).lt.amassash(it-1)) then
            ipeak = it
          endif
c mas 9/10/02
*****

***** dcags.f
c       resuspendablefraction(it)=thickness
```

```
cc SCR472 rwr 9/26/03  removed decay term since "thickness" is now a
cc                  function of time that is determined every
cc                  time step from "amassash(it)"
cc       resuspendablefraction(it)=thickness*100
cc     &                      *dexp(-dlbr*(tim(it)-tim(itoe)))/
cc     &                      resuspendabledepth
       resuspendablefraction(it)=thickness*100/
     &                      resuspendabledepth

cc jrw 12-28-99 added to implement time dependent loading factor
***** DCAGS.F.ORIGINAL
c       resuspendablefraction(it)=thickness
       resuspendablefraction(it)=thickness*100
     &                      *dexp(-dlbr*(tim(it)-tim(itoe)))/
     &                      resuspendabledepth
cc jrw 12-28-99 added to implement time dependent loading factor
*****

***** dcags.f

cc SCR472 rwr 9/26/03  avoid potential array/compiler
cc                  problems if itoe=1 (added the following line)
      if (itoe .gt. 1) then
c
***** DCAGS.F.ORIGINAL

c
*****

***** dcags.f
      end do

cc SCR472 rwr 9/26/03  avoid potential array/compiler
cc                  problems if itoe=1 (added the following line)
      endif

cc
***** DCAGS.F.ORIGINAL
      end do
cc
*****

***** dcags.f
cc    if (gramsashpercm2.eq.0.0d0) then
cc SCR472 rwr 9/26/03  with ash redistribution, don't need
cc                  the following lines
cc      if (amassash(itoe+1).eq.0.0d0) then
cc       do k = 1, nnucldr
cc        ik = indexperiso( namesdr(k) )
cc        do j=1,ntim
cc          remperyrpernuclgs(j,k)=0.0d0
cc        enddo
cc       enddo
cc       return
cc      end if

cc
***** DCAGS.F.ORIGINAL
cc    if (gramsashpercm2.eq.0.0d0) then
      if (amassash(itoe+1).eq.0.0d0) then
       do k = 1, nnucldr
        ik = indexperiso( namesdr(k) )
        do j=1,ntim
```

```
        remperyrpernuclgs(j,k)=0.0d0
       enddo
      enddo
      return
     end if
cc
*****

***** dcags.f

cc SCR472 rwr 9/26/03  avoid division by zero if "amassash()" is zero
      if (amassash(it) .eq. 0.0d0) then
        dcf(it,k) = 0.0d0
      else

cc RRB 04/04/2002 (SCR-382) The dose conversion factor calculation for
***** DCAGS.F.ORIGINAL

cc RRB 04/04/2002 (SCR-382) The dose conversion factor calculation for
*****

***** dcags.f
      dcf(it,k)=dcfde(k)+dcfinga(k)+dcfingp(k)+dcfmlk(k)
cc SCR472 rwr 9/26/03  removed "gramsashpercm2" from DCAGS argument list
cc              ("amassash()" is used instead)
cc    &    +dcfinh(k)/(gramsashpercm2*1.d+04)
     &    +dcfinh(k)/amassash(it)
     &              *(resuspendablefraction(it)*tmassload(it)
***** DCAGS.F.ORIGINAL
      dcf(it,k)=dcfde(k)+dcfinga(k)+dcfingp(k)+dcfmlk(k)
     &    +dcfinh(k)/(gramsashpercm2*1.d+04)
     &              *(resuspendablefraction(it)*tmassload(it)
*****

***** dcags.f
     &               +massloadoffsite*occupancyoffsite)

cc SCR472 rwr 9/26/03  avoid division by zero if "amassash()" is zero
      endif

      end do
***** DCAGS.F.ORIGINAL
     &               +massloadoffsite*occupancyoffsite)
      end do
*****

***** dcags.f

cc SCR472 rwr 9/26/03  avoid division by zero if "amassash()" is zero
      if (amassash(it) .eq. 0.0d0) then
        dcf(it,k) = 0.0d0
      else

cc RRB 04/04/2002 (SCR-382) The dose conversion factor calculation for
***** DCAGS.F.ORIGINAL

cc RRB 04/04/2002 (SCR-382) The dose conversion factor calculation for
*****

***** dcags.f
      dcf(it,k)=dcfde(k)+dcfinga(k)+dcfingp(k)+dcfmlk(k)
cc SCR472 rwr 9/26/03  removed "gramsashpercm2" from DCAGS argument list
cc              ("amassash()" is used instead)
```

```
cc     &     +dcfinh(k)/(gramsashpercm2*1.d+04)
     &     +dcfinh(k)/amassash(it)
     &               *(resuspendablefraction(it)*tmassload(it)
***** DCAGS.F.ORIGINAL
      dcf(it,k)=dcfde(k)+dcfinga(k)+dcfingp(k)+dcfmlk(k)
     &     +dcfinh(k)/(gramsashpercm2*1.d+04)
     &               *(resuspendablefraction(it)*tmassload(it)
*****

***** dcags.f
     &                +massloadoffsite*occupancyoffsite)

cc SCR472 rwr 9/26/03  avoid division by zero if "amassash()" is zero
      endif

      end do
***** DCAGS.F.ORIGINAL
     &                +massloadoffsite*occupancyoffsite)
      end do
*****

***** dcags.f

cc SCR472 rwr 9/26/03  avoid division by zero if "amassash()" is zero
      if (amassash(it) .eq. 0.0d0) then
        dcf(it,k) = 0.0d0
      else

cc RRB 04/04/2002 (SCR-382) The dose conversion factor calculation for
***** DCAGS.F.ORIGINAL

cc RRB 04/04/2002 (SCR-382) The dose conversion factor calculation for
*****

***** dcags.f
cc     &                +massloadoffsite*occupancyoffsite)

cc SCR472 rwr 9/26/03  removed "gramsashpercm2" from DCAGS argument list
cc                  ("amassash()" is used instead)
cc        dcf(it,k)=dcfde(k)*factor2(it)+dcfinh(k)/(gramsashpercm2*1.d+04)
      dcf(it,k)=dcfde(k)*factor2(it)+dcfinh(k)/amassash(it)
     &          *(resuspendablefraction(it)*tmassload(it)*factor1(it)
***** DCAGS.F.ORIGINAL
cc     &                +massloadoffsite*occupancyoffsite)
      dcf(it,k)=dcfde(k)*factor2(it)+dcfinh(k)/(gramsashpercm2*1.d+04)
     &          *(resuspendablefraction(it)*tmassload(it)*factor1(it)
*****

***** dcags.f
     &          +massloadoffsite*occupancyoffsite)

cc SCR472 rwr 9/26/03  avoid division by zero if "amassash()" is zero
      endif

      end do
***** DCAGS.F.ORIGINAL
     &          +massloadoffsite*occupancyoffsite)
      end do
*****

***** dcags.f

cc SCR472 rwr 9/26/03  avoid division by zero if "amassash()" is zero
```

```
        if (amassash(it) .eq. 0.0d0) then
         dcf(it,k) = 0.0d0
        else

cc RRB 04/04/2002 (SCR-382) The dose conversion factor calculation for
***** DCAGS.F.ORIGINAL

cc RRB 04/04/2002 (SCR-382) The dose conversion factor calculation for
*****

***** dcags.f
cc The original dose conversion factor calculation was commented out.

cc SCR472 rwr 9/26/03  removed "gramsashpercm2" from DCAGS argument list
cc                  ("amassash()" is used instead)
cc        dcf(it,k)=dcfde(k)*factor2(it)+dcfinh(k)/(gramsashpercm2*1.d+04)
        dcf(it,k)=dcfde(k)*factor2(it)+dcfinh(k)/amassash(it)
     &           *(resuspendablefraction(it)*tmassload(it)*factor1(it)
***** DCAGS.F.ORIGINAL
cc The original dose conversion factor calculation was commented out.
        dcf(it,k)=dcfde(k)*factor2(it)+dcfinh(k)/(gramsashpercm2*1.d+04)
     &           *(resuspendablefraction(it)*tmassload(it)*factor1(it)
*****

***** dcags.f

cc SCR472 rwr 9/26/03  avoid division by zero if "amassash()" is zero
        endif

        end do
***** DCAGS.F.ORIGINAL

        end do
*****
```

Testing of the unmodified TPA 5.0o code and the modified TPA code was conducted to verify the correct implementation of the proposed changes in the TPA source code.

As an example of this problem in the unmodified TPA 5.0o code with the VOLCANO flag activated for a 100 realization run, the TPA ground surface dose from realization 2 is about 10 million rem/yr (see output below).

```
exec: calling dcags
             Highest annual dose from GS
        Am241  9.2093E+09 [mrem/yr] at  4.357E+02 yr
        Pu240  1.8187E+09 [mrem/yr] at  4.357E+02 yr
        Pu239  1.2614E+09 [mrem/yr] at  4.357E+02 yr
        Pu238  3.5395E+08 [mrem/yr] at  4.357E+02 yr
        Am243  9.0730E+07 [mrem/yr] at  4.357E+02 yr
        Am242m  1.1394E+07 [mrem/yr] at  4.357E+02 yr
```

With the proposed changes implemented, the following doses were computed. These results indicate the modifications were successful in eliminating the unreasonably high doses. The modified code was tested at the CNWRA and passed onto the NRC which tested the code and then accepted those changes. Note that the wind direction used in the unmodified and the modified TPA runs was +90 degrees. This value leads to the very thin ash blanket and the high dose in the unmodified TPA runs. All of these 1000 realizations with the modified TPA code exhibited ground surface doses about 5 order of magnitude less than doses computed with the unmodified TPA code, whose results are shown above.)

Modified TPA 5.0o Results from 1000 realizations

Realization #	Highest Radionuiclide Dose
1	There is no GS release
2	Am243 1.5217E+03 [mrem/yr] at 4.945E+03 yr
3	Pu240 3.1183E+02 [mrem/yr] at 5.971E+03 yr
4	There is no GS release
5	Am243 3.2617E+02 [mrem/yr] at 2.251E+03 yr
6	Pu239 1.2577E+03 [mrem/yr] at 8.293E+03 yr
7	Am243 5.1807E+02 [mrem/yr] at 3.997E+03 yr
8	Am243 5.7884E+01 [mrem/yr] at 4.499E+03 yr
9	Am241 1.9914E+04 [mrem/yr] at 1.854E+03 yr
10	Am241 1.9914E+04 [mrem/yr] at 1.854E+03 yr
etc.	

10/30/03

At the request of R. Jantezke, prepared a list of potentially sensitive words/phrases in the TPA source code. An email was transmitted to R. Janetzke with a list of these words/phrases in a listing that showed a subdirectory for each of the words/phrases and in of these each subdirectories was contained file names for TPA source code files having the word/phrases. A listing of these subdirectories and TPA files follows.

```
Directory of C:\Search_TPA_for_bad_words

.            <DIR>        10-30-03 11:25a .
..           <DIR>        10-30-03 11:25a ..
BUG_DE~1       <DIR>        10-30-03 11:32a bug_debug
JUNK          <DIR>        10-30-03 11:26a junk
STUFF         <DIR>        10-30-03 11:27a stuff
ARBITR~1       <DIR>        10-30-03 11:29a arbitrary
BOGUS         <DIR>        10-30-03 11:31a bogus
UNKNOWN        <DIR>        10-30-03 12:00p unknown
DIR      OUT            0  10-30-03 12:31p dir.out
```

```
GUESS        <DIR>        10-30-03 12:01p guess
!!!          <DIR>        10-30-03 12:04p !!!
WEIRD        <DIR>        10-30-03 12:04p weird
DUM_DU~1     <DIR>        10-30-03 12:06p dum_dummy
WRONG        <DIR>        10-30-03 12:09p wrong
BAD          <DIR>        10-30-03 12:13p bad
UNNECE~1     <DIR>        10-30-03 12:17p unnecessary
NOT_NE~1     <DIR>        10-30-03 12:21p not_needed
NOT_USED     <DIR>        10-30-03 12:26p not_used
REDUND~1     <DIR>        10-30-03 12:28p redundant
        1 file(s)              0 bytes

Directory of C:\Search_TPA_for_bad_words\!!!

.            <DIR>        10-30-03 12:04p .
..           <DIR>        10-30-03 12:04p ..
SNLLHS   F       232,641  07-03-03  6:38a SNLLHS.F
RELEASET F       187,323  07-03-03  6:38a RELEASET.F
EXEC     F       430,094  07-03-03  6:38a EXEC.F
        3 file(s)        850,058 bytes

Directory of C:\Search_TPA_for_bad_words\arbitrary

.            <DIR>        10-30-03 11:29a .
..           <DIR>        10-30-03 11:29a ..
UNCERT~1 F        62,116  07-03-03  6:38a uncertain.f
RELEASET F       187,323  07-03-03  6:38a RELEASET.F
SNLLHS   F       232,641  07-03-03  6:38a SNLLHS.F
IAREADER F        21,918  07-03-03  6:38a IAREADER.F
        4 file(s)        503,998 bytes

Directory of C:\Search_TPA_for_bad_words\bad

.            <DIR>        10-30-03 12:13p .
..           <DIR>        10-30-03 12:13p ..
ITYMUT~1 F        27,564  07-03-03  6:38a itymutils.f
STRTOK~1 F        39,606  07-03-03  6:38a strtokfunc.f
ITYM     I        11,957  07-03-03  6:38a ITYM.I
ESTIMA~1 F        62,680  07-03-03  6:38a estimator.f
RELEASET F       187,323  07-03-03  6:38a RELEASET.F
UZFLOW   I         5,331  07-03-03  6:38a UZFLOW.I
UZFLOW   F        88,348  07-03-03  6:38a UZFLOW.F
UZ_PARMS I         3,818  07-03-03  6:38a UZ_PARMS.I
        8 file(s)        426,627 bytes

Directory of C:\Search_TPA_for_bad_words\bogus

.            <DIR>        10-30-03 11:31a .
..           <DIR>        10-30-03 11:31a ..
NEFMKS   F       317,656  07-03-03  6:38a NEFMKS.F
        1 file(s)        317,656 bytes
```

Directory of C:\Search_TPA_for_bad_words\bug_debug

```
.            <DIR>        10-30-03 11:32a .
..           <DIR>        10-30-03 11:32a ..
GGENII   DEF       14,068  07-03-03  6:38a GGENII.DEF
GGENIIS  DEF       13,386  07-03-03  6:38a GGENIIS.DEF
ACUTE1   F         10,421  07-03-03  6:38a ACUTE1.F
AIRCAL   F          8,964  07-03-03  6:38a AIRCAL.F
ANMCAL   F          8,622  07-03-03  6:38a ANMCAL.F
AQUCAL   F          2,114  07-03-03  6:38a AQUCAL.F
BIOCAL   F          1,262  07-03-03  6:38a BIOCAL.F
CRPCAL   F          5,302  07-03-03  6:38a CRPCAL.F
DKHARV   F          3,961  07-03-03  6:38a DKHARV.F
EDRANM   F          4,079  07-03-03  6:38a EDRANM.F
EDRCRP   F          3,676  07-03-03  6:38a EDRCRP.F
EDRNON   F          2,604  07-03-03  6:38a EDRNON.F
EDRRES   F          2,944  07-03-03  6:38a EDRRES.F
ENV      F         10,906  07-03-03  6:38a ENV.F
EXTCAL   F          6,997  07-03-03  6:38a EXTCAL.F
INHCAL   F          2,940  07-03-03  6:38a INHCAL.F
INTPOL   F          1,909  07-03-03  6:38a INTPOL.F
PACKAG   F          2,411  07-03-03  6:38a PACKAG.F
READIN   F         11,802  07-03-03  6:38a READIN.F
REDCAS   F          6,361  07-03-03  6:38a REDCAS.F
RITENV   F          8,795  07-03-03  6:38a RITENV.F
RITQA    F         27,988  07-03-03  6:38a RITQA.F
EBSFILT  F         18,612  07-03-03  6:38a EBSFILT.F
FAILT    F        107,288  07-03-03  6:38a FAILT.F
MECHFAIL F        134,557  07-03-03  6:38a MECHFAIL.F
NEFMKS   F        317,656  07-03-03  6:38a NEFMKS.F
RELEASET F        187,323  07-03-03  6:38a RELEASET.F
MAKE     BAT        3,131  07-03-03  6:38a Make.bat
DCAGS    F        127,334  07-03-03  6:38a DCAGS.F
DCAGW    F        162,201  07-03-03  6:38a DCAGW.F
EBSREL   F         91,449  07-03-03  6:38a EBSREL.F
EXEC     F        430,094  07-03-03  6:38a EXEC.F
FILEUTIL F          9,218  07-03-03  6:38a FILEUTIL.F
IAREADER F         21,918  07-03-03  6:38a IAREADER.F
NFENV    F        122,240  07-03-03  6:38a NFENV.F
READER   F        158,284  07-03-03  6:38a READER.F
SEISMO2  F         84,413  07-03-03  6:38a SEISMO2.F
SZFT     F        124,489  07-03-03  6:38a SZFT.F
UZFT     F        151,162  07-03-03  6:38a UZFT.F
GGENII   INP       13,377  07-03-03  7:22a GGENII.INP
NEFII    INP       11,849  07-03-03  7:22a NEFII.INP
NEFIISZ  INP       11,849  07-03-03  7:22a NEFIISZ.INP
NEFIIUZ  INP       10,607  07-03-03  7:22a NEFIIUZ.INP
NEFIIUZ  OUT      687,364  07-03-03  7:22a NEFIIUZ.OUT
NEFIISZ  OUT      121,864  07-03-03  7:22a NEFIISZ.OUT
NEFII    OUT      121,720  07-03-03  7:22a NEFII.OUT
        46 file(s)      3,391,511 bytes
```

Directory of C:\Search_TPA_for_bad_words\dum_dummy

```
.            <DIR>        10-30-03 12:06p .
..           <DIR>        10-30-03 12:06p ..
ESTIMA~1 F         62,680  07-03-03  6:38a estimator.f
ITYMUT~1 F         27,564  07-03-03  6:38a itymutils.f
STRTOK~1 F         39,606  07-03-03  6:38a strtokfunc.f
UNCERT~1 F         62,116  07-03-03  6:38a uncertain.f
XQIN     F          5,456  07-03-03  6:38a XQIN.F
ACUTE1   F         10,421  07-03-03  6:38a ACUTE1.F
ACUTEA   F          9,889  07-03-03  6:38a ACUTEA.F
ACUTEC   F          7,350  07-03-03  6:38a ACUTEC.F
AIRCAL   F          8,964  07-03-03  6:38a AIRCAL.F
ANMCAL   F          8,622  07-03-03  6:38a ANMCAL.F
AQUCAL   F          2,114  07-03-03  6:38a AQUCAL.F
BLOCKD   F          4,291  07-03-03  6:38a BLOCKD.F
CANDH    F         13,440  07-03-03  6:38a CANDH.F
CRONMOD  F         10,524  07-03-03  6:38a CRONMOD.F
CRPCAL   F          5,302  07-03-03  6:38a CRPCAL.F
DKHARV   F          3,961  07-03-03  6:38a DKHARV.F
DOSE     F          5,593  07-03-03  6:38a DOSE.F
DRKCAL   F          1,947  07-03-03  6:38a DRKCAL.F
DUMRED   F          1,371  07-03-03  6:38a DUMRED.F
EDRANM   F          4,079  07-03-03  6:38a EDRANM.F
EDRCRP   F          3,676  07-03-03  6:38a EDRCRP.F
EDRNON   F          2,604  07-03-03  6:38a EDRNON.F
EDRRES   F          2,944  07-03-03  6:38a EDRRES.F
ENVLIB   F          4,749  07-03-03  6:38a ENVLIB.F
EXTCAL   F          6,997  07-03-03  6:38a EXTCAL.F
READIN   F         11,802  07-03-03  6:38a READIN.F
REDCAS   F          6,361  07-03-03  6:38a REDCAS.F
REDCHA   F          4,003  07-03-03  6:38a REDCHA.F
REDFLT   F          8,794  07-03-03  6:38a REDFLT.F
RITQA    F         27,988  07-03-03  6:38a RITQA.F
SWCAL    F          8,556  07-03-03  6:38a SWCAL.F
XQCAL    F          9,582  07-03-03  6:38a XQCAL.F
ACCMOD   F         13,180  07-03-03  6:38a ACCMOD.F
NEFMKS   F        317,656  07-03-03  6:38a NEFMKS.F
SNLLHS   F        232,641  07-03-03  6:38a SNLLHS.F
TCCDF    F         24,198  07-03-03  6:38a TCCDF.F
DCAGS    F        127,334  07-03-03  6:38a DCAGS.F
DCAGW    F        162,201  07-03-03  6:38a DCAGW.F
MV       F         17,401  07-03-03  6:38a MV.F
NFENV    F        122,240  07-03-03  6:38a NFENV.F
SAMPLER  F        110,330  07-03-03  6:38a SAMPLER.F
SZFT     F        124,489  07-03-03  6:38a SZFT.F
UZFT     F        151,162  07-03-03  6:38a UZFT.F
        43 file(s)      1,796,178 bytes
```

Directory of C:\Search_TPA_for_bad_words\guess

```
.            <DIR>        10-30-03 12:01p .
```

```
..            <DIR>        10-30-03 12:01p ..
RELEASET F        187,323  07-03-03  6:38a RELEASET.F
FAILT    F        107,288  07-03-03  6:38a FAILT.F
NEFMKS   F        317,656  07-03-03  6:38a NEFMKS.F
SUBAREA  F         39,638  07-03-03  6:38a SUBAREA.F
        4 file(s)       651,905 bytes

Directory of C:\Search_TPA_for_bad_words\junk

.             <DIR>        10-30-03 11:26a .
..            <DIR>        10-30-03 11:26a ..
ZPORTPC  F         48,966  07-03-03  6:38a ZPORTPC.F
SNLLHS   F        232,641  07-03-03  6:38a SNLLHS.F
DCAGS    F        127,334  07-03-03  6:38a DCAGS.F
DCAGW    F        162,201  07-03-03  6:38a DCAGW.F
EBSREL   F         91,449  07-03-03  6:38a EBSREL.F
EXEC     F        430,094  07-03-03  6:38a EXEC.F
NFENV    F        122,240  07-03-03  6:38a NFENV.F
READER   F        158,284  07-03-03  6:38a READER.F
SAMPLER  F        110,330  07-03-03  6:38a SAMPLER.F
ASHPLUMO F         29,192  07-03-03  6:38a ASHPLUMO.F
       10 file(s)     1,512,731 bytes

Directory of C:\Search_TPA_for_bad_words\not_needed

.             <DIR>        10-30-03 12:21p .
..            <DIR>        10-30-03 12:21p ..
FNTDRF   F          2,057  07-03-03  6:38a FNTDRF.F
NFENV    F        122,240  07-03-03  6:38a NFENV.F
DCAGS    F        127,334  07-03-03  6:38a DCAGS.F
        3 file(s)       251,631 bytes

Directory of C:\Search_TPA_for_bad_words\not_used

.             <DIR>        10-30-03 12:26p .
..            <DIR>        10-30-03 12:26p ..
BASECASE INP       98,036  07-03-03  6:38a BASECASE.INP
REVERS~1 INP      257,252  07-03-03  6:38a reversibles.inp
CRONMOD  F         10,524  07-03-03  6:38a CRONMOD.F
ORDER    F          4,374  07-03-03  6:38a ORDER.F
NEFMKS   F        317,656  07-03-03  6:38a NEFMKS.F
RELEASET F        187,323  07-03-03  6:38a RELEASET.F
TPA      INP      102,530  07-03-03  6:38a TPA.INP
EBSREL   F         91,449  07-03-03  6:38a EBSREL.F
EXEC     F        430,094  07-03-03  6:38a EXEC.F
NFENV    F        122,240  07-03-03  6:38a NFENV.F
READER   F        158,284  07-03-03  6:38a READER.F
SUBAREA  F         39,638  07-03-03  6:38a SUBAREA.F
ASHPLUMO F         29,192  07-03-03  6:38a ASHPLUMO.F
       13 file(s)     1,848,592 bytes

Directory of C:\Search_TPA_for_bad_words\redundant
```

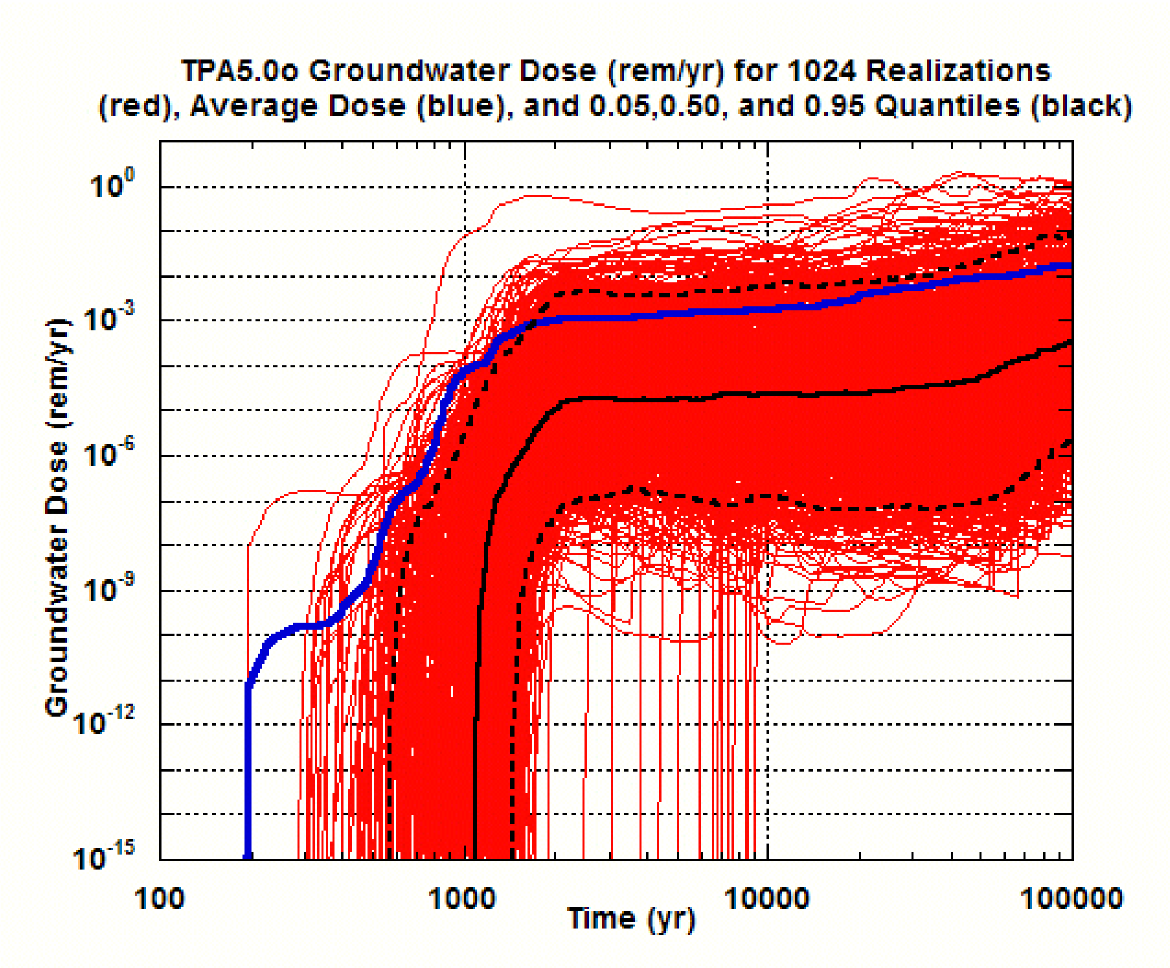
```
.            <DIR>       10-30-03 12:28p .
..           <DIR>       10-30-03 12:28p ..
UZFLOW   F          88,348  07-03-03  6:38a UZFLOW.F
SZFT     F         124,489  07-03-03  6:38a SZFT.F
EXEC     F         430,094  07-03-03  6:38a EXEC.F
        3 file(s)       642,931 bytes

Directory of C:\Search_TPA_for_bad_words\stuff

.            <DIR>       10-30-03 11:27a .
..           <DIR>       10-30-03 11:27a ..
EXEC     F         430,094  07-03-03  6:38a EXEC.F
        1 file(s)       430,094 bytes

Directory of C:\Search_TPA_for_bad_words\unknown

.            <DIR>       10-30-03 12:00p .
..           <DIR>       10-30-03 12:00p ..
ESTIMA~1 F          62,680  07-03-03  6:38a estimator.f
WELDFAIL F          20,402  07-03-03  6:38a WELDFAIL.F
DSFAILT  F          23,900  07-03-03  6:38a DSFAILT.F
EBSFILT  F          18,612  07-03-03  6:38a EBSFILT.F
FAILT    F         107,288  07-03-03  6:38a FAILT.F
MECHFAIL F         134,557  07-03-03  6:38a MECHFAIL.F
NEFMKS   F         317,656  07-03-03  6:38a NEFMKS.F
RELEASET F         187,323  07-03-03  6:38a RELEASET.F
SNLLHS   F         232,641  07-03-03  6:38a SNLLHS.F
ASHPLUME F          97,729  07-03-03  6:38a ASHPLUME.F
TCCDF    F          24,198  07-03-03  6:38a TCCDF.F
ASHPLUMO F          29,192  07-03-03  6:38a ASHPLUMO.F
DCAGS    F         127,334  07-03-03  6:38a DCAGS.F
DCAGW    F         162,201  07-03-03  6:38a DCAGW.F
DSFAIL   F          34,509  07-03-03  6:38a DSFAIL.F
EBSFAIL  F          50,906  07-03-03  6:38a EBSFAIL.F
EBSREL   F          91,449  07-03-03  6:38a EBSREL.F
EXEC     F         430,094  07-03-03  6:38a EXEC.F
IAREADER F          21,918  07-03-03  6:38a IAREADER.F
NFENV    F         122,240  07-03-03  6:38a NFENV.F
READER   F         158,284  07-03-03  6:38a READER.F
SAMPLER  F         110,330  07-03-03  6:38a SAMPLER.F
SEISMO2  F          84,413  07-03-03  6:38a SEISMO2.F
SUBAREA  F          39,638  07-03-03  6:38a SUBAREA.F
UZFLOW   F          88,348  07-03-03  6:38a UZFLOW.F
UZFT     F         151,162  07-03-03  6:38a UZFT.F
       26 file(s)     2,929,004 bytes

Directory of C:\Search_TPA_for_bad_words\unnecessary

.            <DIR>       10-30-03 12:17p .
..           <DIR>       10-30-03 12:17p ..
NEFMKS   F         317,656  07-03-03  6:38a NEFMKS.F
NFENV    F         122,240  07-03-03  6:38a NFENV.F
```

```
        2 file(s)       439,896 bytes

Directory of C:\Search_TPA_for_bad_words\weird

.            <DIR>        10-30-03 12:04p .
..           <DIR>        10-30-03 12:04p ..
STRTOK~1 F          39,606  07-03-03  6:38a strtokfunc.f
SNLLHS   F         232,641  07-03-03  6:38a SNLLHS.F
        2 file(s)       272,247 bytes

Directory of C:\Search_TPA_for_bad_words\wrong

.            <DIR>        10-30-03 12:09p .
..           <DIR>        10-30-03 12:09p ..
NEFMKS   F         317,656  07-03-03  6:38a NEFMKS.F
NFENV    F         122,240  07-03-03  6:38a NFENV.F
EBSREL   F          91,449  07-03-03  6:38a EBSREL.F
        3 file(s)       531,345 bytes

Total files listed:
      173 file(s)    16,796,404 bytes
       50 dir(s)      55,126.91 MB free
```

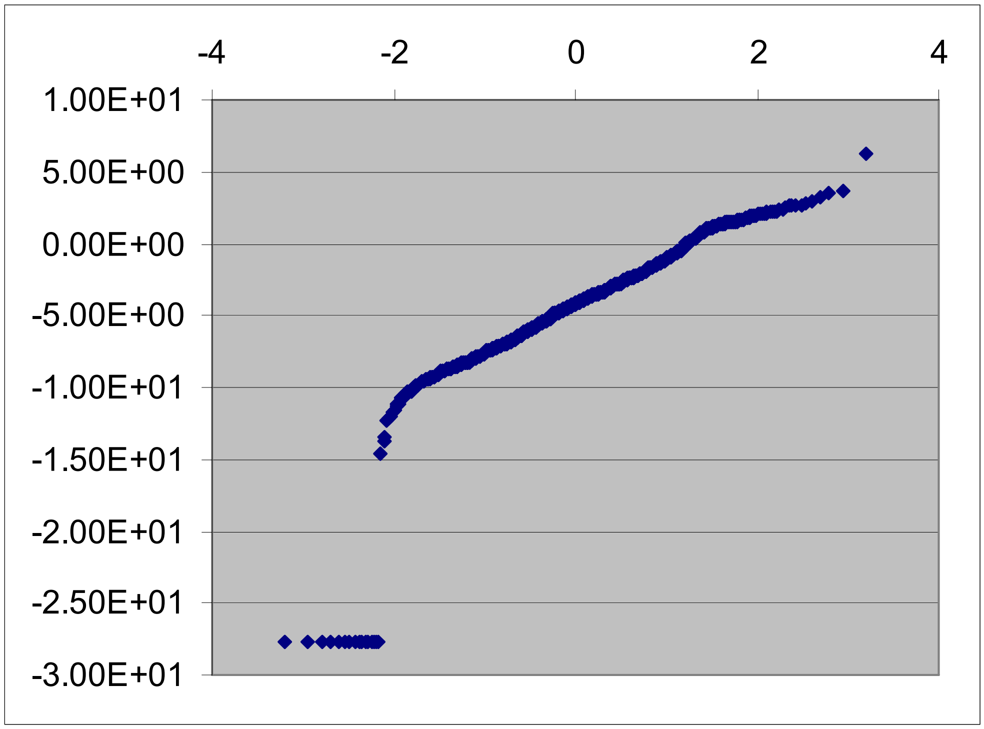
11/7/03

At the request of G. Wittmeyer, prepared plots of TPA 5.0o results showing quantiles and confidence limits. This work began with the goal of establishing confidence limits on the expected dose from a TPA run. The first plot shows expected dose and quantiles, while the second plot illustrates whether, at an single time step of a 1,024 realization TPA run, doses are distributed normally through the use of a normal-probablity-plot. (Note that if the plot is a straight line, then the data are normally distributed and this plot is a straight line except for a couple of extreme points; this second plot indicates that the data normally distributed.)

Plot 1


TPA5.0o Groundwater Dose (rem/yr) for 1024 Realizations
(red), Average Dose (blue), and 0.05,0.50, and 0.95 Quantiles (black)
Groundwater Dose (rem/yr)
10^0
10^-3
10^-6
10^-9
10^-12
10^-15
100
1000
10000
100000
Time (yr)

Plot 2
(from EXCEL)



12/15/03

Prepared a list of items were identified during code testing, validation, and development that should be considered as potential modification to future versions and revisions of the TPA code. This list of items were transmitted as follows via email to R. Janetzke.

12/15/03

Ron,

Here's my short list of items that I have come across in the last few months that may need to be fixed/enhanced in new versions of the TPA code. You and I have talked about most, if not all, of these previously. And more than likely, you already have them on your long list.

If the following changes are not made, it is suggested that the User's Guide be modified, if it already doesn't say so, to state these items are not included or that these are part of the model assumptions.

1. *Couple WP failure with seismic activity (currently, rockfall does not cause WP failure; instead, rockfall affects dripshield integrity). Source: discussion with Doug Gute and others subsequently.*
2. *Chloride ion concentration affects WP failure; however, need to add Fluoride ion concentration to the model of WP failure. This should delay the WP failure time. Source: discussion with Osvaldo Pensado.*
3. *Examine the cause for early WP failures (currently, about 30% of all WPs fail before 2,000 yr, with the remaining WPs failing at around 50,000 - 70,000 yr or so). Look at Chloride concentrations and the WP failure model. Note that there should be a bimodal distribution of the WP failures, but there shouldn't be so many of these early failures). Source: discussion with Osvaldo Pensado.*
4. *Investigate the assumption (and if necessary modify the source code in UZFT) that all flow is in a fracture if the flow rate at any time of a TPA simulation exceeds the matrix hydraulic conductivity. Is it possible to make the matrix/fracture flow split time varying and not "all or nothing"? Source: Gordon Wittmeyer.*
5. *Modify the ASHRMOVO source code to make it easier (more transparent) to read and follow, while not changing results. Source: Michael Smith*
6. *Check the numerical solution in RELEASET for conditions of high release rate. The mass balance error was noted in late July just prior to TPA code delivery when RELEASET results for IMODELs with high release rates (e.g., IMODEL = 5 for glass) had results with more than a 10% mass balance error. Source: This observation was passed on by Rob Rice during a telecon with NRC to Dick Codell who said he'd look into it.*
7. *Modify ASHRMOVO to avoid zero dose when initial ash + incoming ash < ash removal; that is, zero ash is passed on in calculations and for dose determinations even though there is some ash entering and present during the duration of the time step, Source: Michael Smith (12/15/03)*

Please contact me if you have any questions about these items.

Thanks,
Rob Rice
915 373 2472 (cell)
915 581 0853 rwrice@aol.com

01/04/04

The following email details results from TPA4.1jp using different seeds for 6 sets of TPA runs with 331, 500, and 1000 realizations.

> *Subj: Trend With Increasing # Realizations (my results)*
> *Date: 1/4/2004*
> *To: gwittmeyer@swri.org*
>
> *CC: Rwrice@aol.com File:*
>
> *C:\tpa41jp\Results_Summary.doc (275968 bytes) DL Time (32000 bps): < 2 minutes*
>
> *Gordon,*
>
> *As per our conversation in mid-December,*
> *I did some runs with TPA Version 4.1jp with*
> *331, 500, and 1,000 Realizations (I did not go to 4,000).*
> *This version of the code I received from Ron with executables*
> *included.*
>
> *I used 331 because that seemed like a logical starting point*
> *given there are 330 sampled parameters and went to 1,000 realizations*
> *because that is the maximum allowed in TPA Version 4.1jp using*
> *the pre-compiled code.*
>
> *However, this is not a limitation because the results at 331,*
> *500, and 1,000 realizations are quite interesting,*
> *I believe, and do not indicate a problem with sampling, etc.*
>
> *I ran a total of 18 TPA runs, with 6 runs at 331 realizations,*
> *6 runs at 500 realizations, and 6 runs at 1,000 realizations (so it*
> *approximates results in the Sens.; Anal. Report). Each seed for*
> *each of the 18 TPA runs was different.*
>
> *I interpreted the results as follows:*
>
> *1) increasing # realizations gives a trend of a narrower*
>
> *ranges of peak mean dose and a decreasing peak mean dose*

2) I believe 1) occurs because its 10K yr and one realization dominates (the domination I believe is because of the "pre_exp" factor we talked about before) and with increasing # realizations averaging with give a decreasing trend

3) there is not an increasing trend in peak mean dose by # realizations, like is shown in the Sens. Anal. Report

(I have not investigated this completely, but based on my past experience with the TPA results with these types of runs, I do believe this is correct - I can look into the dominant realization if needed, and can analyze further, here but I am intending to really only show you the results).

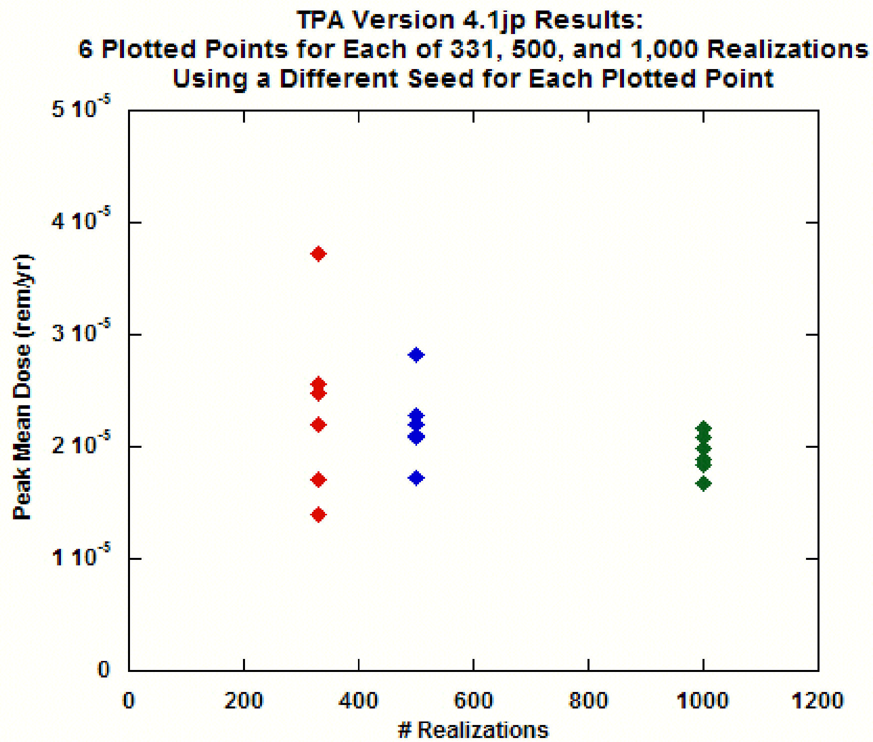
See the attached WORD file for a plot of the results, the results, and a summary of results.

Please contact me if you have any questions and I'll be in touch - I'd like to visit with you in SA in mid-January - please let me know if this works out (I also need to talk with Sitakanta then too).

Take care and hope your holidays were fine,

Rob

The contents of WORD file attached to this email follows. There is 1 plot of the results and a table with a summary of the results and input parameters.


TPA Version 4.1jp Results:
6 Plotted Points for Each of 331, 500, and 1,000 Realizations
Using a Different Seed for Each Plotted Point
Peak Mean Dose (rem/yr)
5 10^-5
4 10^-5
3 10^-5
2 10^-5
1 10^-5
0
0
200
400
600
800
1000
1200
Realizations

Results from TPA Version 4.1jp (pre-compiled executables)

Seed #	Seed Value	# Realizations	Peak Mean Dose (Expected Dose) (rem/yr)	Time of Peak Mean Dose (yr)
13	966798230.0	331	2.20E-05	9,323
14	996679823.0	331	1.40E-05	10,000
15	399667982.0	331	2.56E-05	10,000
16	239966798.0	331	3.73E-05	8,897
17	823996679.0	331	1.71E-05	9,769
18	982399667.0	331	2.48E-05	10,000
1	188910452.0	500	2.20E-05	9,543
2	218891045.0	500	1.72E-05	10,000
3	521889104.0	500	2.10E-05	9,107
4	452188910.0	500	2.28E-05	10,000
5	104521889.0	500	2.82E-05	10,000
6	910452188.0	500	2.09E-05	9,543
7	299021563.0	1000	1.98E-05	10,000
8	329902156.0	1000	1.88E-05	10,000
9	632990215.0	1000	2.08E-05	9,543
10	563299021.0	1000	1.67E-05	10,000
11	156329902.0	1000	2.16E-05	10,000
12	215632990.0	1000	1.84E-05	10,000

Summary of Results from TPA Version 4.1jp (pre-compiled executables)

# Realizations	AVERAGE Peak Mean Dose (Expected Dose) (rem/yr)	STANDARD DEVIATON Peak Mean Dose (Expected Dose) (rem/yr)	RANGE Peak Mean Dose (Expected Dose) (rem/yr)	RATIO OF MAX / MIN Peak Mean Dose (Expected Dose) (rem/yr)
331	2.35E-05	8.13E-06	2.33E-05	**2.66**
500	2.20E-05	3.58E-06	1.10E-05	**1.64**
1000	1.94E-05	1.75E-06	4.88E-06	**1.29**

1/14/04

At the request of S. Mohanty, prepared a table with Chapter 3 figures from the TPA 4.1j Sensitivity Analysis report showing each figure name, the name of the source file used to create the figure (usually a Kaleidagraph or EXCEL file), and a description of the plot and where to get the data in TPA output (or input) files. S. Mohanty provided FORTRAN source code files and the final figures used to create some of these files during a meeting. These files were placed onto a CD.

The following list was prepared and submitted to S. Montany and includes (1) figure name, (2) file name used for the figure, and (3) description

Figure #
Figure file name - Kaleidagraph (or other)
Instructions for Obtaining Plotted Values

Figure 3-1
fig3-01_infilvsMAP_report
MAP: read top of readMAP.f, follow directions for script and execute read MAP.e; output file: avgMAP.plt; MAI: use subroutine sapercflux in singleVectorMakePlot.f; output file: MAIAAIinfil.plt*

Figure 3-2 (a,b,c)
fig3-02(a,b,c)_seep100k_report
Use subroutine sawptemprhwpflow in singleVectorMakePlot.f; output files: seep10k.plt and seep100k.plt (no 1.5kyr file)

Figure 3-3
fig3-03_InfiltrationRate
Read values from infilper.res (has average values for the 3 plotted rates at every 10th time step)

Figure 3-4 (a,b)
fig3-04a_sm and fig3-04b_wptemp_present
Use subroutine sawptemprhwpflow in singleVectorMakePlot.f; output file: wptemp.plt

Figure 3-5
fig3-05
Use subroutine sawptemprhwpflow in singleVectorMakePlot.f; output file: relhum.plt

Figure 3-6
fig3-06
Read Cl values from the 12th column and times from the 1st column of multiflo.dat

Figure 3-7

fig3-07_failt_rthick_present
Read thickness values from the 7th column and times from the 2nd column of corrode.out

Figure 3-8
fig3-08
Read # of failed WPs from wpsfail.res, but can get all information from the screenprint (including initial failures)

Figure 3-9
fig3-09 (EXCEL file)
Read subarea stratigraphic unit thicknesses from tpa.inp (see UZFT section for *_Thickness_*SubArea[m] variable names)

Figure 3-10
fig3-10_cl36norm_ebsuzsz
Use subroutine ebsuzszrel in singleVectorMakePlot.f; output files: relebsAll.plt, reluzAll.plt, and relszAll.plt using Cl column values ** (note: normalize these values with respect to integrated EBS release to arrive at a fraction EBS, UZ, and SZ release)

Figure 3-11
(none)
This is a graphics file. (maybe ArcView or AutoCad?) May need to be updated if streamtube data or water contours change.

Figure 3-12 (a,b)
fig3-12a_nuctotaldose10k_present and fig3-12b_nuctotaldose_present
Use subroutine read_nexpd in singleVectorMakePlot.f; output file: nucdose100k_allnuc.plt **
(note: need to convert these results from mrem/yr to mSv/yr by dividing by 100)

Figure 3-13 (a,b,c)
fig3-13(a,b,c)_inBqs
Use subroutine ebsuzszrel 10kyr values in ebsuzszRelInBqsForMeanVal.f; output files: relebsAllInBq.plt, reluzAllInBq.plt, and relszAllInBq.plt **

Figure 3-14 (a,b)
fig3-14a_meanval_dose_base_faulto_present
For (a) basecase and with Faulting ON and (b) basecase and with IA ON, use subroutine read_expd in singleVectorMakePlot.f; and fig3-14b output file: nucdose10k.plt - will need to modify subroutine read_expd to also read rgssa.tpa and rgwgssa.tpa for (b) (note: need to convert these results from mrem/yr to mSv/yr by dividing by 100)

Figure 3-15 (a,b,c)
fig3-15(a,b,c)_inBqs and fig3-15Legend
(same as Figure 3-13 except use 100 kyr values) **

Figure 3-16 (a-f)
fig3-16(a-f)_inBqs and fig3-16_Legends

Use subroutine ebsuzszrel 100kyr values in ebsuzszRelInBqsForMeanVal.f; output files: relebsInBq.plt, reluzInBq.plt, and relszInBq.plt **

Figure 3-17
fig3-17
Read from dcagw.rlt for Tc99 (there is 1 realilzation since this is the mean value case); extract Tc99 doses by subarea; sum to get total Tc99 dose (note: need to convert these results from mrem/yr to mSv/yr by dividing by 100)

Figure 3-18 (a,b)
fig3-18(a,b) and fig3-18_Legend
There doesn't seem to be a program to compute total dose by subarea. Either (1) write a program to read dcagw.rlt to compute total dose and total dose by subarea or (2) run the TPA code once for each subarea and use total subarea doses from rgwsa.tpa to create this plot. (note: need to convert these results from mrem/yr to mSv/yr by dividing by 100)

Figure 3-19 (a,b)
fig3-19a_meanval_dose_base_faulto_present100k
(same as Figure 3-14 except use 100 kyr values) ** and fig3-19b (note: need to convert these results from mrem/yr to mSv/yr by dividing by 100)

Figure 3-20 (a,b)
fig3-20(a,b)_dose_presentColored
Use read_totdos_c.f; output files: totdos_c.plt (10 kyr) and totdose.plt (100 kyr); for percentiles, not sure where the curve came from - suggest modifying totdos_c.f to determine and then write these percentiles to an output file (note: need to convert these results from mrem/yr to mSv/yr by dividing by 100)

Figure 3-21
fig3-21_infil_avgminmax,Apr18
Use subroutine sapercflux in multiVectorMakePlot.f; output file: infil_avgminmax.plt

Figure 3-22 (a,b)
fig3-22a_wptemp_allsa and fig3-22b_wptempsa1
Use subroutine sawptemprhwpflow in multiVectorMakePlot.f; output file: wptemp.plt

Figure 3-23
fig3-23_fractwpfail
Use subroutine fracwpsfail*** in multiVectorMakePlot.f; output files: fractwpfail.plt and avgfractwpfail.plt

Figure 3-24 (a,b)
fig3-24(a,b)_inBqs
Use subroutine ebsuzszrel in multiVectorMakePlot.f; output files: Tc99_sa1_pkrel.plt and Np237_sa1_pkrel.plt ** (note: need to convert these results from mrem/yr to mSv/yr by dividing by 100 and make sure release rates in Ci/yr are converted to Bq/yr)

Figure 3-25 (a,b)

fig3-25(a,b)_inBqs
Use read_allreleaserateInBqs.f; output files: Tc99_avg_ebsrelInBqs.plt and Np237Tc99_sa1_relebsInBqs.plt for 10 kyr and 100kyr in Subarea 1

Figure 3-26
Fig3-26_inBqs
Use subroutine inventory in inventoryAndCulRelInBqs.f; output files: cumrel10kInBqs.plt and cumrel100kInBqs.plt

Figure 3-27
Fig3-27_inBqs
Use subroutine ebsuzszrel in ebsuzszRelInBecquerels.f and also the average fraction of failed WPs from Figure 3-23; output file: reluz.plt (note: need to be sure the release rates are converted from Ci/yr to Bq/yr)

Figure 3-28 (a,b)
fig3-28(a,b)_inBqs
Use read_allreleaserateInBqs.f; output file: Tc99_avg_uzrelInBqs.plt and Np237Tc99_sa1_reluzInBqs.plt for 10 kyr and 100kyr in Subarea 1

Figure 3-29 (a,b)
fig3-29(a,b)_inBqs
Use read_allreleaserateInBqs.f; output files: Tc99_avg_ebsrelInBqs.plt, Tc99_avg_uzrelInBqs.plt, and Tc99_avg_szrelInBqs.plt for 10 kyr and 100kyr in Subarea 1

Figure 3-30
fig3-30_gwttuzAllSubares(newYMR-TC)
Read and sort into a CCDF the UZ GWTT values for Subareas 1 - 10 and the average UZ GWTT from gwttuzsz.res

Figure 3-31
fig3-31_inBqs
Use subroutine ebsuzszrel in multiVectorMakePlot.f; output file: relsz.plt (note: need to be sure the release rates are converted from Ci/yr to Bq/yr)

Figure 3-32 (a,b)
fig3-32a_inBqs.txt and fig3-32b_inBqs
Use read_allreleaserateInBqs.f; output file: Tc99_avg_szrelInBqs.plt and Np237Tc99_sa1_relszInBqs.plt for 10 kyr and 100kyr in Subarea 1

Figure 3-33
fig3-33_gwttszAllSubares(newYMR-TC)
Read and sort into a CCDF the SZ GWTT values for Subareas 1 - 10 and the average SZ GWTT from gwttuzsz.res

Figure 3-34 (a,b)
fig3-34(a,b)_percentpkdose10k

Read total and nuclide peak GW doses from gwpkds_c.res (10 kyr) and gwpkdos.res (100 kyr) and compute % of total dose for each realization

Figure 3-35 (a,b)
fig3-35a_nucdose10k, fig3-35b, and fig3-35a_Legend
Use subroutine read_nexpd in multiVectorMakePlot.f; output file: nucdose100k_allnuc.plt ** (note: need to convert these results from mrem/yr to mSv/yr by dividing by 100)

Figure 3-36 (a,b)
fig3-36a_DissolutionModelsUsingExpDoseAt10k
Use mean values and set tpa.inp variable values according to the Fuel-Dissolution Models specified in Section 3.5.1; obtain GW dose from

fig3-36b_DissolutionModelsUsingExpDoseAt100k the rgwsa.tpa file (note: need to convert these results from rem/yr to mSv/yr by multiplying by 10)

Figure 3-37 (a,b)
fig3-37a_fuelwettingUsingNewCladM1_10k and fig3-37b_fuelwettingUsingNewCladM1_100k
Use mean values and set tpa.inp variable values according to the Fuel-Wetting Assumptions specified in Section 3.5.2; obtain GW dose from the rgwsa.tpa file (note: need to convert these results from rem/yr to mSv/yr by multiplying by 10)

Figure 3-38 (a,b)
fig3-38a_TransportAlternatives10k and fig3-38b_TransportAlternatives100k
Use mean values and set tpa.inp variable values according to the Transport Assum ptions specified in Section 3.5.3; obtain GW dose from the rgwsa.tpa file (note: need to convert these results from rem/yr to mSv/yr by multiplying by 10)

Figure 3-39
fig3-39_seishaz_present
Read from the SEISMIC Hazard Curve variable set in tpa.inp

Figure 3-40
fig3-40_vertextrockfall_present
Read from the VerticalExtentOfRockFall*_*[m] variable set in tpa.inp

Figure 3-41
fig3-41_seisjoint_present
Read from the SEISMOJointSpacing*[m] and DistributionJointSpacing*forSEISMO variables set in tpa.inp

Figure 3-42
fig3-42_seis_fractarea
Read from the FractionAreaForGroundMotion* variable set in tpa.inp

Figure 3-43 (a,b)
fig3-43a_faulting_present and fig3-43b_MikeMullersCvolc

For (a) basecase and with Faulting ON, use subroutine read_expd in multiVectorMakePlot.f; output file: dose100k.plt
For (b) basecase and with IA ON, use IA dose from Figure 3-45 (probability weighted) note that the 2 basecase doses are from Figure 3-20(a) and (b)

Figure 3-44
fig3-44expdoseForEachETEventInMilliSieverts
It appears that the following two source codes were used, combinev.f and cvolc5.f, to determine the Figure 3-44 and 3-45 plots (the former file reads totdose.res from a TPA run with IA ON [i.e., preprocesses volcanism dose to get average at each timestep]; the latter probability weights results from a number of TPA IA runs <= 10kyr) So, need to do a number of TPA IA runs and then set-up the cvolc5.f input file

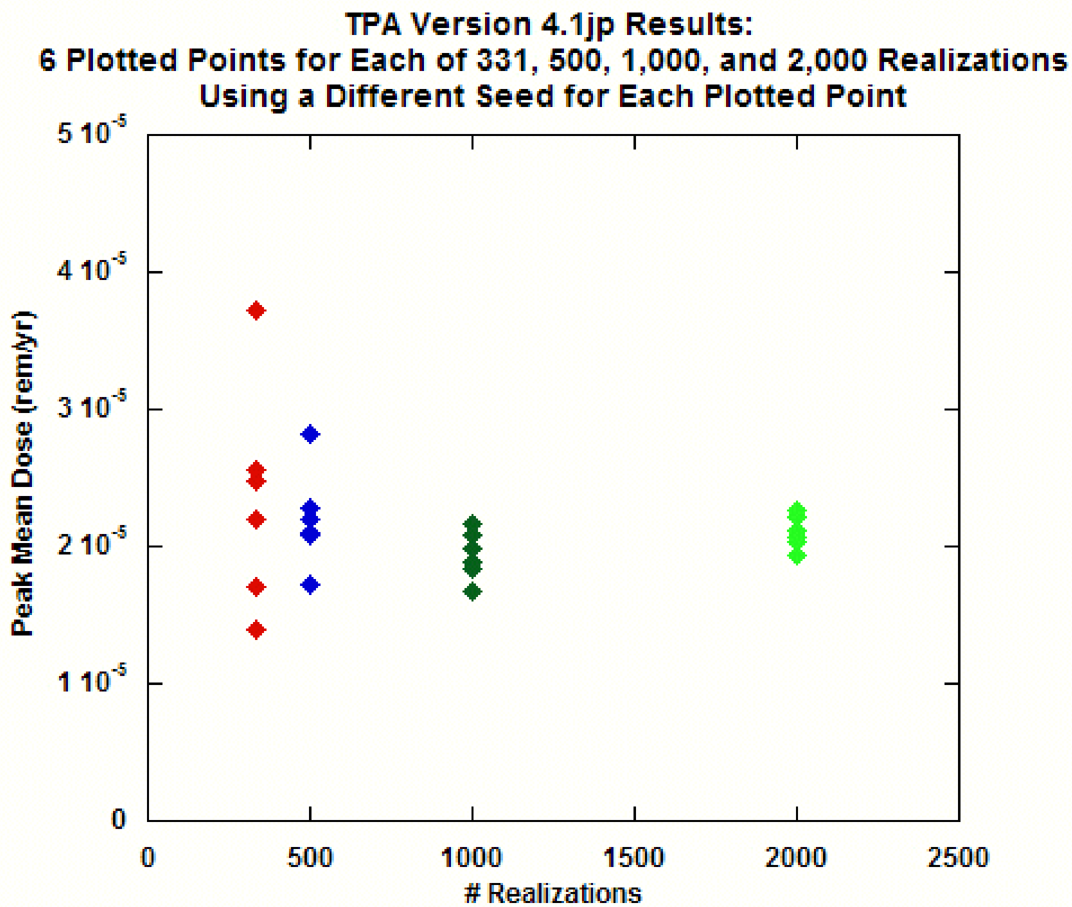
Figure 3-45
fig3-45_doseaftreposclose
(see Figure 3-44)

* = will need to change source code to reflect 1 realization instead of 350 realizations
** = check to be sure the radionuclide order in singleVectorMakePlot.f matches the order in tpa.inp
*** = it's not clear that the WP failed fraction is correct since the source code divides by 10 (should divide by fraction of total WPs in the subarea)

NOTE 1: some of the plots do not match the format shown in the December 2002 report
NOTE 2: hard-coded values in source code will need modifications if the number of subareas and/or subarea coordinants change

02/03/04

At the request of Gordon Wittmeyer, from the end of the previous entry to the date of this entry, also performed 6 runs with different seeds using TPA4.1jp for 2,000 realizations. A plot of those results and a table summarizing the results and input parameters is provided below.



Results from TPA Version 4.1jp (pre-compiled executables)

Seed #	Seed Value	# Realizations	Peak Mean Dose (Expected Dose) (rem/yr)	Time of Peak Mean Dose (yr)
13	966798230.0	331	2.20E-05	9,323
14	996679823.0	331	1.40E-05	10,000
15	399667982.0	331	2.56E-05	10,000
16	239966798.0	331	3.73E-05	8,897
17	823996679.0	331	1.71E-05	9,769
18	982399667.0	331	2.48E-05	10,000
1	188910452.0	500	2.20E-05	9,543
2	218891045.0	500	1.72E-05	10,000
3	521889104.0	500	2.10E-05	9,107
4	452188910.0	500	2.28E-05	10,000
5	104521889.0	500	2.82E-05	10,000
6	910452188.0	500	2.09E-05	9,543
7	299021563.0	1000	1.98E-05	10,000
8	329902156.0	1000	1.88E-05	10,000
9	632990215.0	1000	2.08E-05	9,543
10	563299021.0	1000	1.67E-05	10,000
11	156329902.0	1000	2.16E-05	10,000
12	215632990.0	1000	1.84E-05	10,000
19	300132674.0	2000	2.03E-05	10,000
20	430013267.0	2000	1.94E-05	10,000
21	743001326.0	2000	2.06E-05	10,000
22	674300132.0	2000	2.26E-05	10,000
23	267430013.0	2000	2.11E-05	10,000
24	326743001.0	2000	2.22E-05	9,543

Summary of Results from TPA Version 4.1jp (pre-compiled executables)

# Realizations	AVERAGE Peak Mean Dose (Expected Dose) (rem/yr)	STANDARD DEVIATON Peak Mean Dose (Expected Dose) (rem/yr)	RANGE Peak Mean Dose (Expected Dose) (rem/yr)	RATIO OF MAX / MIN Peak Mean Dose (Expected Dose) (rem/yr)
331	2.35E-05	8.13E-06	2.33E-05	**2.66**
500	2.20E-05	3.58E-06	1.10E-05	**1.64**
1000	1.94E-05	1.75E-06	4.88E-06	**1.29**
2000	2.10E-05	1.20E-06	3.20E-06	**1.11**

03/16/04

Working with S. Mohanty, completed FORTRAN coding and testing for a post-processing code of TPA5.0r output files that create text files (named *.plt) utilized to generate the plots consistent with figures in Chapter 3 of the TPA Version 4.1 Sensitivity Analysis report. This work was first broached during a December meeting with S. Mohanty. The work began in late-January.

This post-processing source code is called “TPAPP.F” with an include file “TPAPP.I” and an input file “TPAPP.INP”. The first version of these “TPAPP“ files along with example TPA Version 5.0r output files used to create the *.plt files were transmitted in a CD on 3/16/04 to S. Mohanty.

By activating a flag in the “TPAPP.INP” file, information used to create any of the figures in Chapter 3 TPA Version 4.1 Sensitivity Analysis report can be generated from a TPA Version 5.0o run.

There are four types of runs that the “TPAPP” code addresses. These four types and a description of these four types are listed below.

1) **mean_value** - a single realization run that uses the “tpameans.out” file created as the result of a TPA run with the basecase “tpa.inp” file

2) **multi_vector** - uses the basecase “tpa.inp” file with a number of realizations greater than the number of sampled parameters which ensures stratified LHS sampling (e.g., 400 for TPA Version 5.0o, since there are about 381 sampled parameters)

3) **other #1** - the screenprint from “TPAPP.F”, with the associated flag activated in “TPAPP.INP” for the activated plot(s), identifies the requirements for generating these Chapter 3 plots (e.g., Figure 3-43 requires the merging of two files from TPA runs w/ and w/o Igneous Activity; Figure 3-44 requires the execution of a separate, standalone code [identified in the screenprint] that uses output files for dose from a number of TPA runs

4) **other #2** - these Chapter 3 figures provide either maps of the Yucca Mountain area (e.g., Figure 3-11) or data from the primary TPA input file “tpa.inp” (e.g., Figures 3-39 through 3-42). These types of figures may be deleted modified because the SEISMO model has changed, the conceptual model is different, or data was up-dated.

The screenprint from a TPA 5.0r run with all the “**mean_value**” case flag activated in the “TPAPP.INP” file is shown below.

```
==============================================================================
     exec: Welcome to TPA Version 5.0r
    Job started: Mon Feb 09 11:19:43 2004
==============================================================================
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    7061.6       895

Total Area [acre]         =    1165.73439756614
Total Buried Waste [MTU]  =    70039.5300000000
Repository AML [MTU/acre] =    60.0818935653192

Specified Global Parameters:

          Compliance Period =  10000.0 (yr)
    Maximum Simulation Time = 100000.0 (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)<<<**


***>>> 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.     <<<***


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  10         realization    1 of    1
----------------------------------------------------------------------
exec: calling uzflow
UZFLOW: Uncertainty parameter:    0.0000E+00
       Mean Annual Infiltration at Start(AAI0):    8.5000E+00
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
    ebsfail: No Weld Failure
    ebsfail: time of WP failure   =    69400.0  yr
exec: calling volcano
exec: failed WPs from INITIAL   event =      7 at time =      0.0 yr
exec: failed WPs from CORROSION event =   1455 at time =  69400.0 yr
 *** failed WPs: all WPs failed (       1462) ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
             Highest release rates from Sub Area          1
          Tc99    3.6926E-01 [Ci/yr/SA] at  7.030E+04 yr
          Cs135   1.0043E-01 [Ci/yr/SA] at  7.030E+04 yr
          I129    6.8109E-03 [Ci/yr/SA] at  7.030E+04 yr
          Se79    4.9627E-03 [Ci/yr/SA] at  7.030E+04 yr
          Cl36    3.7487E-03 [Ci/yr/SA] at  7.030E+04 yr
          Pu239   3.5143E-03 [Ci/yr/SA] at  8.020E+04 yr
exec: calling uzft
                Highest release rates from UZ
          Tc99    3.2664E-01 [Ci/yr/SA] at  7.030E+04 yr
          I129    6.0267E-03 [Ci/yr/SA] at  7.030E+04 yr
          Cl36    3.3163E-03 [Ci/yr/SA] at  7.030E+04 yr
          Se79    1.0913E-03 [Ci/yr/SA] at  7.390E+04 yr
          Cs135   2.7242E-04 [Ci/yr/SA] at  1.000E+05 yr
          Np239   1.7479E-04 [Ci/yr/SA] at  8.020E+04 yr
exec: calling szft
                Highest release rates from SZ
          Tc99    2.4089E-01 [Ci/yr/SA] at  7.120E+04 yr
          I129    4.4519E-03 [Ci/yr/SA] at  7.120E+04 yr
          Cl36    2.4457E-03 [Ci/yr/SA] at  7.120E+04 yr
          Se79    2.9318E-04 [Ci/yr/SA] at  8.650E+04 yr
          Pu239   1.5850E-04 [Ci/yr/SA] at  1.000E+05 yr
          U234    7.9346E-05 [Ci/yr/SA] at  8.560E+04 yr
----------------------------------------------------------------------
   subarea   2 of  10         realization    1 of    1
----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
    ebsfail: No Weld Failure
    ebsfail: time of WP failure   =    69400.0  yr
exec: failed WPs from INITIAL   event =      8 at time =      0.0 yr
exec: failed WPs from CORROSION event =   1541 at time =  69400.0 yr
```

```
 *** failed WPs: all WPs failed (       1567) ***
 *** ejected WPs:           4
exec: calling ebsrel
     ebsrel: running spent fuel waste form
            Highest release rates from Sub Area          2
        Tc99    3.8635E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   1.0513E-01 [Ci/yr/SA] at  7.030E+04 yr
        C14     1.8585E-02 [Ci/yr/SA] at  4.945E+03 yr
        I129    7.1293E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    5.1943E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    3.9227E-03 [Ci/yr/SA] at  7.030E+04 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    3.8635E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   1.0513E-01 [Ci/yr/SA] at  7.030E+04 yr
        I129    7.1293E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    5.1943E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    3.9227E-03 [Ci/yr/SA] at  7.030E+04 yr
        Pu239   3.8683E-03 [Ci/yr/SA] at  7.840E+04 yr
exec: calling szft
              Highest release rates from SZ
        Tc99    2.6687E-01 [Ci/yr/SA] at  7.120E+04 yr
        I129    4.9316E-03 [Ci/yr/SA] at  7.120E+04 yr
        Cl36    2.7090E-03 [Ci/yr/SA] at  7.120E+04 yr
        Se79    4.9963E-04 [Ci/yr/SA] at  8.110E+04 yr
        Pu239   3.7199E-04 [Ci/yr/SA] at  8.020E+04 yr
        U234    7.0336E-05 [Ci/yr/SA] at  8.020E+04 yr
----------------------------------------------------------------------
   subarea   3 of  10          realization    1 of    1
----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
    ebsfail: No Weld Failure
    ebsfail: time of WP failure    =    69400.0  yr
exec: failed WPs from INITIAL   event =       4 at time =      0.0 yr
exec: failed WPs from CORROSION event =     762 at time =  69400.0 yr
 *** failed WPs: all WPs failed (        771) ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
            Highest release rates from Sub Area          3
        Tc99    1.9290E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   5.2470E-02 [Ci/yr/SA] at  7.030E+04 yr
        C14     6.6228E-03 [Ci/yr/SA] at  4.945E+03 yr
        I129    3.5582E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    2.5926E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    1.9582E-03 [Ci/yr/SA] at  7.030E+04 yr
exec: calling uzft
              Highest release rates from UZ
        Tc99    1.5906E-01 [Ci/yr/SA] at  7.030E+04 yr
        I129    2.9354E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    1.6149E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    3.8229E-04 [Ci/yr/SA] at  7.930E+04 yr
        Np239   9.4406E-05 [Ci/yr/SA] at  7.930E+04 yr
        U234    4.2302E-05 [Ci/yr/SA] at  7.840E+04 yr
exec: calling szft
```

```
            Highest release rates from SZ
        Tc99    1.1928E-01 [Ci/yr/SA] at  7.120E+04 yr
        I129    2.2046E-03 [Ci/yr/SA] at  7.120E+04 yr
        Cl36    1.2108E-03 [Ci/yr/SA] at  7.120E+04 yr
        Se79    1.5266E-04 [Ci/yr/SA] at  9.190E+04 yr
        Pu239   8.5091E-05 [Ci/yr/SA] at  1.000E+05 yr
        U234    3.7166E-05 [Ci/yr/SA] at  8.470E+04 yr
---------------------------------------------------------------------
  subarea   4 of  10         realization    1 of    1
---------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
   ebsfail: No Weld Failure
   ebsfail: time of WP failure   =    69400.0  yr
exec: failed WPs from INITIAL   event =      2 at time =      0.0 yr
exec: failed WPs from CORROSION event =    426 at time =  69400.0 yr
 *** failed WPs: all WPs failed (        429) ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
          Highest release rates from Sub Area          4
        Tc99    1.0218E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   2.7815E-02 [Ci/yr/SA] at  7.030E+04 yr
        I129    1.8864E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    1.3743E-03 [Ci/yr/SA] at  7.030E+04 yr
        C14     1.3523E-03 [Ci/yr/SA] at  4.945E+03 yr
        Cl36    1.0377E-03 [Ci/yr/SA] at  7.030E+04 yr
exec: calling uzft
            Highest release rates from UZ
        Tc99    7.6087E-02 [Ci/yr/SA] at  7.030E+04 yr
        I129    1.4056E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    7.7285E-04 [Ci/yr/SA] at  7.030E+04 yr
        Se79    1.1242E-04 [Ci/yr/SA] at  8.110E+04 yr
        Jp239   4.9390E-05 [Ci/yr/SA] at  7.480E+04 yr
        U234    1.6850E-05 [Ci/yr/SA] at  7.480E+04 yr
exec: calling szft
            Highest release rates from SZ
        Tc99    6.1147E-02 [Ci/yr/SA] at  7.120E+04 yr
        I129    1.1314E-03 [Ci/yr/SA] at  7.120E+04 yr
        Cl36    6.2108E-04 [Ci/yr/SA] at  7.120E+04 yr
        Se79    5.9694E-05 [Ci/yr/SA] at  9.910E+04 yr
        Pu239   4.4740E-05 [Ci/yr/SA] at  1.000E+05 yr
        U234    1.2829E-05 [Ci/yr/SA] at  8.110E+04 yr
---------------------------------------------------------------------
  subarea   5 of  10         realization    1 of    1
---------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
   ebsfail: No Weld Failure
   ebsfail: time of WP failure   =    69400.0  yr
exec: failed WPs from INITIAL   event =      4 at time =      0.0 yr
exec: failed WPs from CORROSION event =    743 at time =  69400.0 yr
 *** failed WPs: all WPs failed (        758) ***
exec: calling ebsrel
```

```
    ebsrel: running spent fuel waste form
          Highest release rates from Sub Area       5
        Tc99    1.8772E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   5.1068E-02 [Ci/yr/SA] at  7.030E+04 yr
        C14     1.5882E-02 [Ci/yr/SA] at  4.945E+03 yr
        I129    3.4632E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    2.5233E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    1.9058E-03 [Ci/yr/SA] at  7.030E+04 yr
exec: calling uzft
            Highest release rates from UZ
        Tc99    1.3808E-01 [Ci/yr/SA] at  7.030E+04 yr
        I129    2.5490E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    1.4020E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    2.0196E-04 [Ci/yr/SA] at  8.110E+04 yr
        Jp239   8.9644E-05 [Ci/yr/SA] at  7.930E+04 yr
        Cs135   5.3219E-05 [Ci/yr/SA] at  6.040E+04 yr
exec: calling szft
            Highest release rates from SZ
        Tc99    1.0906E-01 [Ci/yr/SA] at  7.120E+04 yr
        I129    2.0163E-03 [Ci/yr/SA] at  7.120E+04 yr
        Cl36    1.1073E-03 [Ci/yr/SA] at  7.120E+04 yr
        Se79    1.0081E-04 [Ci/yr/SA] at  9.820E+04 yr
        Pu239   8.0332E-05 [Ci/yr/SA] at  1.000E+05 yr
        U234    3.1951E-05 [Ci/yr/SA] at  8.650E+04 yr
----------------------------------------------------------------------
  subarea   6 of  10        realization    1 of    1
----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
   ebsfail: No Weld Failure
   ebsfail: time of WP failure   =    69400.0  yr
exec: failed WPs from INITIAL   event =       4 at time =       0.0 yr
exec: failed WPs from CORROSION event =     844 at time =  69400.0 yr
 *** failed WPs: all WPs failed (       849) ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
          Highest release rates from Sub Area       6
        Tc99    2.0760E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   5.6505E-02 [Ci/yr/SA] at  7.030E+04 yr
        I129    3.8320E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    2.7919E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    2.1083E-03 [Ci/yr/SA] at  7.030E+04 yr
        Pu239   1.9263E-03 [Ci/yr/SA] at  7.930E+04 yr
exec: calling uzft
            Highest release rates from UZ
        Tc99    1.0814E-01 [Ci/yr/SA] at  7.030E+04 yr
        I129    1.9985E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    1.0985E-03 [Ci/yr/SA] at  7.030E+04 yr
        Jp239   9.4291E-05 [Ci/yr/SA] at  7.930E+04 yr
        Se79    5.4520E-05 [Ci/yr/SA] at  1.000E+05 yr
        U234    2.3105E-05 [Ci/yr/SA] at  7.750E+04 yr
exec: calling szft
            Highest release rates from SZ
        Tc99    1.0395E-01 [Ci/yr/SA] at  7.120E+04 yr
        I129    1.9242E-03 [Ci/yr/SA] at  7.120E+04 yr
        Cl36    1.0561E-03 [Ci/yr/SA] at  7.120E+04 yr
```

```
        Pu239   8.6226E-05 [Ci/yr/SA] at  1.000E+05 yr
        Se79    2.4966E-05 [Ci/yr/SA] at  1.000E+05 yr
        U234    1.9564E-05 [Ci/yr/SA] at  8.380E+04 yr
-----------------------------------------------------------------------
   subarea   7 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
    ebsfail: No Weld Failure
    ebsfail: time of WP failure   =    69400.0  yr
exec: failed WPs from INITIAL   event =       2 at time =       0.0 yr
exec: failed WPs from CORROSION event =     322 at time =  69400.0 yr
 *** failed WPs: all WPs failed (         324) ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
            Highest release rates from Sub Area           7
        Tc99    7.8676E-02 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   2.1416E-02 [Ci/yr/SA] at  7.030E+04 yr
        I129    1.4524E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    1.0582E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    7.9907E-04 [Ci/yr/SA] at  7.030E+04 yr
        Pu239   7.0464E-04 [Ci/yr/SA] at  7.840E+04 yr
exec: calling uzft
              Highest release rates from UZ
        Tc99    4.2428E-02 [Ci/yr/SA] at  7.120E+04 yr
        I129    7.8339E-04 [Ci/yr/SA] at  7.120E+04 yr
        Cl36    4.3045E-04 [Ci/yr/SA] at  7.120E+04 yr
        Jp239   3.4418E-05 [Ci/yr/SA] at  7.840E+04 yr
        U234    7.4563E-06 [Ci/yr/SA] at  7.570E+04 yr
        U238    2.4770E-06 [Ci/yr/SA] at  7.840E+04 yr
exec: calling szft
              Highest release rates from SZ
        Tc99    3.8054E-02 [Ci/yr/SA] at  7.120E+04 yr
        I129    7.0459E-04 [Ci/yr/SA] at  7.120E+04 yr
        Cl36    3.8667E-04 [Ci/yr/SA] at  7.120E+04 yr
        Pu239   3.1674E-05 [Ci/yr/SA] at  1.000E+05 yr
        U234    6.4481E-06 [Ci/yr/SA] at  9.100E+04 yr
        U238    2.1115E-06 [Ci/yr/SA] at  8.470E+04 yr
-----------------------------------------------------------------------
   subarea   8 of  10          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
    ebsfail: No Weld Failure
    ebsfail: time of WP failure   =    69400.0  yr
exec: failed WPs from INITIAL   event =       4 at time =       0.0 yr
exec: failed WPs from CORROSION event =     836 at time =  69400.0 yr
 *** failed WPs: all WPs failed (         845) ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
            Highest release rates from Sub Area           8
        Tc99    2.1178E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   5.7609E-02 [Ci/yr/SA] at  7.030E+04 yr
```

```
        C14    6.6248E-03 [Ci/yr/SA] at  4.945E+03 yr
        I129   3.9068E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79   2.8465E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36   2.1500E-03 [Ci/yr/SA] at  7.030E+04 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   2.1178E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135  5.7609E-02 [Ci/yr/SA] at  7.030E+04 yr
        I129   3.9068E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79   2.8465E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36   2.1500E-03 [Ci/yr/SA] at  7.030E+04 yr
        Pu239  2.0912E-03 [Ci/yr/SA] at  7.930E+04 yr
exec: calling szft
            Highest release rates from SZ
        Tc99   1.4940E-01 [Ci/yr/SA] at  7.120E+04 yr
        I129   2.7606E-03 [Ci/yr/SA] at  7.120E+04 yr
        Cl36   1.5167E-03 [Ci/yr/SA] at  7.120E+04 yr
        Se79   2.2766E-04 [Ci/yr/SA] at  8.110E+04 yr
        Pu239  2.0048E-04 [Ci/yr/SA] at  8.110E+04 yr
        U234   4.3632E-05 [Ci/yr/SA] at  8.200E+04 yr
-----------------------------------------------------------------------
  subarea   9 of  10        realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
   ebsfail: No Weld Failure
   ebsfail: time of WP failure   =    69400.0  yr
exec: failed WPs from INITIAL   event =       5 at time =      0.0 yr
exec: failed WPs from CORROSION event =     972 at time =  69400.0 yr
 *** failed WPs: all WPs failed (        977) ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
           Highest release rates from Sub Area          9
        Tc99   2.4537E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135  6.6765E-02 [Ci/yr/SA] at  7.030E+04 yr
        I129   4.5277E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79   3.2989E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36   2.4916E-03 [Ci/yr/SA] at  7.030E+04 yr
        Pu239  2.2073E-03 [Ci/yr/SA] at  7.930E+04 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   2.4537E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135  6.6765E-02 [Ci/yr/SA] at  7.030E+04 yr
        I129   4.5277E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79   3.2989E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36   2.4916E-03 [Ci/yr/SA] at  7.030E+04 yr
        Pu239  2.2073E-03 [Ci/yr/SA] at  7.930E+04 yr
exec: calling szft
            Highest release rates from SZ
        Tc99   1.7513E-01 [Ci/yr/SA] at  7.120E+04 yr
        I129   3.2389E-03 [Ci/yr/SA] at  7.120E+04 yr
        Cl36   1.7790E-03 [Ci/yr/SA] at  7.120E+04 yr
        Pu239  2.0969E-04 [Ci/yr/SA] at  8.110E+04 yr
        Se79   1.8128E-04 [Ci/yr/SA] at  8.200E+04 yr
```

```
        U234    4.2354E-05 [Ci/yr/SA] at  8.290E+04 yr
---------------------------------------------------------------------
   subarea  10 of  10         realization    1 of    1
---------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling dsfail
exec: calling seismo
exec: calling ebsfail
    ebsfail: No Weld Failure
    ebsfail: time of WP failure   =    69400.0  yr
exec: failed WPs from INITIAL   event =      5 at time =      0.0 yr
exec: failed WPs from CORROSION event =    880 at time =  69400.0 yr
 *** failed WPs: all WPs failed (        895) ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
             Highest release rates from Sub Area          10
        Tc99    2.2032E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   5.9949E-02 [Ci/yr/SA] at  7.030E+04 yr
        C14     1.4573E-02 [Ci/yr/SA] at  4.945E+03 yr
        I129    4.0656E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    2.9621E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    2.2370E-03 [Ci/yr/SA] at  7.030E+04 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    2.2032E-01 [Ci/yr/SA] at  7.030E+04 yr
        Cs135   5.9949E-02 [Ci/yr/SA] at  7.030E+04 yr
        I129    4.0656E-03 [Ci/yr/SA] at  7.030E+04 yr
        Se79    2.9621E-03 [Ci/yr/SA] at  7.030E+04 yr
        Cl36    2.2370E-03 [Ci/yr/SA] at  7.030E+04 yr
        Pu239   2.1206E-03 [Ci/yr/SA] at  7.840E+04 yr
exec: calling szft
              Highest release rates from SZ
        Tc99    1.5920E-01 [Ci/yr/SA] at  7.120E+04 yr
        I129    2.9437E-03 [Ci/yr/SA] at  7.120E+04 yr
        Cl36    1.6167E-03 [Ci/yr/SA] at  7.120E+04 yr
        Pu239   2.0203E-04 [Ci/yr/SA] at  8.020E+04 yr
        Se79    1.8146E-04 [Ci/yr/SA] at  8.200E+04 yr
        U234    3.6982E-05 [Ci/yr/SA] at  8.200E+04 yr
exec: calling dcagw
              Highest annual dose GW pathway
        I129    2.5354E+00 [mrem/yr]  at  7.120E+04 yr
        Pu239   1.8101E+00 [mrem/yr]  at  1.000E+05 yr
        Tc99    7.0375E-01 [mrem/yr]  at  7.120E+04 yr
        Pu240   8.3550E-02 [mrem/yr]  at  1.270E+04 yr
        Am243   6.2669E-02 [mrem/yr]  at  4.093E+03 yr
        Am241   5.3411E-02 [mrem/yr]  at  3.384E+03 yr
       At end of TPI, annual dose GW pathway
        Pu239   1.8101E+00 [mrem/yr]
        Np237   4.6765E-02 [mrem/yr]
        U234    1.3172E-02 [mrem/yr]
        Th230   1.0371E-02 [mrem/yr]
        Tc99    5.4956E-03 [mrem/yr]
        U238    3.7831E-03 [mrem/yr]
          sum  1.8969E+00 [mrem/yr]
exec: calling ashplumo
exec: calling ashrmovo
exec: calling dcags
```

```
       Highest annual dose from GS
    Pu240  4.4841E+02 [mrem/yr] at  4.945E+03 yr
    Pu239  4.4290E+02 [mrem/yr] at  4.945E+03 yr
    Am243  3.3444E+02 [mrem/yr] at  5.063E+03 yr
    Sn126  9.6753E+01 [mrem/yr] at  5.063E+03 yr
     Nb94  5.8611E+01 [mrem/yr] at  5.063E+03 yr
    Am241  4.9775E+00 [mrem/yr] at  5.063E+03 yr
exec: end realizations

exec: Peak Mean Dose is 9.75100E-01 rem/yr at   4945.1 yr, based on     1 realizations.

exec:  Run Successfully Completed
```

Using the “tpameans.out” file from a basecase TPA 5.0r run as the “tpa.inp” file with the APPEND option activated to generate TPA output files and after running the “TPAPP.F” code with all of the “mean_value” flags activated in “TPAPP.INP” provides the following screenprint.

```
   *******************************************
     Welcome to "TPAPP" - TPA Post-Processor
    (  this program screenprints input data  )
    ( and the status of the simulation; files)
    (for plotting, with *.plt extensions, are)
    (  written according to flags set in the )
    (          input file tpapp.inp          )
   *******************************************

entering tpa data reader
echo: from tpa.inp, nreal=          1
echo: from tpa.inp, ntim_d=         201
echo: from tpa.inp, ntim_a=         100
echo: from tpa.inp, time_cp=    10000.0000000000
echo: from tpa.inp, time_max=    100000.000000000
echo:therefore, ntim,ntim_c=         301         201
echo: from tpa.inp, nsubarea=          10
echo: sa i,pt j, (x,y) subarea coordinates=          1          1
   547514.880000000         4079310.61000000
echo: sa i,pt j, (x,y) subarea coordinates=          1          2
   548069.200000000         4079136.50000000
echo: sa i,pt j, (x,y) subarea coordinates=          1          3
   547847.300000000         4077816.20000000
echo: sa i,pt j, (x,y) subarea coordinates=          1          4
   547370.950000000         4077922.04000000
echo: sa i,pt j, (x,y) subarea coordinates=          2          1
   548069.200000000         4079136.50000000
echo: sa i,pt j, (x,y) subarea coordinates=          2          2
   548569.320000000         4078981.00000000
echo: sa i,pt j, (x,y) subarea coordinates=          2          3
   548504.060000000         4077664.24000000
echo: sa i,pt j, (x,y) subarea coordinates=          2          4
   547847.300000000         4077816.20000000
echo: sa i,pt j, (x,y) subarea coordinates=          3          1
   547370.950000000         4077922.04000000
echo: sa i,pt j, (x,y) subarea coordinates=          3          2
   547847.300000000         4077816.20000000
echo: sa i,pt j, (x,y) subarea coordinates=          3          3
```

```
  548322.700000000       4077192.20000000
echo: sa i,pt j, (x,y) subarea coordinates=       3        4
  547474.700000000       4077281.60000000
echo: sa i,pt j, (x,y) subarea coordinates=       4        1
  547847.300000000       4077816.20000000
echo: sa i,pt j, (x,y) subarea coordinates=       4        2
  548504.060000000       4077664.24000000
echo: sa i,pt j, (x,y) subarea coordinates=       4        3
  548479.710000000       4077173.06000000
echo: sa i,pt j, (x,y) subarea coordinates=       4        4
  548322.700000000       4077192.20000000
echo: sa i,pt j, (x,y) subarea coordinates=       5        1
  547474.700000000       4077281.60000000
echo: sa i,pt j, (x,y) subarea coordinates=       5        2
  547887.300000000       4077238.10000000
echo: sa i,pt j, (x,y) subarea coordinates=       5        3
  547897.790000000       4076045.46000000
echo: sa i,pt j, (x,y) subarea coordinates=       5        4
  547655.970000000       4076123.07000000
echo: sa i,pt j, (x,y) subarea coordinates=       6        1
  547887.300000000       4077238.10000000
echo: sa i,pt j, (x,y) subarea coordinates=       6        2
  548322.700000000       4077192.20000000
echo: sa i,pt j, (x,y) subarea coordinates=       6        3
  548155.700000000       4075962.63000000
echo: sa i,pt j, (x,y) subarea coordinates=       6        4
  547897.790000000       4076045.46000000
echo: sa i,pt j, (x,y) subarea coordinates=       7        1
  548322.700000000       4077192.20000000
echo: sa i,pt j, (x,y) subarea coordinates=       7        2
  548479.710000000       4077173.06000000
echo: sa i,pt j, (x,y) subarea coordinates=       7        3
  548455.000000000       4076674.51000000
echo: sa i,pt j, (x,y) subarea coordinates=       7        4
  548155.700000000       4075962.63000000
echo: sa i,pt j, (x,y) subarea coordinates=       8        1
  547645.270000000       4079656.06000000
echo: sa i,pt j, (x,y) subarea coordinates=       8        2
  548588.980000000       4079377.55000000
echo: sa i,pt j, (x,y) subarea coordinates=       8        3
  548569.320000000       4078981.00000000
echo: sa i,pt j, (x,y) subarea coordinates=       8        4
  547514.880000000       4079310.61000000
echo: sa i,pt j, (x,y) subarea coordinates=       9        1
  547732.820000000       4080960.00000000
echo: sa i,pt j, (x,y) subarea coordinates=       9        2
  548251.910000000       4080817.50000000
echo: sa i,pt j, (x,y) subarea coordinates=       9        3
  548116.890000000       4079516.81000000
echo: sa i,pt j, (x,y) subarea coordinates=       9        4
  547645.270000000       4079656.06000000
echo: sa i,pt j, (x,y) subarea coordinates=      10        1
  548251.910000000       4080817.50000000
echo: sa i,pt j, (x,y) subarea coordinates=      10        2
  548664.550000000       4080675.00000000
echo: sa i,pt j, (x,y) subarea coordinates=      10        3
  548588.980000000       4079377.55000000
echo: sa i,pt j, (x,y) subarea coordinates=      10        4
  548116.890000000       4079516.81000000
```

```
echo: from tpa.inp,naqueous=        20
echo: from tpa.inp,ncolloid=        11
echo: from tpa.inp,nnucl=        31
echo: from tpa.inp,nstart=         1
echo: from tpa.inp,nstart=         0

NOTE: for reading the number of WPs in each subarea,
    need to have the screenprint from a TPA run
    in a file called "tpa.out"

echo: from tpa.out,nwps in subarea          1        1462
echo: from tpa.out,nwps in subarea          2        1567
echo: from tpa.out,nwps in subarea          3         771
echo: from tpa.out,nwps in subarea          4         429
echo: from tpa.out,nwps in subarea          5         758
echo: from tpa.out,nwps in subarea          6         849
echo: from tpa.out,nwps in subarea          7         324
echo: from tpa.out,nwps in subarea          8         845
echo: from tpa.out,nwps in subarea          9         977
echo: from tpa.out,nwps in subarea         10         895
exiting tpa data reader simulation


entering input_data_reader
echo:iflag_fig3_1=          1
echo:iflag_fig3_2=          1
echo:iflag_fig3_3=          1
echo:iflag_fig3_4=          1
echo:iflag_fig3_5=          1
echo:iflag_fig3_6=          1
echo:iflag_fig3_7=          1
echo:iflag_fig3_8=          1
echo:iflag_fig3_9=          1
echo:iflag_fig3_10=          1
echo:iflag_fig3_11=          1
echo:iflag_fig3_12=          1
echo:iflag_fig3_13=          1
echo:iflag_fig3_14a=          1
echo:iflag_fig3_14b=          0
echo:iflag_fig3_15=          1
echo:iflag_fig3_16=          1
echo:iflag_fig3_17=          0
echo:iflag_fig3_18=          0
echo:iflag_fig3_19=          1
echo:iflag_fig3_20=          0
echo:iflag_fig3_21=          0
echo:iflag_fig3_22=          0
echo:iflag_fig3_23=          0
echo:iflag_fig3_24=          0
echo:iflag_fig3_25=          0
echo:iflag_fig3_26=          0
echo:iflag_fig3_27=          0
echo:iflag_fig3_28=          0
echo:iflag_fig3_29=          0
echo:iflag_fig3_30=          0
echo:iflag_fig3_31=          0
echo:iflag_fig3_32=          0
echo:iflag_fig3_33=          0
echo:iflag_fig3_34=          0
```

echo:iflag_fig3_35= 0
echo:iflag_fig3_36= 1
echo:iflag_fig3_37= 1
echo:iflag_fig3_38= 1
echo:iflag_fig3_39= 1
echo:iflag_fig3_40= 1
echo:iflag_fig3_41= 1
echo:iflag_fig3_42= 1
echo:iflag_fig3_43a= 0
echo:iflag_fig3_43b= 0
echo:iflag_fig3_44= 1
echo:iflag_fig3_45= 1
exiting input_data_reader simulation

entering the fig3_1 subroutine
****
Figure 3-1 is requested - MAP and MAI vs. Time
- the following files are needed from a MEAN VALUE run:
dcagw.ech
uzflow.rlt

The output file is: fig3_1.plt

Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp
****
exiting the fig3_1 subroutine

entering the fig3_2 subroutine
****
Figure 3-2 is requested - Seepage Flux vs. Time
- the following file is needed from a MEAN VALUE run:
ebsrel.ech

The output file is: fig3_2.plt

Verify this is a MEAN VALUE run file
note that the # realizations should be 1,
and it is set at 1 in tpa.inp
****
exiting the fig3_2 subroutine

entering the fig3_3 subroutine
****
Figure 3-3 is requested - Infiltration Rate vs. Time
- the following file is needed from a MEAN VALUE run:
infilper.res

The output file is: fig3_3.plt

Verify this is a MEAN VALUE run file
note that the # realizations should be 1,
and it is set at 1 in tpa.inp
****
exiting the fig3_3 subroutine

```
entering the fig3_4 subroutine
**********************************************************
Figure 3-4 is requested - WP Temperature vs. Time
- the following file is needed from a MEAN VALUE run:
  ebsrel.ech

The output file is: fig3_4.plt

Verify this is a MEAN VALUE run file
note that the # realizations should be 1,
    and it is set at          1 in tpa.inp
**********************************************************
exiting the fig3_4 subroutine


entering the fig3_5 subroutine
**********************************************************
Figure 3-5 is requested - Relative Humidity vs. Time
- the following file is needed from a MEAN VALUE run:
  ebsrel.ech

The output file is: fig3_5.plt

Verify this is a MEAN VALUE run file
note that the # realizations should be 1,
    and it is set at          1 in tpa.inp
**********************************************************
exiting the fig3_5 subroutine


entering the fig3_6 subroutine
**********************************************************
Figure 3-6 is requested - Chloride Conc. vs. Time
- the following file is needed:
  chlrdmf.dat

The output file is: fig3_6.plt

(note: "chlrdmf.dat" is created/overwritten)
(        for each subarea            )

Verify this is a MEAN VALUE run file
note that the # realizations should be 1,
    and it is set at          1 in tpa.inp
**********************************************************
exiting the fig3_6 subroutine


entering the fig3_7 subroutine
**********************************************************
Figure 3-7 is requested - WP Wall Thickness vs. Time
- the following file is needed:
  corrode.out

The output file is: fig3_7.plt

(note: "corrode.out" is created/overwritten)
```

(for each subarea)

Verify this is a MEAN VALUE run file
note that the # realizations should be 1,
and it is set at 1 in tpa.inp
****
exiting the fig3_7 subroutine

entering the fig3_8 subroutine
****
Figure 3-8 is requested - Cumulative WPs Failed vs. Time
- the following file is needed:
ebsrel.ech

The output file is: fig3_8.plt

Verify this is a MEAN VALUE run file
note that the # realizations must be 1,
and it is set at 1 in tpa.inp
****
exiting the fig3_8 subroutine

entering the fig3_9 subroutine
****
Figure 3-9 is requested - UZ Unit Thicknesses by Subarea
- the following file is needed:
tpa.inp

The output file is: fig3_9.plt

The 7 tpa.inp units: TSw,CHnv,CH_Total,PPw,UCF,BFw,UFZ
If these are not correct, then modify this program
****
exiting the fig3_9 subroutine

entering the fig3_10 subroutine
****
Figure 3-10 is requested - Cl36 Release Rates vs. Time
- the following files are needed from a MEAN VALUE run:
ebsrel.rlt
szft.ech
szft.rlt

The output file is: fig3_10.plt

Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp
****
exiting the fig3_10 subroutine

entering the fig3_11 subroutine
****
Figure 3-11 is requested - SZ Streamtube and Subarea Map

This figure is a graphics file.

*There is no *.plt file for Figure 3-11.*

*This figure contains water-level contours,
the repository outline (including subareas),
streamtubes 1-3, well locations, the 10km and
20km boundaries, and the Highway U.S. 95 location.*

*Check that this information has not changed to
ensure that the figure does not need to be updated.*
****
exiting the fig3_11 subroutine

entering the fig3_12 subroutine
****
*Figure 3-12 is requested - GW Dose vs. Time
- the following file is needed from a MEAN VALUE run:
rgwna.tpa*

The output file is: fig3_12.plt

*Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp*
****
exiting the fig3_12 subroutine

entering the fig3_13 subroutine
****
*Figure 3-13 is requested - Release Rates vs. Time(10kyr)
- the following files are needed from a MEAN VALUE run:
ebsrel.rlt
szft.ech
szft.rlt*

*The output files are: fig3_13a.plt (EBS)
fig3_13b.plt (UZ)
fig3_13c.plt (SZ)*

*Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp*
****
exiting the fig3_13 subroutine

entering the fig3_14a subroutine
****
*Figure 3-14a is requested - GW Dose vs. Time
(i.e., Basecase Dose and w/ Faulting Dose vs. Time)
- the following file is needed from a MEAN VALUE run:
rgwsa.tpa*

The output file is: fig3_14a.plt

THE USER NEEDS TO RUN TPAPP TWICE: ONCE WITH RESULTS

*FROM THE BASECASE TPA.INP FILE AND ONCE WITH RESULTS
FROM THE FAULTING FLAG ACTIVATED AND THRESHOLD=0.1*

*AFTER EACH OF THESE 2 TPAPP RUNS, THE FIG3_14A.PLT FILES
NEED TO BE MERGED TO GENERATE THE FIGURE 3-14A PLOT*

*Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp*
****
exiting the fig3_14a subroutine

entering the fig3_15 subroutine
****
*Figure 3-15 is requested-Release Rates vs. Time(100kyr)
- the following files are needed from a MEAN VALUE run:
ebsrel.rlt
szft.ech
szft.rlt*

*THIS FIGURE CAN BE GENERATED USING THE OUTPUT FILES
FROM FIGURE 3-13 LISTED BELOW EXCEPT WITH 100KYR RESULTS*

*The output files are: fig3_13a.plt (EBS)
fig3_13b.plt (UZ)
fig3_13c.plt (SZ)*

*Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp*
****
exiting the fig3_15 subroutine

entering the fig3_16 subroutine
****
*Figure 3-16 is requested -
Subarea Np237 and Tc99 Release Rates vs. Time(10kyr)
- the following files are needed from a MEAN VALUE run:
ebsrel.rlt
szft.ech
szft.rlt*

*The output files are: fig3_16a.plt (EBS)
fig3_16b.plt (UZ)
fig3_16c.plt (SZ)*

*Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp*
****
exiting the fig3_16 subroutine

entering the fig3_19 subroutine
****
*Figures 3-19a and 3-19b are requested - GW Dose vs. Time
(i.e., Basecase Dose and w/ Faulting Dose vs. Time)*

*(and Basecase Dose, IA GW Dose, IA GS Dose,
IA GW+GS Dose vs. Time)*

*- the following files are needed from a MEAN VALUE run:
rgwsa.tpa
rgssa.tpa*

*THIS FIGURE CAN BE GENERATED USING THE OUTPUT FILES
FROM FIGURES 3-14a AND 3-14b LISTED BELOW EXCEPT
USING 100KYR RESULTS*

*The output files are: fig3_14a.plt (Faulting)
fig3_14b.plt (IA)*

*Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp*
****
exiting the fig3_19 subroutine

entering the fig3_36 subroutine
****
*Figure 3-36 is requested - GW Dose vs. Time
for the Fuel-Dissolution Alternative Conceptual Models*

*- the following file is needed from a MEAN VALUE run:
rgwsa.tpa*

The output file is: fig3_36.plt

*THE USER NEEDS TO RUN TPAPP FOUR TIMES (SEE NOTE):
(1) WITH RESULTS FROM THE BASECASE TPA.INP FILE
(2) WITH RESULTS USING MODEL 1
(3) WITH RESULTS USING NATURAL ANALOG
(4) WITH RESULTS USING SCHOEPITE*

*(NOTE: SECTIONS 2.3 AND 3.5 OF THE SENSITIVITY ANALYSIS
REPORT FOR "tpa.inp" PARAMETER SETTINGS
NEEDED IN THESE FOUR CASES)*

*AFTER EACH OF THESE 4 TPAPP RUNS, THE FIG3_36.PLT FILES
NEED TO BE MERGED TO GENERATE THE FIGURE 3-36 PLOT*

*Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp*
****
exiting the fig3_36 subroutine

entering the fig3_37 subroutine
****
*Figure 3-37 is requested - GW Dose vs. Time
for the Fuel-Wetting Alternative Conceptual Models*

*- the following file is needed from a MEAN VALUE run:
rgwsa.tpa*

The output file is: fig3_37.plt

THE USER NEEDS TO RUN TPAPP SIX TIMES (SEE NOTE):
(1) WITH RESULTS FROM THE BASECASE TPA.INP FILE
(2) WITH RESULTS USING FLWTHRU-2
(3) WITH RESULTS USING FLWTHRU-1
(4) WITH RESULTS USING FOCFLOW
(5) WITH RESULTS USING CLAD-M1
(6) WITH RESULTS USING GRAIN1

(NOTE: SECTIONS 2.3 AND 3.5 OF THE SENSITIVITY ANALYSIS
REPORT FOR "tpa.inp" PARAMETER SETTINGS
NEEDED IN THESE SIX CASES)

AFTER EACH OF THESE 6 TPAPP RUNS, THE FIG3_37.PLT FILES
NEED TO BE MERGED TO GENERATE THE FIGURE 3-37 PLOT

Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp
****
exiting the fig3_37 subroutine

entering the fig3_38 subroutine
****
Figure 3-38 is requested - GW Dose vs. Time
for the Transport Alternative Conceptual Models

- the following file is needed from a MEAN VALUE run:
rgwsa.tpa

The output file is: fig3_38.plt

THE USER NEEDS TO RUN TPAPP FIVE TIMES (SEE NOTE):
(1) WITH RESULTS FROM THE BASECASE TPA.INP FILE
(2) WITH RESULTS USING NORET
(3) WITH RESULTS USING NOMATDIF
(4) WITH RESULTS USING NOSOLLIMIT(BATHTUB)
(5) WITH RESULTS USING NOSOLLIMIT(FLOWTHRU)

(NOTE: SECTIONS 2.3 AND 3.5 OF THE SENSITIVITY ANALYSIS
REPORT FOR "tpa.inp" PARAMETER SETTINGS
NEEDED IN THESE FIVE CASES)

AFTER EACH OF THESE 5 TPAPP RUNS, THE FIG3_38.PLT FILES
NEED TO BE MERGED TO GENERATE THE FIGURE 3-38 PLOT

Verify these are MEAN VALUE run files
note that the # realizations should be 1,
and it is set at 1 in tpa.inp
****
exiting the fig3_38 subroutine

entering the fig3_39 subroutine
****
Figure 3-39 is requested - SEISMO Seismic Hazard Curve
Magnitude vs. Recurrence Time

- the following file is needed:
tpa.inp

The output file is: fig3_39.plt
****
exiting the fig3_39 subroutine

entering the fig3_40 subroutine
****
Figure 3-40 is requested -
Vertical Extent of Rockfall(m) vs. Event Type
for all Rock Types

- the following file is needed:
tpa.inp

This information has been replaced in the SEISMO section
of "tpa.inp"

CONSIDER REPLACING FIGURE 3-40 WITH OTHER SEISMO DATA
****
exiting the fig3_40 subroutine

entering the fig3_41 subroutine
****
Figure 3-41 is requested -
SEISMO Joint Spacing (m) vs. Rock Type
and Distribution Joint Fraction vs. Rock Type

- the following file is needed:
tpa.inp

This information has been replaced in the SEISMO section
of "tpa.inp"

CONSIDER REPLACING FIGURE 3-41 WITH OTHER SEISMO DATA
****
exiting the fig3_41 subroutine

entering the fig3_42 subroutine
****
Figure 3-42 is requested -
Fraction Area for Ground Motion vs. Event Type

- the following file is needed:
tpa.inp

This information has been replaced in the SEISMO section
of "tpa.inp"

CONSIDER REPLACING FIGURE 3-42 WITH OTHER SEISMO DATA
****
exiting the fig3_42 subroutine

```
entering the fig3_44 subroutine
*******************************************************
Figure 3-44 is requested -
        Igneous Activity COnditional Dose vs. Time

This figure needs to be generated using files such as
the following:

 COMBINEV.F
 CVOLC5.F

There is no *.plt file for Figure 3-44.

Refer to the Sensitivity Analysis Report for
a description of the contents of this plot.
*******************************************************
exiting the fig3_44 subroutine


entering the fig3_45 subroutine
*******************************************************
Figure 3-45 is requested -
    Total (GW+GS prob weighted) Expected Dose vs. Time

This figure needs to be generated using files such as
the following:

 COMBINEV.F
 CVOLC5.F

There is no *.plt file for Figure 3-45.

Refer to the Sensitivity Analysis Report for
a description of the contents of this plot.
*******************************************************
exiting the fig3_45 subroutine
```

With all of the “multi_vector” flags activated in “TPAPP.INP” from a basecase TPA 5.0r run having 10 realizations set in the “tpa.inp” file and the APPEND option activated (this case was used as an example) and after running the “TPAPP.F” code provides the following screenprint.

```
   *******************************************
    Welcome to "TPAPP" - TPA Post-Processor
   (  this program screenprints input data  )
   ( and the status of the simulation; files)
   (for plotting, with *.plt extensions, are)
   (  written according to flags set in the )
   (          input file tpapp.inp          )
   *******************************************

entering tpa data reader
echo: from tpa.inp, nreal=        10
echo: from tpa.inp, ntim_d=        201
echo: from tpa.inp, ntim_a=        100
echo: from tpa.inp, time_cp=   10000.0000000000
```

```
echo: from tpa.inp, time_max=    100000.000000000
echo:therefore, ntim,ntim_c=         301         201
echo: from tpa.inp, nsubarea=          10
echo: sa i,pt j, (x,y) subarea coordinates=           1           1
   547514.880000000       4079310.61000000
echo: sa i,pt j, (x,y) subarea coordinates=           1           2
   548069.200000000       4079136.50000000
echo: sa i,pt j, (x,y) subarea coordinates=           1           3
   547847.300000000       4077816.20000000
echo: sa i,pt j, (x,y) subarea coordinates=           1           4
   547370.950000000       4077922.04000000
echo: sa i,pt j, (x,y) subarea coordinates=           2           1
   548069.200000000       4079136.50000000
echo: sa i,pt j, (x,y) subarea coordinates=           2           2
   548569.320000000       4078981.00000000
echo: sa i,pt j, (x,y) subarea coordinates=           2           3
   548504.060000000       4077664.24000000
echo: sa i,pt j, (x,y) subarea coordinates=           2           4
   547847.300000000       4077816.20000000
echo: sa i,pt j, (x,y) subarea coordinates=           3           1
   547370.950000000       4077922.04000000
echo: sa i,pt j, (x,y) subarea coordinates=           3           2
   547847.300000000       4077816.20000000
echo: sa i,pt j, (x,y) subarea coordinates=           3           3
   548322.700000000       4077192.20000000
echo: sa i,pt j, (x,y) subarea coordinates=           3           4
   547474.700000000       4077281.60000000
echo: sa i,pt j, (x,y) subarea coordinates=           4           1
   547847.300000000       4077816.20000000
echo: sa i,pt j, (x,y) subarea coordinates=           4           2
   548504.060000000       4077664.24000000
echo: sa i,pt j, (x,y) subarea coordinates=           4           3
   548479.710000000       4077173.06000000
echo: sa i,pt j, (x,y) subarea coordinates=           4           4
   548322.700000000       4077192.20000000
echo: sa i,pt j, (x,y) subarea coordinates=           5           1
   547474.700000000       4077281.60000000
echo: sa i,pt j, (x,y) subarea coordinates=           5           2
   547887.300000000       4077238.10000000
echo: sa i,pt j, (x,y) subarea coordinates=           5           3
   547897.790000000       4076045.46000000
echo: sa i,pt j, (x,y) subarea coordinates=           5           4
   547655.970000000       4076123.07000000
echo: sa i,pt j, (x,y) subarea coordinates=           6           1
   547887.300000000       4077238.10000000
echo: sa i,pt j, (x,y) subarea coordinates=           6           2
   548322.700000000       4077192.20000000
echo: sa i,pt j, (x,y) subarea coordinates=           6           3
   548155.700000000       4075962.63000000
echo: sa i,pt j, (x,y) subarea coordinates=           6           4
   547897.790000000       4076045.46000000
echo: sa i,pt j, (x,y) subarea coordinates=           7           1
   548322.700000000       4077192.20000000
echo: sa i,pt j, (x,y) subarea coordinates=           7           2
   548479.710000000       4077173.06000000
echo: sa i,pt j, (x,y) subarea coordinates=           7           3
   548455.000000000       4076674.51000000
echo: sa i,pt j, (x,y) subarea coordinates=           7           4
   548155.700000000       4075962.63000000
```

echo: sa i,pt j, (x,y) subarea coordinates= 8 1
547645.270000000 4079656.06000000
echo: sa i,pt j, (x,y) subarea coordinates= 8 2
548588.980000000 4079377.55000000
echo: sa i,pt j, (x,y) subarea coordinates= 8 3
548569.320000000 4078981.00000000
echo: sa i,pt j, (x,y) subarea coordinates= 8 4
547514.880000000 4079310.61000000
echo: sa i,pt j, (x,y) subarea coordinates= 9 1
547732.820000000 4080960.00000000
echo: sa i,pt j, (x,y) subarea coordinates= 9 2
548251.910000000 4080817.50000000
echo: sa i,pt j, (x,y) subarea coordinates= 9 3
548116.890000000 4079516.81000000
echo: sa i,pt j, (x,y) subarea coordinates= 9 4
547645.270000000 4079656.06000000
echo: sa i,pt j, (x,y) subarea coordinates= 10 1
548251.910000000 4080817.50000000
echo: sa i,pt j, (x,y) subarea coordinates= 10 2
548664.550000000 4080675.00000000
echo: sa i,pt j, (x,y) subarea coordinates= 10 3
548588.980000000 4079377.55000000
echo: sa i,pt j, (x,y) subarea coordinates= 10 4
548116.890000000 4079516.81000000
echo: from tpa.inp,naqueous= 20
echo: from tpa.inp,ncolloid= 11
echo: from tpa.inp,nnucl= 31
echo: from tpa.inp,nstart= 1
echo: from tpa.inp,nstart= 0

NOTE: for reading the number of WPs in each subarea,
need to have the screenprint from a TPA run
in a file called "tpa.out"

echo: from tpa.out,nwps in subarea 1 1462
echo: from tpa.out,nwps in subarea 2 1567
echo: from tpa.out,nwps in subarea 3 771
echo: from tpa.out,nwps in subarea 4 429
echo: from tpa.out,nwps in subarea 5 758
echo: from tpa.out,nwps in subarea 6 849
echo: from tpa.out,nwps in subarea 7 324
echo: from tpa.out,nwps in subarea 8 845
echo: from tpa.out,nwps in subarea 9 977
echo: from tpa.out,nwps in subarea 10 895
exiting tpa data reader simulation

entering input_data_reader
echo:iflag_fig3_1= 0
echo:iflag_fig3_2= 0
echo:iflag_fig3_3= 0
echo:iflag_fig3_4= 0
echo:iflag_fig3_5= 0
echo:iflag_fig3_6= 0
echo:iflag_fig3_7= 0
echo:iflag_fig3_8= 0
echo:iflag_fig3_9= 1
echo:iflag_fig3_10= 0
echo:iflag_fig3_11= 1

```
echo:iflag_fig3_12=     0
echo:iflag_fig3_13=     0
echo:iflag_fig3_14a=     0
echo:iflag_fig3_14b=     0
echo:iflag_fig3_15=     0
echo:iflag_fig3_16=     0
echo:iflag_fig3_17=     0
echo:iflag_fig3_18=     0
echo:iflag_fig3_19=     0
echo:iflag_fig3_20=     1
echo:iflag_fig3_21=     1
echo:iflag_fig3_22=     1
echo:iflag_fig3_23=     1
echo:iflag_fig3_24=     1
echo:iflag_fig3_25=     1
echo:iflag_fig3_26=     1
echo:iflag_fig3_27=     1
echo:iflag_fig3_28=     1
echo:iflag_fig3_29=     1
echo:iflag_fig3_30=     1
echo:iflag_fig3_31=     1
echo:iflag_fig3_32=     1
echo:iflag_fig3_33=     1
echo:iflag_fig3_34=     1
echo:iflag_fig3_35=     1
echo:iflag_fig3_36=     0
echo:iflag_fig3_37=     0
echo:iflag_fig3_38=     0
echo:iflag_fig3_39=     1
echo:iflag_fig3_40=     1
echo:iflag_fig3_41=     1
echo:iflag_fig3_42=     1
echo:iflag_fig3_43a=     1
echo:iflag_fig3_43b=     1
echo:iflag_fig3_44=     1
echo:iflag_fig3_45=     1
exiting input_data_reader simulation


entering the fig3_9 subroutine
*******************************************************
Figure 3-9 is requested - UZ Unit Thicknesses by Subarea
- the following file is needed:
  tpa.inp

The output file is: fig3_9.plt

The 7 tpa.inp units: TSw,CHnv,CH_Total,PPw,UCF,BFw,UFZ
If these are not correct, then modify this program
*******************************************************
exiting the fig3_9 subroutine


entering the fig3_11 subroutine
*******************************************************
Figure 3-11 is requested - SZ Streamtube and Subarea Map

This figure is a graphics file.
```

*There is no *.plt file for Figure 3-11.*

This figure contains water-level contours,
the repository outline (including subareas),
streamtubes 1-3, well locations, the 10km and
20km boundaries, and the Highway U.S. 95 location.

Check that this information has not changed to
ensure that the figure does not need to be updated.
****
exiting the fig3_11 subroutine

entering the fig3_20 subroutine
****
Figure 3-20 is requested - GW Dose vs. Time
- the following file is needed from a MULTI-VECTOR run:
rgwsr.tpa

A hair diagram with total dose for each realization will
will be plotted together with expected dose and 25, 50,
and 75 percentile values for 10kyr (Figure 3-20a) and
and 100kyr (Figure 3-20b)

The output files are:
fig3_20a.plt (hair diagram)
fig3_20b.plt (exp & quantile doses)

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_20 subroutine

entering the fig3_21 subroutine
****
Figure 3-21 is requested - Infiltration Rate vs. Time
(average, maximum,minimum)

- the following file is needed from a MULTI-VECTOR run:
uzflow.rlt

The output file is: fig3_21.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_21 subroutine

entering the fig3_22 subroutine
****
Figure 3-22 is requested - WP Temperature vs. Time
(subarea- and repository-average temperatures and
Subarea 1 average, minimum, and maximum temperatures

- the following file is needed from a MULTI-VECTOR run:

ebsrel.ech

The output file is: fig3_22.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_22 subroutine

entering the fig3_23 subroutine
****
Figure 3-23 is requested - Fraction WP Failures vs. Time
(including the average fraction WPs failed)

- the following file is needed from a MULTI-VECTOR run:
ebsfail.rlt

The output files are: fig3_23a.plt (all realizations)
fig3_23b.plt (average)

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_23 subroutine

entering the fig3_24 subroutine
****
Figure 3-24 is requested -
Peak GW Dose vs. Tc99 and Np237 Peak Release Rate

-the following files are needed from a MULTI-VECTOR run:
ebsrel.rlt
gwpkdos.res

The output file is: fig3_24.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_24 subroutine

entering the fig3_25 subroutine
****
Figure 3-25 is requested -
Realization and Average Subarea 1 Tc99 EBS
Release Rate vs. Time
(note: Figures 3-25a & 3-25b are for 10kyr and 100kyr)
*(and both times are included in these *.plt files)*

-the following file is needed from a MULTI-VECTOR run:
ebsrel.rlt

The output files are: fig3_25a.plt (all realizations) *fig3_25b.plt (average)*

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_25 subroutine

entering the fig3_26 subroutine
****
Figure 3-26 is requested -
(1) Tc EBS, UZ, and SZ Release Rates,
(2) Repository Inventory,
and (3) Fraction of Failed WPs vs. Time

-the following files are needed from a MULTI-VECTOR run:
ebsrel.rlt
szft.ech
szft.rlt
ebsfail.rlt
tpa.inp

The output file is: fig3_26.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
echo: from tpa.inp, total_rep_mtu= 70040.0000000000
echo: from tpa.inp, glass_fraction= 0.00000000000000
echo: from tpa.inp, equiv_glass_mtu= 1.63000000000000
echo: from tpa.inp, wp_payload= 7.89000000000000
echo: calc, anumber_wps_non_glass= 8877.05956907478
echo: calc, anumber_wps_glass= 0.00000000000000
exiting the fig3_26 subroutine

entering the fig3_27 subroutine
****
Figure 3-27 is requested -
Average Tc99, Np237, and Pu239 UZ Release Rates and
Fraction of Failed WPs vs. Time

-the following files are needed from a MULTI-VECTOR run:
szft.ech
ebsfail.rlt

The output file is: fig3_27.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_27 subroutine

entering the fig3_28 subroutine
****

Figure 3-28 is requested -
Realization and Average Subarea 1 Tc99 UZ
Release Rate vs. Time
(note: Figures 3-28a & 3-28b are for 10kyr and 100kyr)
*(and both times are included in these *.plt files)*

-the following file is needed from a MULTI-VECTOR run:
szft.ech

The output files are: fig3_28a.plt (all realizations)
fig3_28b.plt (average)

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_28 subroutine

entering the fig3_29 subroutine
****
Figure 3-29 is requested -
Tc EBS, UZ, and SZ Release Rates vs. Time
-the following files are needed from a MULTI-VECTOR run:
ebsrel.rlt
szft.ech
szft.rlt

The output file is: fig3_29.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_29 subroutine

entering the fig3_30 subroutine
****
Figure 3-30 is requested -
UZ Subarea Average and UZ average GWTT as
an Exceedance Probabality

-the following file is needed from a MULTI-VECTOR run:
gwttuzsz.res

The output file is: fig3_30.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_30 subroutine

entering the fig3_31 subroutine
****
Figure 3-31 is requested -
Average Tc99, Np237, and Pu239 SZ Release Rate vs. Time

-the following file is needed from a MULTI-VECTOR run:
szft.rlt

The output file is: fig3_31.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_31 subroutine

entering the fig3_32 subroutine
****
Figure 3-32 is requested -
Realization and Average Subarea 1 Tc99 SZ
Release Rate vs. Time
(note: Figures 3-32a & 3-32b are for 10kyr and 100kyr)
*(and both times are included in these *.plt files)*

-the following file is needed from a MULTI-VECTOR run:
szft.rlt

The output files are: fig3_32a.plt (all realizations)
fig3_32b.plt (average)

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_32 subroutine

entering the fig3_33 subroutine
****
Figure 3-33 is requested -
SZ Subarea Average and SZ average GWTT as
an Exceedance Probabality

-the following file is needed from a MULTI-VECTOR run:
gwttuzsz.res

The output file is: fig3_33.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_33 subroutine

entering the fig3_34 subroutine
****
Figure 3-34 is requested - % Contribution to GW Dose
by Radionuclide and Realization

-the following files are needed from a MULTI-VECTOR run:
gwpkds_c.res (10kyr)

gwpkdos.res (100kyr)

The output files are:
fig3_34a.plt (10kyr)
fig3_34b.plt (100kyr)

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_34 subroutine

entering the fig3_35 subroutine
****
Figure 3-35is requested - GW Dose vs. Time
- the following file is needed from a MULTI-VECTOR run:
rgwna.tpa

The output file is: fig3_35.plt

Verify these are MULTI-VECTOR run files
note that the # realizations should be > 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_35 subroutine

entering the fig3_39 subroutine
****
Figure 3-39 is requested - SEISMO Seismic Hazard Curve
Magnitude vs. Recurrence Time

- the following file is needed:
tpa.inp

The output file is: fig3_39.plt
****
exiting the fig3_39 subroutine

entering the fig3_40 subroutine
****
Figure 3-40 is requested -
Vertical Extent of Rockfall(m) vs. Event Type
for all Rock Types

- the following file is needed:
tpa.inp

This information has been replaced in the SEISMO section
of "tpa.inp"

CONSIDER REPLACING FIGURE 3-40 WITH OTHER SEISMO DATA
****
exiting the fig3_40 subroutine

entering the fig3_41 subroutine

****
Figure 3-41 is requested -
SEISMO Joint Spacing (m) vs. Rock Type
and Distribution Joint Fraction vs. Rock Type

- the following file is needed:
tpa.inp

This information has been replaced in the SEISMO section
of "tpa.inp"

CONSIDER REPLACING FIGURE 3-41 WITH OTHER SEISMO DATA
****
exiting the fig3_41 subroutine

entering the fig3_42 subroutine
****
Figure 3-42 is requested -
Fraction Area for Ground Motion vs. Event Type

- the following file is needed:
tpa.inp

This information has been replaced in the SEISMO section
of "tpa.inp"

CONSIDER REPLACING FIGURE 3-42 WITH OTHER SEISMO DATA
****
exiting the fig3_42 subroutine

entering the fig3_43a subroutine
****
Figure 3-43a is requested - GW Dose vs. Time
(i.e., Basecase Dose and w/ Faulting Dose vs. Time)
- the following file is needed from a MULTI-VECTOR run:
rgwsa.tpa

The output file is: fig3_43a.plt

THE USER NEEDS TO RUN TPAPP TWICE: ONCE WITH RESULTS
FROM THE BASECASE TPA.INP FILE AND ONCE WITH RESULTS
FROM THE FAULTING FLAG ACTIVATED

AFTER EACH OF THESE 2 TPAPP RUNS, THE FIG3_43A.PLT FILES
NEED TO BE MERGED TO GENERATE THE FIGURE 3-43A PLOT

Verify these are MULTI-VECTOR run files
note that the # realizations should be 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_43a subroutine

entering the fig3_43b subroutine
****
Figure 3-43b is requested - GW Dose vs. Time
(i.e., Basecase Dose, IA GW Dose, IA GS Dose,

IA GW+GS Dose vs. Time)
-the following files are needed from a MULTI-VECTOR run:
rgwsa.tpa
rgssa.tpa

The output file is: fig3_43b.plt

THE USER NEEDS TO RUN TPAPP TWICE: ONCE WITH RESULTS FROM THE BASECASE TPA.INP FILE (USE FIGURE 3-43A FOR THIS) AND ONCE WITH RESULTS WITH IA FLAG ACTIVATED

AFTER EACH OF THESE 2 TPAPP RUNS, THE FIG3_43A.PLT FILE NEEDS TO BE MERGED WITH FIG3_43B.PLT TO GENERATE THE FIGURE 3-43B PLOT

ADDITIONALLY, NEED TO PROBABILITY WEIGHT THE GS DOSES FOR THIS FIGURE

Verify these are MULTI-VECTOR run files
note that the # realizations should be 1,
and it is set at 10 in tpa.inp
****
exiting the fig3_43b subroutine

entering the fig3_44 subroutine
****
Figure 3-44 is requested -
Igneous Activity COnditional Dose vs. Time

This figure needs to be generated using files such as the following:

COMBINEV.F
CVOLC5.F

*There is no *.plt file for Figure 3-44.*

Refer to the Sensitivity Analysis Report for a description of the contents of this plot.
****
exiting the fig3_44 subroutine

entering the fig3_45 subroutine
****
Figure 3-45 is requested -
Total (GW+GS prob weighted) Expected Dose vs. Time

This figure needs to be generated using files such as the following:

COMBINEV.F
CVOLC5.F

*There is no *.plt file for Figure 3-45.*

Refer to the Sensitivity Analysis Report for a description of the contents of this plot.

****

exiting the fig3_45 subroutine

The *.plt files listed above for the "mean_value" and the "multi_vector" cases (i.e., the *.plt files with the appropriate flags activated in the 'TPAPP.INP" file) from a TPA 5.0r run can be used to supply information to "Kaleidagraph" data files and plots created from the final TPA 4.1j "Kaleidagraph" files (used as templates). Plots from TPA 4.1j and 5.0r runs can be compared to determine differences in output caused by changes in the (1) input data and (2) conceptual model and for preparing the next Sensitivity Analysis report, if needed.

The names of "mean_value" *.plt files from a mean value TPA run are listed below.

```
02/16/2004  07:05 AM          20,240 fig3_1.plt
02/16/2004  07:05 AM          24,462 fig3_10.plt
02/16/2004  07:05 AM         161,271 fig3_12.plt
02/16/2004  07:05 AM         236,778 fig3_13a.plt
02/16/2004  07:05 AM         236,775 fig3_13b.plt
02/16/2004  07:05 AM         236,775 fig3_13c.plt
02/16/2004  07:05 AM          10,275 fig3_14a.plt
02/16/2004  07:05 AM         181,513 fig3_16a.plt
02/16/2004  07:05 AM         181,512 fig3_16b.plt
02/16/2004  07:05 AM         181,491 fig3_16c.plt
02/16/2004  07:05 AM          90,911 fig3_2.plt
02/16/2004  07:05 AM           3,147 fig3_3.plt
02/16/2004  07:05 AM          10,275 fig3_36.plt
02/16/2004  07:05 AM          10,275 fig3_37.plt
02/16/2004  07:05 AM          10,275 fig3_38.plt
02/16/2004  07:05 AM             580 fig3_39.plt
02/16/2004  07:05 AM          88,194 fig3_4.plt
02/16/2004  07:05 AM          88,796 fig3_5.plt
02/16/2004  07:05 AM          12,691 fig3_6.plt
02/16/2004  07:05 AM          11,797 fig3_7.plt
02/16/2004  07:05 AM          12,692 fig3_8.plt
02/16/2004  07:05 AM           2,318 fig3_9.plt
              22 File(s)      1,813,043 bytes
```

The names of "multi_vector" *.plt files from a 10 realization run are listed below.

```
02/16/2004  06:59 AM          85,916 fig3_20a.plt
02/16/2004  06:59 AM          34,850 fig3_20b.plt
02/16/2004  06:59 AM          26,580 fig3_21.plt
02/16/2004  06:59 AM         122,018 fig3_22.plt
02/16/2004  06:59 AM          86,202 fig3_23a.plt
02/16/2004  06:59 AM          10,278 fig3_23b.plt
02/16/2004  06:59 AM             971 fig3_24.plt
02/16/2004  06:59 AM          86,202 fig3_25a.plt
02/16/2004  06:59 AM          10,281 fig3_25b.plt
02/16/2004  06:59 AM          48,926 fig3_26.plt
02/16/2004  06:59 AM          34,732 fig3_27.plt
02/16/2004  06:59 AM          86,200 fig3_28a.plt
02/16/2004  06:59 AM          10,280 fig3_28b.plt
02/16/2004  06:59 AM          26,581 fig3_29.plt
02/16/2004  06:59 AM           3,763 fig3_30.plt
```

02/16/2004 06:59 AM   26,583 fig3_31.plt
02/16/2004 06:59 AM   86,200 fig3_32a.plt
02/16/2004 06:59 AM   10,280 fig3_32b.plt
02/16/2004 06:59 AM   3,763 fig3_33.plt
02/16/2004 06:59 AM   5,602 fig3_34a.plt
02/16/2004 06:59 AM   5,602 fig3_34b.plt
02/16/2004 06:59 AM   161,271 fig3_35.plt
02/16/2004 06:59 AM   580 fig3_39.plt
02/16/2004 06:59 AM   10,275 fig3_43a.plt
02/16/2004 06:59 AM   25,374 fig3_43b.plt
02/16/2004 06:59 AM   2,318 fig3_9.plt

September 21, 22, 23, and 24, 2004

Subject: Long TPA runs using the TPA Version 4.1jpd code

Goals:

- determine the ability of the TPA code to perform long runs using as many as 20,001 time steps (delta time = 50 years)
- verify the results are correct at these longer times and increased number of time steps
- document the modifications to the source code
- record results from verification testing at these longer times and increased number of time steps

Summary of Achievements: The TPA Version 4.1jpd code compiled using LF95 and running on the high-end Xeon GIS machine successfully completed execution for 1,000,000 years and 17,000 time steps. Follow-up verification work is needed in a number of areas.

Chronology of Activities:

1. After talking with R. Janetzke, we determined that the correct version of the TPA code to use for this work would be Version 4.1jpd. This version, with all the source code, exists on the home directory of R. Janetzke for SUN FORTRAN. These files were copied to a CD. Note that there was no PC version of TPA 4.1j with source code, so this version is appropriate.

2. Created the LF90 Make files to use on my laptop. These files replaced the SUN FORTRAN Make files. Successfully compiled Version 4.1jpd on the laptop.

3. Compared results from the laptop compiled LF90 TPA Version 4.1jpd code with results from the TPA Version 4.1j code that was available with only executables on a CD. The basecase tpa.inp file (i.e., the file that was present on the CD) was used and the results from the two runs were consistent. This exercise served as an installation test and showed the TPA Version 4.1jpd was successfully compiled and gave the same results as the CD version.

4. Developed a plan to first increase the simulation time to well-beyond 100,000 years (1,000,000 years selected as the new maximum simulation time). Then the number of time steps would be increased from the initial maximum value of 401 to 20,001

5. Performed TPA runs to increase the simulation time by modifying the following files: uzflow.def, climato2.dat, exec.f, and tpa.inp. These files were identified previously in an email from R. Rice to S. Mohanty and allowed 500,000 yr TPA runs. The first two data files needed the time

period extended from 100,000 years to the longer time (1,000,000 years). The exec.f file needed the maximum number of seismic events increased to 6,000. The tpa.inp file needed simulation parameters (maximum time) to be increased. Additionally, the parameter mnClits in uz_parms.i was increased from 1001 to 2001 and in failt.f, "1X" was added on line number 336 to allow for a larger time to be written to ebstrh.dat.

6. With the above TPA code modifications, using a maximum time of 1,000,000 years and 401 time steps for subarea 1, the TPA code execution was successful. The next task was to increase from 401 time steps to 20,001 time steps and the approach was to slowly increase so that there would be confounding effects arising from more than one area of the TPA code. Thus, debugging and solving the problem (if any) would be simplified.

7. To successfully conduct a TPA code run using 7,000 time steps, the following files were modified: releaset.f, maxntime.i, exec.f, failt.f, and nintv.i. The first file needed maxste, maxtim, and maxbin to be increased from 502. The second file needed maxntime increased. The third file needed kMaxTimeSteps increased. The fourth and fifth files both needed nintv increased.

8. With the above TPA code modifications, using a maximum time of 1,000,000 years and 7,000 time steps for subarea 1, the TPA code execution was successful. However, to go beyond 7,001 time steps, my laptop needed more RAM (currently has 512MB) because of requirements for RELEASET.

9. To go beyond 7,001 time steps, faster computers in the GIS Lab (Xeon machine) and Vermont in Marty's office were used. A simulation using 8,001 time steps nearly completed successfully, however the gentpa code generated an error that is associated with the PIV chip. Therefore, the LF95 compiler was needed (this compiler does not yield these gentpa code errors on machine with the new PIV chips).

10. The LF95 Make files for TPA Version 5.0z were used as templates (i.e., the *.fig files in the various directories) and then modified accordingly to account for the presence of different source code in Versions 5.0z and 4.1jpd and to remove reference to "sh" and "system" integer and external statements from about 8 of the source code files (e.g., uzft.f, szft.f, dcagw.f, ashplumo.f, exec.f, zportpc.f, etc.) Also, the format in ebsrel.f to write the number of failed WPs by scenario needed to be modified from a real to an integer.

11. With the above modifications to the TPA Version 5.0z code Make files to adapt them to the work with the TPA Version 4.1jpd code, the TPA code compiled successfully.

12. The TPA Version 4.1jpd code, compiled on the GIS Xeon machine (since it has LF95), successfully completed execution of the TPA code for 1,000,000 years and 17,001 time steps (this is a delta time of about 59 years). Note that the modifications stated in #7 above needed to be completed appropriately to increased the time steps to this level.

13. At 17,501 time steps and greater, compiling the TPA code generated an executable for RELEASET generated an error and that was characterized by the XP Operating System as accepting to use an "Invalid Win32 Application".

14. The TPA code was executed for all subareas in a single realization run and during Subarea 8 calculations, there was a problem identified in UZFT execution and TPA code execution stopped. The problem was fixed by increasing in uzft.f the variable maxnumdis from 99999 to 999999. Also, the write statement to nefii.dis for the number of NEFTRAN time steps needed to be changed from I5 to I6 in nefmks.f. This problem arose because this subarea yielded an UZFT nefii.dis file with over 100,000 time steps for the release rate.

15. The TPA code was executed at 1,000 year number of time step increments to determine the stability of the peak dose and the time of the peak dose printed at the end of TPA execution. The effects of using the default time stepping in the tpa.inp file and using uniform time steps on the peak dose and time of the peak dose was also evaluated. The results show a large difference in these results at certain time steps (almost a factor of 2 difference and times of the peak dose that varied by as much as a few 100,000 years).

16. The TPA code simulation time increased from about 1 minute/realization (301 time steps and 100,000 years) to about 10 minutes/realization (8,001 time steps and 1,000,000 years).

Recommendations:

- perform TPA runs using multiple realizations to identify other potential problems
- determine the reasons for the Win32 Application error for RELEASET so that simulations could be extended beyond 17,001 time steps
- once an acceptable number of time steps is achieved, perform verification testing of the results to ensure the results are correct an consistent (i.e., the results do not have a no time step dependence as it appears in #15 above)
- check on the reasons why the number of WPs ejected appeared on the screen print during a 8,001 time step TPA run as a number with 8 digits (meaning the value was spurious)

September 27, 28, 29, and 30, 2004

1. Used a Remote Desktop on VERMONT to run the 1e6 yr and 15,001 time step TPA4.1jpd LF95 code. Also, ran this code on GRYPHON. In a 331 realization BEMORE run, found that the TPA code execution stopped for Realization 18 and Subarea 2. Did some debugging and discovered that the reason was attributable to running EBSFILT (for the first time in that TPA simulation). Upon inspection of the source code, noted that EBSFILT has its maximum number of time steps and associated array dimensioning set at two different values - 402 and 201. So, consistent with modifications made to TPA Version 5.0, changed these values in ebsfilt.f to 15,002 and 15,001, respectively, in the EBSFILT source code and recompiled. Restarted the 331 realization, 1e6 yr, 15,001 time step TPA4.1jpd LF95 code on GRYPHON.

2. From the GRYPHON run, found that execution time was 17 minutes/realization (versus 22 minutes/realization on BEMORE; that is, GRYPHON appears to be about 30% faster than BEMORE). Also, note that the 331 realization TPA run would be expected to take about 4 days on the faster GRYPHON computer.

3. Noted, and reported to R. Janetzke, that TPA code screenprint with both TPA Versions 4.1jp and Version 5.0 includes the number of WPs ejected, even though the VOLCANISM flag is not activated and that this occurs for Subarea 2. It was noted by R. Janetzke, who indicated he would take care of any necessary modifications to the TPA code.

4. Compared TPA code results using the Command Prompt utility "fc" from (a) the executables on CD for TPA4.1jp from Ron, (b) the LF90 compiled TPA4.1jpd code from the SUN, and (c) the LF95 TPA4.1jpd code for 1e6 yr and 15,001 time steps. Concluded that the results from these different source codes were consistent. Noted that just a few values showed differences in the 4th or 5th significant digit and that the screenprint had more spaces in the LF90 compiled code compared to the LF95 compiled code. The totdose.res, rgwnr.tpa, rgwna.tpa, and rgwsa.tpa files were identical except for the header time and date.

5. Plotted dose results for 10kyr compliance period from the (c) code above from three different runs - 10kyr, 100kyr, and 1,000kyr TPA runs. Then plotted dose results for 100kyr from the (c) code above from two different runs - 100kyr and 1,000kyr TPA runs. A final plot of 1,000kyr dose results was also generated. (see these plots in the subdirectory "Long_Runs_Check_Results". Also, see these three plots are Figures 1, 2, and 3 at the end of this report. (Note that (c) only TPA runs are sufficient since (a) through (c) results were consistent.)

6. Noted during the debugging above, the TPA code execution do not complete successfully when Start/Stop for a Realization and for a Subarea are specified. This appears to be related to the FindPeakMean subroutine towards the end of exec.f. The cause of this problem will be investigated and corrected during this work.

7. A proposed time stepping scheme with suggested values for tpa.inp file parameters was developed. The scheme is intended to be used for TPA runs utilizing the full, time-step capabilities of this long simulation TPA code. That is, the following TPA code tpa.inp file parameters and associated values should be:

```
**
constant
DurationOfCompliancePeriod[yr]
1.0e4
**
constant
MaximumTime[yr]
1.0e6
**
** Sum of pre- and post-compliance time steps must not exceed 15001
**
iconstant
NumberOfTimeStepsInCompliancePeriod
401
**
constant
RatioOfLastToFirstTimeStepInCompliancePeriod
10.0
**
iconstant
NumberOfTimeStepsAfterCompliancePeriod
14600
**
constant
RatioOfLastToFirstTimeStepAfterCompliancePeriod
1.0
**
```

The proposed settings will yield the time steps shown in Figure 4. These time steps have the desired characteristics of finer discretization at the beginning of the TPA code simulation (the time step is about 6.4 years), which geometrically increases to a value of about 64 years in time step 401 at the end the 10,000 year Compliance Period. This discretization is desirable because it captures events occurring at the beginning of the simulation. Additionally, the 14,600 equal time steps following the 10,000 year Compliance Period (from 10,000 to 1,000,000 years) have a 67.8 year time step, which provides a smooth transition from time step 401 to time step 402. Also shown in Figure 4 are the 10,000 year Compliance Period time stepping scheme for the TPA4.1jpd Basecase with 201 time steps and a 100.0 first to last time step ratio and for Equal time steps with 201 time steps and a 1.0 first to last time step ratio. These two time stepping schemes illustrate the reason why the time stepping needs to be modified, as presented in the context of the proposed time stepping also shown in this figure.

The TPA code user should note that when the time stepping scheme proposed above for 15,001 time steps is not implemented and a decreased number of time steps is chosen (possibly for reasons related to the need to desire the TPA code execution time), care should be taken to select appropriate values for the above tpa.inp file time step input parameters. Figure 5 shows that when the user decreases to 10,001 time steps (using the same other tpa.inp file time step parmeters above), the proposed time stepping scheme shows a greater (and undesirable) transitions. This is also true for the Basecase and Equal time step cases displayed in Figure 5. Therefore, the TPA code user consider the implications of changing the tpa.inp file time step parameter presented previously to ensure results are not affected by that new time step scheme.

8. The potential impacts on groundwater dose of using time steps other than the one presented previously are shown in Figures 6 through 11. The impacts do not appear to be caused by code errors, do not have a large impact dose (just the time of the peak dose), and are not found in every different time stepping scheme. The impacts can appear to be significant. That is, Figures 6 through 11 are for 15,001 and 10,001 time steps, using the basecase, equal, and proposed schemes discussed previously, and show about a 40% increase in the peak dose which is shifted in time from about 130,000 years to 430,000 years. (Note that the results are for one realization and for subarea 1 - code testing will be conducted for all subareas and multiple realizations, up to and exceeding 331 realizations for LHS shuffling.) For a complete TPA4.1jpd code run with all subareas and SNLLHS shuffling, based on this analysis the effects are not expected to significantly change the groundwater dose (less than 1% change in the peak expected [mean] dose),.

9. To further illustrate the analysis and conclusions presented in #8 above, Figures 12 through 15 show the flow rates that are inputs into the UZFLOW, EBSREL/EBSFAIL, and UZFT TPA code modules for a number of time periods, including 0-1,000,000 years, 0-500,000 years, 200,000-700,000 years, and 500,000-1,000,000 years. These time intervals were chosen because the figures are useful in explaining the increase in the peak dose and the shift in the time of that peak dose. At this time, the explanation for this increase and shift is under investigation. Findings to date, suggest the interpolation algorithm in uzft.f, which determines which velocities and time are written to the UZ NEFTRAN input file NEFII.VEL, sets the increased flow rates shown in Figure 12 at times of about 420,000, 620,000, and 820,000 years because of the particular occurrences of

time steps at these 200,000 year intervals. Again, the oscillating occurrence of this peak flow rate will be addressed during this work and/or during follow-up work.

10. Noted that the peak dose coincides with the UZFLOW/NEFTRAN rate up until about 600,000 years, at which time the dose drops about 2 or 3 orders of magnitude and follows similar cycles that coincide with the UZFLOW/NEFTRAN flow rate. The reasons for the large drop in dose at about 600,000 years is attributable to NP237 and its complete release from the WP and then to the receptor location (i.e., source depletion and transport of NP237 out of the system). Also, note that NP237 is basically the sole contributor (i.e., 95+%) to dose from about 100,000 years through about 600,000 years. Therefore, the dose is from TH230 (about 90%) and U238 (the remaining about 10%).

11. While running the code and using the start and stop at subarea and realization options in the tpa.inp file, noticed that the Peak Mean Dose was printed to the screen as -9999. The reasons behind printing this value to the screen were investigated in exec.f and that file modified accordingly. Source code was also modified to print useful values to the pkmndose.out file. (Note that this situation was addressed in the TPA Version 5.0 code. Also, talked to R. Janetzke about the contents of the pkmndose.out file and the *.out extension for this file; he included this in a new SCR.)

12. Since it appears that most of the changes to the TPA 4.1jpd code have been made, a "clean" version of the source code and data file is being prepared, including consistent comments and removal of extra/development files. This version is named TPA4.1jpdls (the "ls" for long simulation", with the "p" and "d" designating PC version and disclaimers added, respectively).

13. Verified with S. Painter and R. Fedors that extending the data in the multiflo.dat and climato2.dat files, respectively, to 1e6 yrs or beyond was reasonable and defendable. Both agreed that in the TPA4.1j code, this is reasonable and defendable. Currently, there do not appear to be other assumptions like these that need to be verified with CNWRA experts.

14. Based on a 1 realization TPA4.1jpdls run with the basecase tpa.inp file that was run on BEMORE, the disk space requirements are approximately equal to 230MB + 5 MB per realization (for the *.res and *.tpa files that increase in size with each realization). Therefore, a 1 realization TPA run would require about 235 MB of disk space, whereas a 331 realization TPA run (i.e., with LHS shuffling) would require about 2 GB of disk space.

15. Verified that the TPA4.1jpdls code (i.e., the developed codes that was cleaned up and had extra developmental files removed) gave results that were consistent with the developed code. The results were determined to be consistent by comparing output files from a basecase TPA run. Therefore, the TPA41.jpdls code became the controlled version. (It was noted that the number of

ejected WPs is printed to the screen although the VOLCANO flag is not activated - this number is an overflow value (meaningless value) and that value together with the time and date of the runs were the only differences in the files compared from the two runs. Again, this was described to R. Janetzke who noted this as a possible TPA Version 5.0 change.)

Recommendations
- Run the TPA4.1jpdls code for 331 realizations or more using the TPA4.1jpdls basecase tpa.inp file settings. Need to use a dedicated computer, with minimum capabilities of BEMORE or GRYPHON. Check for successful execution. Plot and visually inspect results to check for reasonableness.
- Run the TPA4.1jpdls code using various tpa.inp file flags (e.g., VOLCANISM, alternative models, etc.).
- Check TPA input, intermediate, and output files for format and reasonable values.
- Through debugging UZFT, determine whether the peak flow rates (see below) are correctly determined.
- Check whether the timing of the peak dose from the basecase 1 realization TPA4.1jpdls code (occurs at about 330,000 years) is reasonable and correct; need to do the same for other files such as *.res and *.tpa files.
- Look at ways to force early WP failures to mimic Version 5.0 (mentioned by S. Mohanty at the beginning of this work)
- Similar to the previous item, look at seismic failures (as mentioned by S. Mohanty).
- OTHER ITEMS (follow-up previous Recommendations list that hasn't yet been addressed)?

October 4, 5, 6, and 7, 2004

1. Performed a basecase TPA4.1jpdls run with the "Append" option selected for all append files and 1 realization. Found the disk space requirement for the *rlt and *.ech files was about 315 MB. Recommend changing the screenprint that states the amount of disk space required for the append files (e.g., extrapolating for a 331 realization TPA run, about 105 GB of disk space would be required). This is important to note for the user since a long TPA run could be lost if there was not sufficient disk space available. (Also, it was previously noted that about 230 MB are needed for a 1 realization [non-Append] TPA simulation.)

2. In the TPA run described in #1 above, noted that the *.cum files were not written because the PC version (LF) doesn't recognize 'cat'. This should be modified in the TPA Version. 5.0 code and in this version (TPA4.1jpdls), since the TPA code will be run more using the PC version.

3. Found and corrected the zportpc.f source code for using "type" instead of "cat". A system message was generated when the "Append" option was activated because the *.cum could not be

written using the "cat" command; instead, "type" should be used in zportpc.f. Note that this change was already made to the TPA Version 5.0 code.

4. Suggest using 12,375 time steps following the Compliance Period (this will yield 80 year time steps from 10kyr to 1,000 kyr) and an associated first/last ratio of 1.0; for the Compliance Period, suggest using 501 time steps with an associated first/last ratio of 40.0 (this yields an initial time of about 2.0 years, which is similar to the current basecase initial time, and a final time step of about 79.67 years, which provide a smooth transition to the uniform time steps from 10,000 to 1,000,000 years. See these values in the TPA41jpdls code from 10/4/04.

5. If the user chooses to modify these time steps (and time steps don't coincide 100kyr, 200kyr, 300kyr, etc. cycles in the climato2.dat data, a warning should be issued to the screen stating the new time steps don't match input data cycles at times greater than 100,000 years and the results could be affected (see previously discussion and figures that show flow rates about potential impacts of the time step on the flow rates and dose results.

6. Noted that the number of ejected WPs is in the screenprint (see some comments above). Modified exec.f to only screenprint the number of ejected WPs when the volcano flag is activated (i.e., changed from "if(ivolmodel .eq. 1) then" to "if(ivolmodel .eq. 1 .and. iflagvolcano .eq. 1) then").

7. Modified the tpa.inp file parameter for determining the time steps written to the NEFTRAN input file NEFII.VEL "UnsaturatedZoneMinimumVelocityChangeFactor[Fraction]" from 0.4 to 0.1. This change increased the number of flow rates written to NEFII.VEL (and therefore may also increase the NEFTRAN runtime), however the benefit to this change is that using a value of 0.1 has thus far successfully resulted in peak flow rates in the NEFII.VEL file that repeat every 100,000 yr (thus coinciding with the climato2.dat information and the qm3peryrintoloweruz values used in UZFT to create the NEFII.VEL file.

8. Successfully executed the TPA code for 1, 2, and 3 realizations with the "Append" option activated. Examination of the resources utilized indicates an execution time of about 24, 25, and 31 minutes/realization, respectively on BEMORE (XEON CPU) (the increased time needed for 3 realizations is probably due to EBSFILT and UZ NEFTRAN runtimes). Additionally, the total disk space requirements are 739, 792, and 1,330 MB, respectively (note the 1 realization TPA run required more disk space because of a UZ NEFTRAN run), with the "Append" option files needing about 499, 627, and 1,159 MB, respectively. Thus, to update the previous estimate, a TPA simulation with 331 realizations (i.e., with LHS shuffling) will required about 150 GB of disk space (or about 443 MB/realization [average] - note that this could be higher because of UZ NEFTRAN simulations). Results from a successful 25 realization TP41jpdls code run needed 9 GB of disk

space (or about 120 GB of disk space for a 331 realization run). Therefore, the Append option will not be activated for 331 realization TPA code runs.

9. Ran the TPA code for Subarea 1 in Realization 3 of the 3 realization run noted in #8 above. Figures 16 -20 below display EBS, UZFT, and SZFT releases for NP237 together with the total dose and the input flow rate to UZFT NEFTRAN. These results were chosen because the peak dose (from NP237) occurs at 313,280 yrs - which was noticed because many other cases show the peak dose/releases occur at about 140,000 years or so. The results are reasonable (as shown by the series to EBS through SZFT release rate and dose). That is, this is in contract to Subarea 3 in Realization 1 results which has corrosion failure at 49,280 years versus at 64,400 years for the Subarea 3 in Realization 1 example.

10. Plotted dose for individual realizations from 1, 2, and 3 realization simulations and the total dose for those three realizations. The results are provided in Figures 21 and 22 and are reasonable and consistent.

11. Plotted results from TPA simulations using mean values for the TPA41jpdls code and the TPA41jp1k (Controlled Version on a CD from R. Janetzke). The former for 1e6 years and 12,850 time steps and the latter for 100,000 years using 301 and 401 time steps. The results are provided in Figures 23 through 25 (for 1,000, 100, and 10 kyr, respectively) and are reasonable and consistent.

12. Ran the TPA41jpdls code overnight for 25 realizations (no Append) on BEMORE (this was the same run with Append that stopped previously on Realization 4). The run was successfully completed.

13. Ran the TPA41jpdls code overnight for 331 realizations (no Append) on GRYPHON. Code execution was unsuccessful and stopped on Subarea 4 in Realization 23. The error was from NEFTRAN UZ and was repeatable. Modified the velocity change factor from 0.1 to 0.15 and tested the code for that subarea/realization and execution was successful. Restarted that run on BEMORE in "331real_try2". Talked with R. Janetzke about monitoring the process of the run in my absence.

14. Noted an error in execution when Start/Stop Subarea and Realization are used. A checkpoint file is created and the TPA41jpdls code will not run at all when another TPA run is initiated. The user needs to remove/delete the "check.pnt" file in these instances to allow the TPA code to execute.

15. Observed formatting of the number of the time steps in the Append files needs to be modified (e.g., "I4" is used and should probably be "I5").

16. Conversed with M. Menchaca about his sensitivity analysis study using TPA41jpdls and the location and features of that code. M. Menchaca will be interacting with S. Mohanty about the approach and resource availability.

Recommendations

- Modify the screenprint to state the new disk space requirements for the TPA4.1jpdls code for the "Append" option activated, since 15,001 time steps (or the 12,850 time steps recommended in the tpa.inp file) significantly increases those requirements.
- Change the 'cat' commands to an acceptable PC (LF) command so that the *.cum files will be generated when the"Append" option is activated in the tpa.inp file.(ACCOMPLISHED)
- Add a screenprint message described in #5 above.
- Consider adding screenprint or comment in the tpa.inp file (or both) about how the time steps affect the flow rates and that could lead to movement of peak dose by potentially hundred(s) of thousands of years - really need to investigate the interpolation and figure out why the cycles are not repeated.
- Need to modify some Append files for formatting (i..e., "*****" is printed in some files) and probably other files (see #15 above).
- See previous Recommendations

October 18, 19, 20, and 22, 2004

1. During the previous week, R. Janetzke conducted TPA Version 4.1jpdls code runs. He needed to modify "SIZES.INC" and increased the array dimensions to attempt to allow NEFTRAN UZ to execute successfully. In a 331 realization run, he noted that the TPA Version 4.1jpdls code execution stopped on GRYPHON in Realization 126, Subarea 7 - so he increased the velocity change factor from 0.15 to 0.4. On GRYPHON, RELEASET didn't run successfully on October 18, 2004, however NEFTRAN execution was not stopped. Note that the following modifications (also in the TPA Version 5.0 code) were made to "SIZES.INC":

```
Comparing files SIZES.INC and ..\..\SIZES.INC
***** SIZES.INC
    PARAMETER (MXGRD=100000, NDDF=45500, NDSF=15500)
    PARAMETER (NDJPN=20000, NDBF=150000, MXELEM=30)
    PARAMETER (MXTDV=500, MXQSC=500)
***** ..\..\SIZES.INC
    PARAMETER (MXGRD=100000, NDDF=45500, NDSF=15500)
cc rwj 10-11-04
c    PARAMETER (NDJPN=20000, NDBF=150000, MXELEM=30)
    PARAMETER (NDJPN=20000, NDBF=600000, MXELEM=30)
```

```
      PARAMETER (MXTDV=500, MXQSC=500)
*****
```

2. Using BEMORE, recreated the Realization 126, Subarea 7 NEFTRAN problem and debugged the reasons for the error. The source of the problem is related to the times and flow rates in the NEFTRAN input flow file NEFII.VEL. Investigated different velocity change factors in tpa.inp and 0.2 seems to be working without the TPA code execution stopping. Verified this in a 1-50 realization run in which the code successfully executed. Ran for the Realization 126, Subarea 7 case and there wasn't a problem. Followed this TPA code run with a Realization 101-150 out of 331 total realization TPA code run on BEMORE.

3. Found that NEFTRAN is sensitive to the peak flows (more so than for the low flows) in terms of cyclical behavior caused by the climate information.

4. In uzft.f, at the advise of R. Janetzke, changed the assignment of "gwttmin" from 10.0d0 to 20.0d0. This change is in TPA Version 5.0 and is intended to avoid problems associated with NEFTRAN execution.

5. Discovered that the shift in peak mean flows during the 100,000 year cycles was most probably caused by an interpolation in uzft.f using the maplist subroutine. The interpolation set flow rates in NEFII.VEL at 500 year time steps. Modified uzft.f to use flow rates at TPA time steps and thus avoid the interpolation. The changes made to uzft.f are as follows:

```
Comparing files uzft.f and UZFT.F.ORIGINAL
***** uzft.f
      implicit integer (i-n)

cc rwr 10/20/04 modified for long TPA simulations
cc    include 'max500yr.i'

***** UZFT.F.ORIGINAL
      implicit integer (i-n)
      include 'max500yr.i'

*****

***** uzft.f
      character*6 names(nnucl)
cc rwr 10/20/04 modified for long TPA simulations
```

```
cc     dimension tim(max500yr)
cc     dimension qm3peryrinsa( max500yr )
      dimension tim(ntimg)
      dimension qm3peryrinsa( ntimg )

      dimension timg(ntimg)
***** UZFT.F.ORIGINAL
      character*6 names(nnucl)
      dimension tim(max500yr)
      dimension qm3peryrinsa( max500yr )
      dimension timg(ntimg)
*****

***** uzft.f
C

cc rwr 10/20/04 modified for long TPA simulations
cc     REAL*8 gwtt(max500yr, MAXLYR)
      REAL*8 gwtt(ntimg, MAXLYR)
      REAL*8 avgwtt(MAXLYR)
***** UZFT.F.ORIGINAL
C
      REAL*8 gwtt(max500yr, MAXLYR)
      REAL*8 avgwtt(MAXLYR)
*****

***** uzft.f
C

cc rwr 10/20/04 modified for long TPA siumulations
cc     DIMENSION INFIL(max500yr)
cc
cc     DOUBLE PRECISION repvel(max500yr)

      DIMENSION INFIL(ntimg)

      DOUBLE PRECISION repvel(ntimg)

***** UZFT.F.ORIGINAL
```

```
C
      DIMENSION INFIL(max500yr)

      DOUBLE PRECISION repvel(max500yr)

*****

***** uzft.f
      DIMENSION SATM(MAXLYR),SATF(MAXLYR)

cc rwr 10/20/04 modified for long TPA siumulations
cc    DIMENSION vell(max500yr,MAXLYR)
cc
cc    DIMENSION tvel(max500yr,MAXLYR)

      DIMENSION vell(ntimg,MAXLYR)

      DIMENSION tvel(ntimg,MAXLYR)

C
***** UZFT.F.ORIGINAL
      DIMENSION SATM(MAXLYR),SATF(MAXLYR)

      DIMENSION vell(max500yr,MAXLYR)

      DIMENSION tvel(max500yr,MAXLYR)

C
*****

***** uzft.f
      dimension vellast(MAXLYR)

cc rwr 10/20/04 modified for long TPA siumulations
cc    dimension vtim(max500yr)
      dimension vtim(ntimg)

***** UZFT.F.ORIGINAL
      dimension vellast(MAXLYR)
```

```
     dimension vtim(max500yr)

*****

***** uzft.f

cc rwr 10/20/04 modified for long TPA siumulations
cc       ntim = 1 + nint( timg(ntimg) / 500.d0 )
      ntim = ntimg

cc rwr 10/20/04 modified for long TPA siumulations
cc       tim(1) = 0.d0
      tim(1) = timg(1)
      itime_c = 2
***** UZFT.F.ORIGINAL

      ntim = 1 + nint( timg(ntimg) / 500.d0 )

      tim(1) = 0.d0
      itime_c = 2
*****

***** uzft.f
      do itime = 2, ntim
cc rwr 10/20/04 modified for long TPA siumulations
cc          tim(itime) = tim(itime-1) + 500.d0
         tim(itime) = timg(itime)
cc itime_c will contain the index for the last time in the
***** UZFT.F.ORIGINAL
      do itime = 2, ntim
         tim(itime) = tim(itime-1) + 500.d0
cc itime_c will contain the index for the last time in the
*****

***** uzft.f

cc rwr 10/20/04 modified for long TPA runs
cc       call maplist( ntimg, timg(1), qm3peryrinsag(1), ntim, tim(1),
cc     &              qm3peryrinsa(1) )
```

```
      do itime = 1, ntim
        qm3peryrinsa(itime)= qm3peryrinsag(itime)
      enddo
cc
***** UZFT.F.ORIGINAL

      call maplist( ntimg, timg(1), qm3peryrinsag(1), ntim, tim(1),
     &              qm3peryrinsa(1) )
cc
*****

***** uzft.f
CC they both should be the same value

cc rwr 10/20/04 modified for long TPA simulations
cc      call writevelocities( max500yr, itm, vtim, nefleg,
cc     &                    repvel, tvel)
      call writevelocities( mxntime, itm, vtim, nefleg,
     &                    repvel, tvel)
***** UZFT.F.ORIGINAL
CC they both should be the same value
      call writevelocities( max500yr, itm, vtim, nefleg,
     &                    repvel, tvel)
*****
```

6. Performed runs with the above modifications and found some problems that required further investigation. That is, for example, increasing time steps still shows some shifts in the peak.

7. Conducted a mean value run with Th229 (and U233 added). Plotted the results. See Figure 26.

October 26, 27, 28, and 29, 2004

1. The aqueousnuclide U233 and Th229 will be added to current list in the tpa.inp file and included in the modifications to the TPA code delivered to the NRC at the end of this week.

2. Found the long (331 realization and 8001 time step) TPA runs left for execution over the weekend did not unsuccessfully complete (used both GRYPHON and BEMORE). The cause of the

problem was from UZ NEFTRAN execution arising from the cyclical flow rate in NEFII.VEL which actually was attributable to the cyclical data in climato2.dat. This is the latest of a number of problems associated with long TPA simulations and making sure that the user set number of time steps dfoes not change results. It was determined that these problems, which prevent the successful completion of a TPA code run, are from the following four areas (all are related to setting longer simulation times and using cyclical climate data with different number of time steps): (i) longer simulation times results in more velocities in the UZ NEFTRAN input file NEFII.VEL (fixed by increasing array dimensions in the NEFTRAN INCLUDE file SIZES.INC); (ii) the cyclical climate data yielded unexpected peaks (e.g., the MAPLIST interpolation could result in flow rates with peaks occurring every 200,000 years) in the flow rates in the UZ NEFTRAN NEFII.VEL file when different number of time steps are set in the tpa.inp file (fixed by modifying the use of the MAPLIST subroutine in UZFT - instead of mapping times and flow rates to 500 year time intervals, TPA times and flow rates at those time are used to determine the UZ NEFTRAN input file NEFII.VEL) - also note that to fix this problem of unexpected flow rate peaks occurring because of interpolation, the velocity change factor in the UZFT portion of the tpa.inp file was decreased from 0.4 to 0.1 (caused more array out-of-bounds problems), then from 0.4 to 0.15 (again, caused more array out-of-bounds problems), and then to 0.2 (this value was not fully tested because computer resources were not available for this work) ; (iii) with fixes discussed in (i) and (ii) above, TPA output was not stable in the UZ NEFTRAN release rates (especially note Np-237) with unexpected peaks occurring at 419,000 years instead of at 119,000 years (not fixed because this result seems to be tied to the cyclical input flow rates and to the fluctuating release rates from RELEASET); and (iv) as tied to (iii), there are fluctuating release rates from RELEASET that seem to be caused by the cyclical input flow rates (also, not fixed). To address the above issues (with the goals of providing (1) a stable TPA code regardless of the user selected time steps and (2) results that are consistent with the verified TPA Version 4.1jpd code), the decision was made by R. Janetzke and S. Mohanty (as recommended by R. Rice) that the climate data in climato2.dat be set at a constant value from 41,000 through the end of the simulation (i.e., the cyclical flows would be removed), although the initial increase in flow rates through the 10,000 year compliance period (as specified in the climato2.dat file) would be left unchanged. The new ("steady") climato2.dat file is:

0	0	0
1000	0	0
2000	0.0253339	0.0253339
3000	0.0560985	0.0560985
4000	0.0906067	0.0906067
5000	0.128457	0.128457
6000	0.169215	0.169215
7000	0.21242	0.21242
8000	0.257593	0.257593

9000	0.304244	0.304244
10000	0.35188	0.35188
11000	0.40001	0.40001
12000	0.448158	0.448158
13000	0.495864	0.495864
14000	0.542693	0.542693
15000	0.588244	0.588244
16000	0.63215	0.63215
17000	0.674086	0.674086
18000	0.713773	0.713773
19000	0.750977	0.750977
20000	0.785517	0.785517
21000	0.817261	0.817261
22000	0.846128	0.846128
23000	0.872084	0.872084
24000	0.895148	0.895148
25000	0.915377	0.915377
26000	0.932875	0.932875
27000	0.947779	0.947779
28000	0.960259	0.960259
29000	0.970511	0.970511
30000	0.978751	0.978751
31000	0.98521	0.98521
32000	0.990123	0.990123
33000	0.993732	0.993732
34000	0.996268	0.996268
35000	0.997955	0.997955
36000	0.998999	0.998999
37000	0.999583	0.999583
38000	0.999865	0.999865
39000	0.999972	0.999972
40000	0.999998	0.999998
41000	1	1
50000	1	1
1000000	1	1

2. Testing of the TPA code with the modification discussed in #1 above, will determine a recommended number of time steps and whether there are any issues associated with the time steps that cause instability in the results. Results from the testing are shown in Figures 27 - 29. The

results indicate the steady climate flow rates lead to an earlier time of peak dose, with the peak dose being about the same.

3. By adding U233 and Th229 to the aqueousnuclides in tpa.inp, found an array out of bounds message in UZ NEFTRAN. After consultation with R. Janetzke, increased the "NDBF" value from 600000 to 1500000 in SIZES.INC. This change allowed for successful completion of UZ NEFTRAN for the 1e6 yr, constant climate, 331 total realizations, Subarea 1, Realization 30 case (all else basecase tpa.inp values)

4. Modified nfenv.f to remove the hardcoded 10,000 year end of reflux specification. The 10,000 year time was set in the reflux2 and the reflux3 subroutines. In the revision, the end of reflux was set to tim(ntim) (i.e., the maximum simulation time).

5. The "n3" variable dimension in the reflux2.i include file was reset from a value of 100000 to 1000000. This value is used in the NFENV module and used in the reflux2 and reflux3 subroutines (see the change for #4 above). These calculations had been done on a yearly basis, so increasing the maximum "n3" to 1,000,000 was reasonable.

6. The exec.f source code was modified to set the variable "nwphumed"to "0" and thus print values of "0" to the files ashout.res and ebsrel.ech files when the VOLCANO flag is NOT activated. Without this change, these files would contain "****" or a bogus "garbage number" for the number of exhumed WPs (because the variable "nwpexhumed" was not initialized if VOLCANO is not activated; however a value is printed to these files). NOTE that a similar change was accomplished previously in EXEC when the number of exhumed WPs was written to the screen for Subarea 2, even though VOLCANO was not activated (again, a bogus "garbage number" was written in the screenprint).

7. In the exec.f source code, the screenprint related to the estimated disk space required for a TPA code run with the APPPEND option activated was modified to reflect the increased requirements arising from the increased number of time steps. Those estimated requirements, as determined from TPA code simulations (Version 41jpdls_beta2) were 90 megs (base), 2 megs per realization after the first, and 130 megs per realization for the APPEND files (*.ech, *.rlt, and *.cum).

8. Found what appears to be a double counting of failed WPs - when VOLCANO is activated and # exhumed WPs is > 0, the RELEASET calculations include those ejected WPs in the release calculations for CORROSION failure (if there is CORROSION failure).

9. During testing, G. Adams noted that there was a change in the magnitudes of the seismic event when the new and old versions of the TPA code are compared. These differences are attributable to the increased array dimensioning associated with the long simulations (i.e., the maximum number of seismic events was increased in exec.f to accommodate the long simulations). Testing by decreasing this dimensioning in the TPA41jpdls_beta3 code exec.f file to the previous value (1000) showed the same magnitudes of seismic events in the TPA41jpdls_beta3 (new) code and in the TPA41j (old) code.

10. During developer testing of #4 above, found that the REFLUX3 model would show reflux during the entire 1e6 period (even though the temperature dropped below 100 deg C at about 2,000 years and was about 50 deg for most of the simulation). Modified, again, the NFENV to arrive at the TPA41jpdls_beta3 code which sets the end of reflux period at 20,000 years (note that this time is consistent with Figure 3-3 in the March 2004 TPA 4.1 Sensitivity Analysis Report)

11. Results from TPA41jpdls_beta3 for 10,000, 100,000, and 1,000,000 years are provided in Figures 27, 28, and 29 for 350 realizations, respectively. Note that the peak mean dose was about 35 mrem/yr occurring at 14,260 years for this basecase simulation (only the number of realizations was changed in the TPA41jpdls_beta3 tpa.inp file for this simulation - from 1 to 350 realizations).

November 15, 16, 17, and 18, 2004

1. The work is this was related to preparing the TPA code for delivery to NRC on Friday, November 19, 2004 (i.e., modifications were made to TPA41jpdls_beta3 in preparation of delivery of TPA41jpdls_beta4). Work, initiated from an email from T. McCartin, was conducted to investigate TPA41jpdls_beta3 code results when the dilution model was activated and the user-supplied dilution volume se to 3,000 acre-f/yr. Results showed this user-set dilution model in the TPA41j version, though it was present as a flag, was never utilized in calculations (the pumping rate was set at a sampled value based on a uniform distribution from about 3.2 to 9.2 M gal/day) and, though the user could activate this flag, the TPA code would use the sampled pumping rate in calculations. The dcagw.f file was modified to activate a flag that would allow the user to specify a dilution volume in the tpa.inp file so that dilution volume would always be used calculations. The following information is an "fc" (file comparison) between the dcagw.f file before and after these modifications. These modifications will be tested prior to delivery of the next version of the TPA code (TPA41jpdls_beta4).

```
Comparing files dcagw.modified.f and DCAGW.ORIGINAL.F
***** dcagw.modified.f
      dilutionvolume=pump
      if (dilflg .eq. 1) dilutionvolume = userdilutionvolume
```

```
     &                        * 365.25d0 / 264.172d0

***** DCAGW.ORIGINAL.F
      dilutionvolume=pump
*****

***** dcagw.modified.f
      dilutionvolume=pump
      if (dilflg .eq. 1) dilutionvolume = userdilutionvolume
     &                        * 365.25d0 / 264.172d0

***** DCAGW.ORIGINAL.F
      dilutionvolume=pump
*****
```

2. Investigated reasons why UZ NEFTRAN stops execution because of the BF array dimensions being exceeded for certain realizations/subareas (e.g., realization 165 of 400 for Subarea 1; realization 22 of 500 for Subarea 1; realization 279 of 450 for Subarea 1). After consultation with P. Bertetti and based on his email, modified the tpa.inp file. The email contents are:

Please use Cm sorption values (Kds or Rds) that are equivalent to the values used for Am. This is consistent with values used in other portions of TPA 4.1 and is consistent with recent summaries of Cm and Am chemical behavior.

e.g. Runde, W. 2000. "The Chemical Interactions of Actinides in the Environment". In Challenges in Plutonium Science, Vol II. Los Alamos Science, No. 26. LA-UR-00-4100. Los Alamos, MN: Los Alamos National Laboratory. pp 392

Consequently, the tpa.inp file was modified to make the distributions for Cm and Am in the UZ Matrix KD the same. The following information provides the "fc" (file comparison) between the TPA41jpdls_beta3 and TPA41jpdls_beta4 tpa.inp files (NOTE: also included in the modifications shown below, as related to #1 above, dilution model was also activated and the user-supplied dilution volume set at 2676394 gal/day or 3000 acre-ft/ and the plume capture model was also activated to capture all of the plume).

```
Comparing files tpa.modified.inp and TPA.ORIGINAL.INP
***** tpa.modified.inp
title
```

```
 Input file tpa.inp as supplied with the TPA41jpdls_beta4 Code.
 Base case.
***** TPA.ORIGINAL.INP
title
 Input file tpa.inp as supplied with the TPA41jpdls_beta2 Code.
 Base case.
*****
***** tpa.modified.inp
**
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.
**
***** TPA.ORIGINAL.INP
**
```

```
constant
MatrixKD_TSw_Cm[m3/kg]
0.0
**
constant
MatrixKD_CHnvCm[m3/kg]
0.0
**
constant
MatrixKD_CHnzCm[m3/kg]
0.0
**
constant
MatrixKD_PPw_Cm[m3/kg]
0.0
**
constant
MatrixKD_UCF_Cm[m3/kg]
0.0
**
constant
MatrixKD_BFw_Cm[m3/kg]
0.0
**
constant
MatrixKD_UFZ_Cm[m3/kg]
0.0
**
*****
***** tpa.modified.inp
PlumeCaptureModel
1
**
***** TPA.ORIGINAL.INP
PlumeCaptureModel
0
**
*****
```

***** tpa.modified.inp
DilutionModel
1
**
***** TPA.ORIGINAL.INP
DilutionModel
0
**
*****

***** tpa.modified.inp
UserDefinedDilutionVolume[gal/day]
2676394.
** 3000 acre-feet per year = 2676394 gallons per day.
**
***** TPA.ORIGINAL.INP
UserDefinedDilutionVolume[gal/day]
10901787.249406d0
**
*****

These modifications will be tested prior to delivery of the next version of the TPA code (TPA41jpdls_beta4).

Development testing showed that activating plume capture was working properly. The TPA code always captures the entire plume at 20km. At 10 km, if plume capture is not activated, it is possible that less than 100% of the plume will be captured (this depends on values for the pumping rates/user-supplied dilution). At 10km, if plume capture is activated, 100% of the plume is captured. This development testing used the basecase TPA41jpdls_beta4 tpa.inp file, modified to run Subarea 1 only, and with the aforementioned modifications associated with activating plume capture, activating dilution model, and modifying the user-supplied dilution volume. Note that the tpa.inp file contains a value of 1.0 for the fraction of the plume captured (this is used when the plume capture model is activated).

January 27 and 28, 2005; February 2, 3 and 4, 2005

Subject: Long TPA runs using the TPA Version 5.0.0.f code

Goals:

- modify the TPA Version 5.0.0.f code to allow "long simulations" in a manner that is consistent with similar modifications made to the TPA Version 4.1jpd code
- verify the results are correct at these longer times and increased number of time steps
- document the modifications to the source code
- record results from verification testing at these longer times and increased number of time steps

Summary of Achievements: The TPA Version 5.0.0f code was modified and compiled using LF95 and, running on the high-end Xeon GIS machine, successfully completed execution for 1,000,000 years and 5,000 time steps. Follow-up verification work is needed in a number of areas.

Chronology of Activities:

1. Received direction from R. Janetzke during a 1/24/05 meeting to begin this work.

2. Obtained the TPA code for Versions 4.1jpdls_beta4 and 5.0.0.f from Vermont.

3. Identified files (using file dates) that were modified while enhancing the capabilities of TPA Version 4.1jpd to do "long simulations". These files were:

(In main TPA directory)

ashplumo.f
dcags.f
dcagw.f
ebsrel.f
exec.f
maxntime.i
nfenv.f
nintv.i
reflux2.i
sampler.f
samplerv.i
seismo.f
szft.f
tpa.inp
uzft.f
uz_parms.i
zportpc.f

(In codes subdirectory)

ebsfilt.f
failt.f

nefmks.f
releaset.f
SIZES.INC

(In data subdirectory)

climato2.dat
multiflo.dat
tpanames.dbs
wpflow.def

4. The files from TPA Version 4.1jpdls_beta4 were compared with the TPA Version 4.1jpd files using the “fc” command. The outputs from this file comparison were saved and printed. The changes introduced for the “long simulations” were then transferred to files for TPA Version 5.0.0.f.

5. The files “ashplumo.f”, “dcags.f”, “dcagw.f”, and “ebsrel.f” (although they were modified for the TPA Version 4.1jpdls_beta4 code) did not need to be changed because all of the relevant changes were incorporated into the TPA code during code development from Versions 4.1 to 5.0.0.f.

6. For the “exec.f” file (instead of modifying “maxseismicevents” in that file), in Version 5.0.0.f this parameter is contained in the seisadj.i file. This file was modified by increasing “maxseismicevents” from 1500 to 6000.

7. 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.)

8. 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)
```

9. The other modifications to the TPA Version 4.1jpdls_beta4 code “exec.f” file were already contained in the TPA Version 5.0.0.f code “exec.f” file.

10. 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 )
```

11. 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
```

12. 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)
```

13. 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)
```

14. Modifications to the TPA Version 4.1jpdls_beta4 code “sampler.f” file were already contained in the TPA Version 5.0.0.f code “sampler.f” file. Also, although the file date indicated there was a change made in the “samplerv.i” file”, this file is the same in both the 4.1jpdls_beta4 and 5.0.0.f versions of the TPA code.

15. In the development of TPA Version 5.0.0.f from Version 4.1jpdls_beta4, the file “seismo.f” was replaced with “seismo2.f” and the “sh” and “system” references are not contained in the “seismo2.f” file. No change needed to be made.

16. Modifications to the TPA Version 4.1jpdls_beta4 code “szft.f” file were already contained in the TPA Version 5.0.0.f code “szft.f” file.

17. 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".

18. 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.

19. Verified values for all dilution-related parameters in TPA Version 4.1jpdls_beta4 were already included in the tpa.inp file for TPA Version 5.0.0.f. All values were consistent.

20. 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)
```

21. In “uzft.f”, did not modify the source code to print only TPA code time steps to the “NEFII.VEL” file, as was done in the TPA Version 4.1jpdls_beta4 code (this was done to help remove the instability of flow rates into UZ NEFTRAN). However, because other

TPA 5.0.0.f development work is currently being done in this area, this modification was put on hold.

22. Noted that the file "max500yr.i" was already dimensioned at 1e6/500 + 1 timesteps; so no change in the parameter "max500yr" needed to be made.

23. 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)
```

24. 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)
```

25. Modifications to the TPA Version 4.1jpdls_beta4 code "zportpc.f" file were already contained in the TPA Version 5.0.0.f code "zportpc.f" file.

26. Noted in "ebsfilt.f" that moving from the TPA Version 4.1jpdls_beta4 code to TPA Version 5.0.0.f code, the time step dimensions had been moved to the "maxntime.i" file instead of using multiple hard-coded values. No changes needed to be made in TPA Version 5.0.0.f..

27. 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)
```

28. Also in failt.f, it appears as though a write statement to “ebstrh.dat” that allows the possibility to write numbers with one more place value (i.e., numbers greater than or equal to one million) had been added to the TPA code during modifications from Version 4.1jpd to 5.0.0.f. Testing will verify the implementation of this modification.

29. 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)
```

30. Noted in “releaset.f” that moving from the TPA Version 4.1jpdls_beta4 code to TPA Version 5.0.0.f code, the time step dimensions had been moved to the “maxntime.i” file instead of using multiple hard-coded values. No changes needed to be made in TPA Version 5.0.0.f.

31. 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)
```

32. 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

33. Noted that the file "multoflo.dat", though it was used in the TPA Version 4.1jpdls_beta4 code, has been deleted from the TPA Version 5.0.0.f code.

34. 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
```

35. 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
```

36. Created a subdirectory called c:\tpa500f_ls and copied the TPA Version 5.0.0.f code into that subdirectory. Then, also copied into this subdirectory any files that were modified (i.e., as documented above) and overwrote those files. The contents of this subdirectory were burned onto a CD and BEMORE used for compiling. Runs will be done on either BEMORE or GRYPHON.

February 8, 9, 10, and 11, 2005; February 15, 16, 17, and 18, 2005

1. Performed a TPA code simulation with the modifications listed previously and found through a screenprint error message that the “maxseismicevents” in the seisadj.i file needed to be increased. This value was modified from 6000 to 10000 and the TPA code execution was successful.

2. 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.

3. 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

4. Ran the TPA code and noted that the number of ejected WPs is listed as 2012602235 (a bogus number). This was corrected in the exec.f file for the TPA Version 4. 1jpdls_beta4 code and needs to be corrected in the TPA Version 5.0.0.f code. Communicated with R. Janetzke who stated this needed change will be accomplished through SCR 519.

5. 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
**
```

6. 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
```

7. 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.

8. As a follow-up to #5, 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

9. 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.)

10. 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.

11. Needed to test #6 list above (i.e., 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 in #6, 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:

12. NOTE: During testing for #11, noted that the partitioning of aqueousnuclides that are entering the UZ into colloids and aqueousnuclides assumes the aqueousnuclides are not decreased. In fact, during #11 testing, 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

13. Received a version of the tpa.inp file from C. Scherer on 2/16/05 (10:26 a.m.) That includes the current final TPA code data. This file is called "tpa_dosverified.inp". Ran the TPA code with this new file.

14. Using the file from #11, made modifications to the tpa.inp file discussed previously in this documentation to enable long simulations.

March 10 and 11, 2005

1. 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.

2. 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.

3. Executed the above code on GRYPHON successfully for the basecase (execution time was 5 minutes). Then, ran this code 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).

4. 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, u_parms.i, and failtadj.i. Comment #1 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.)

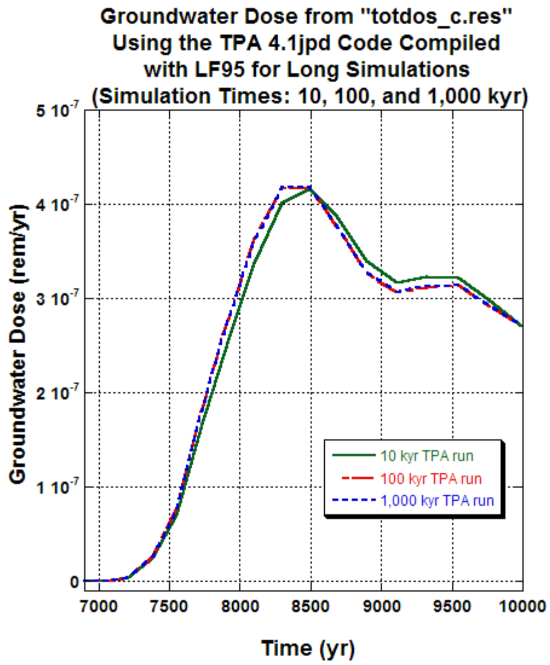


Figure 1.

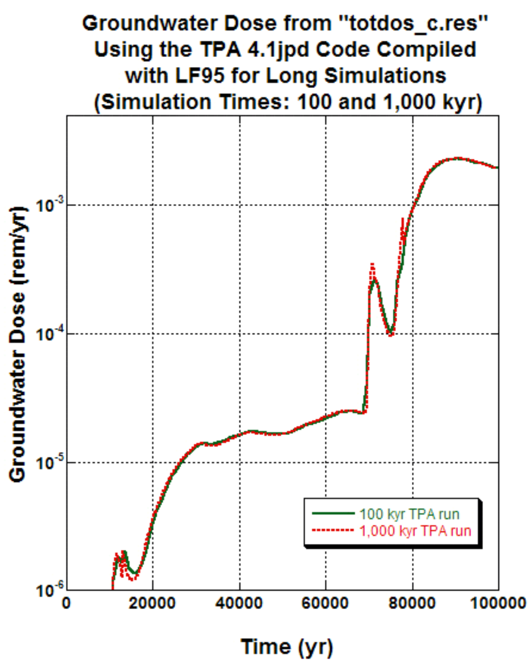


Figure 2.

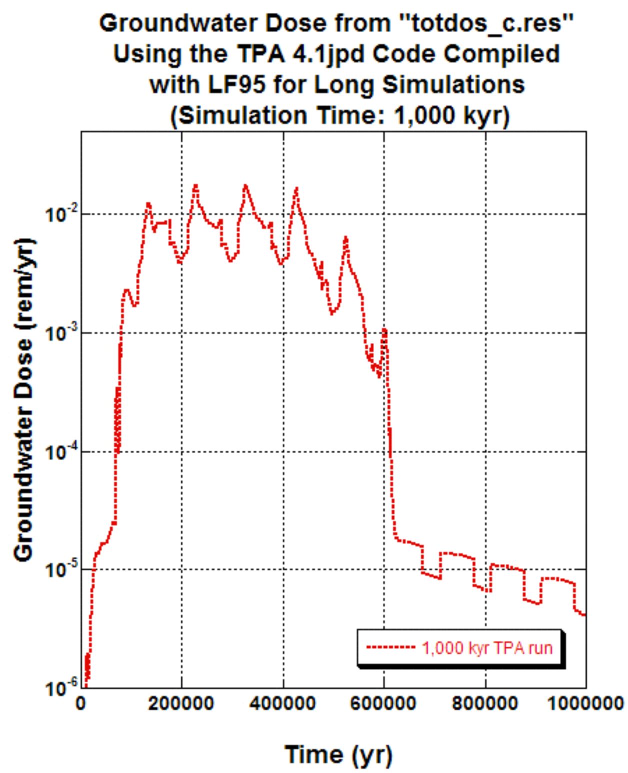

Groundwater Dose from "totdos_c.res"
Using the TPA 4.1jpd Code Compiled
with LF95 for Long Simulations
(Simulation Time: 1,000 kyr)
Groundwater Dose (rem/yr)
10^-2
10^-3
10^-4
10^-5
10^-6
0
200000
400000
600000
800000
1000000
Time (yr)
1,000 kyr TPA run

Figure 3.

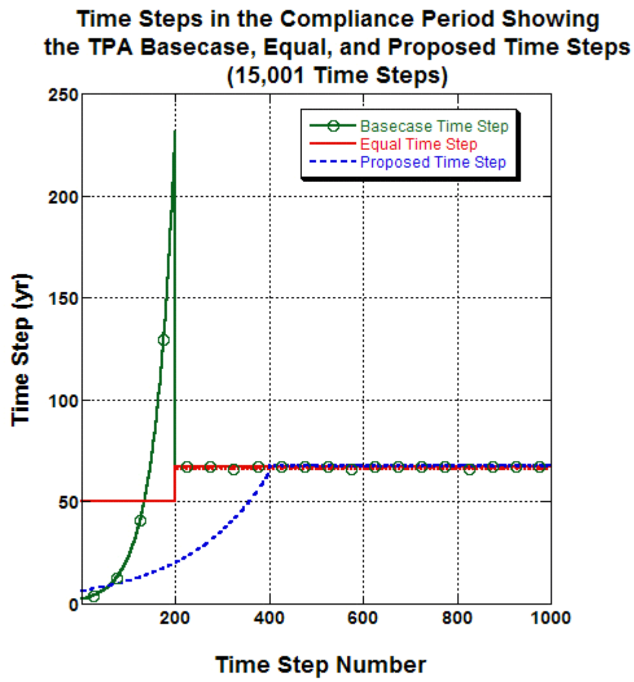


Figure 4.

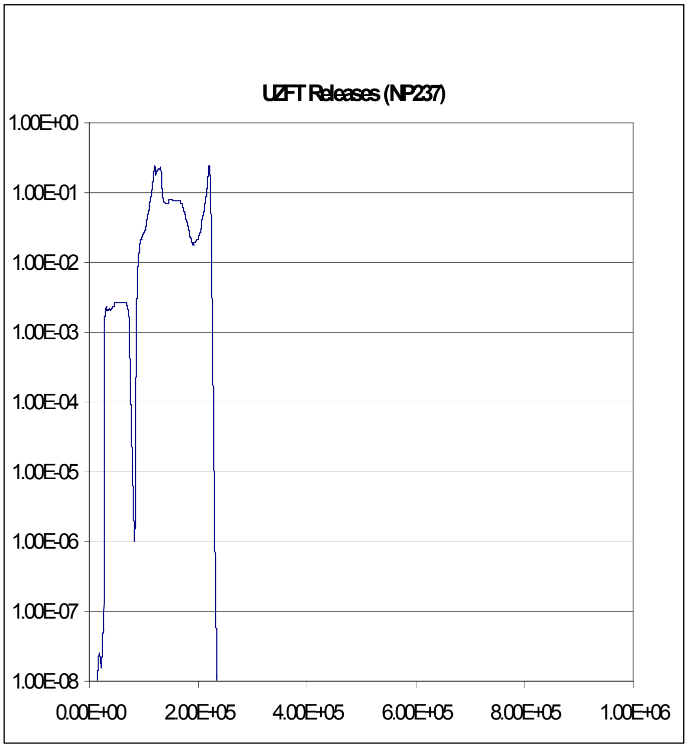


Figure 5.

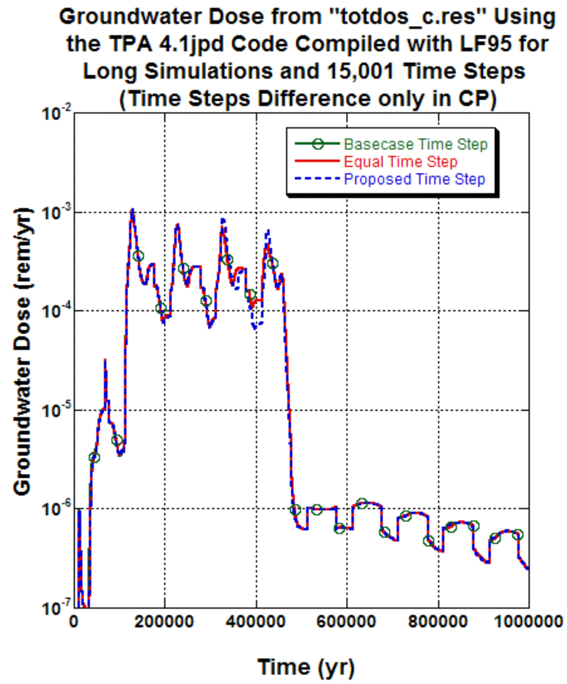


Figure 6.

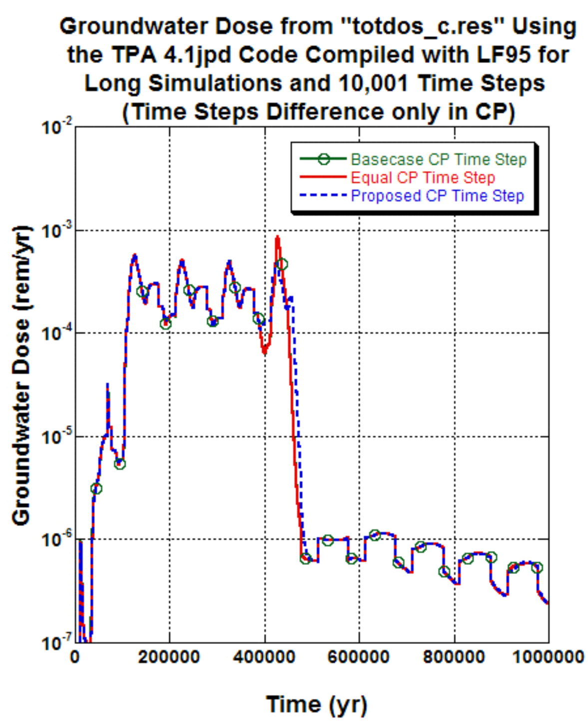


Figure 7.

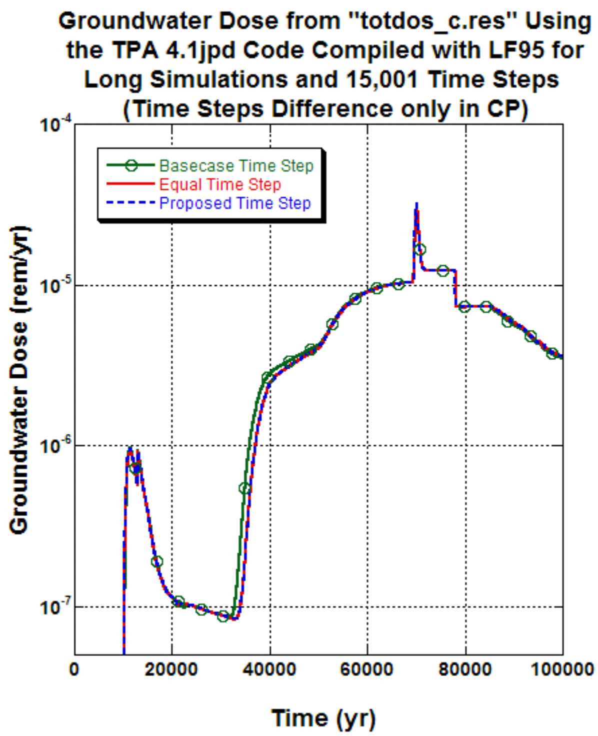


Figure 8.

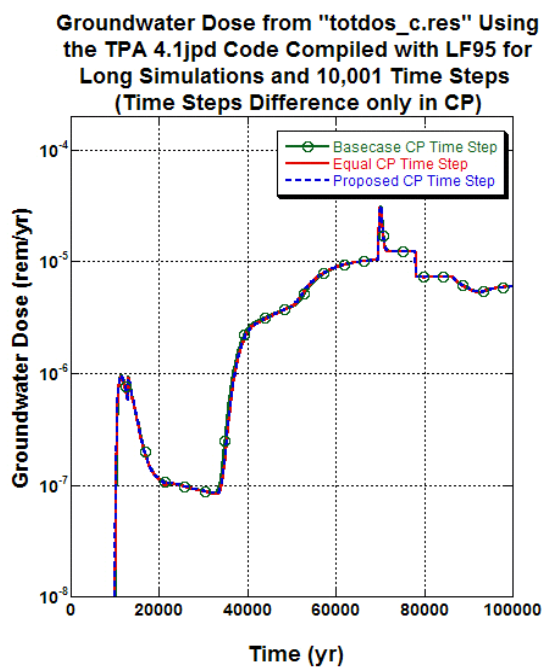


Figure 9.

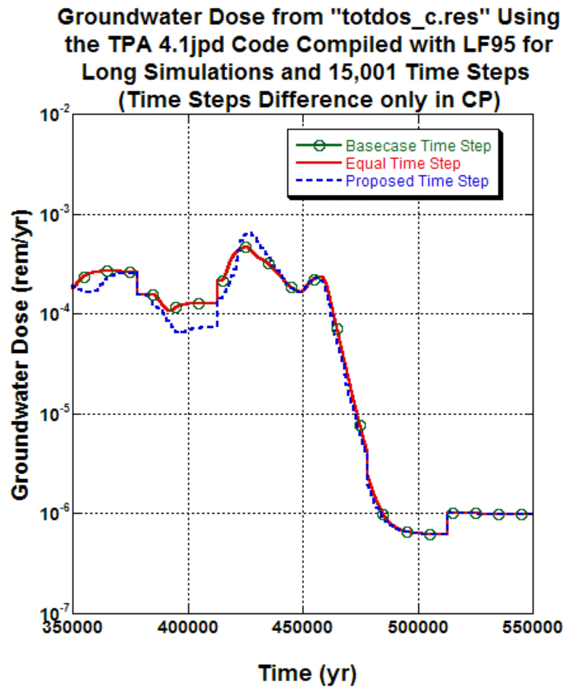


Figure 10.

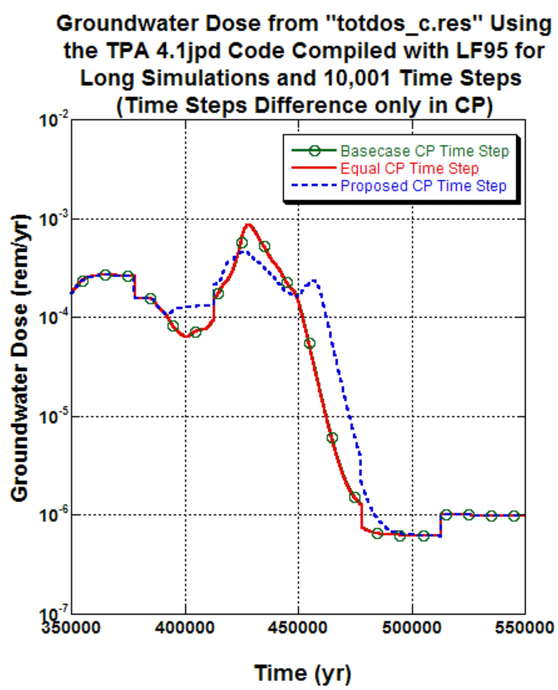


Figure 11.

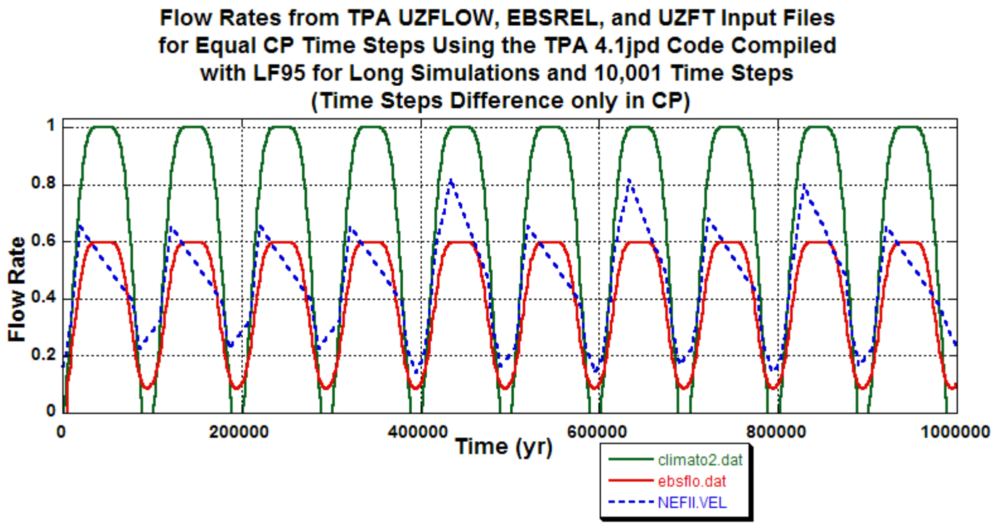


Figure 12.

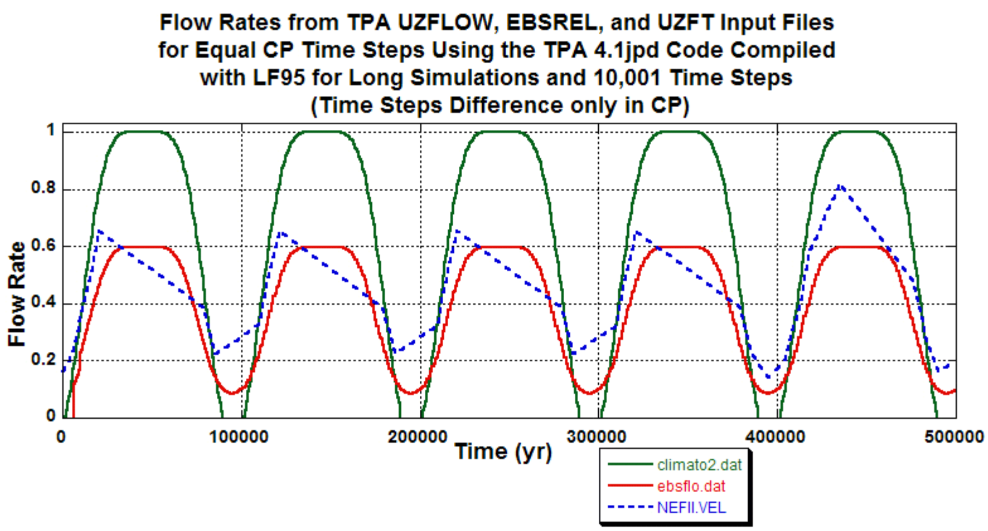


Figure 13.

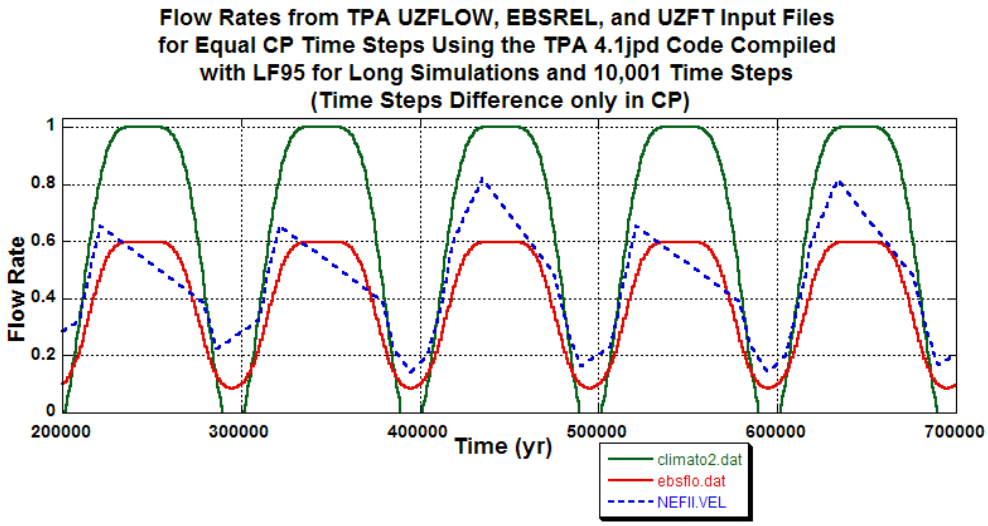


Figure 14.

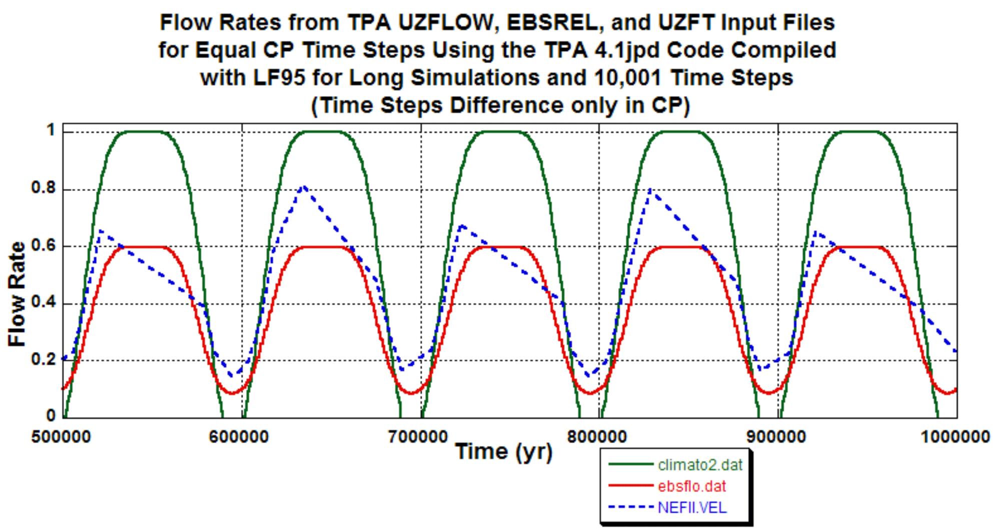


Figure 15.

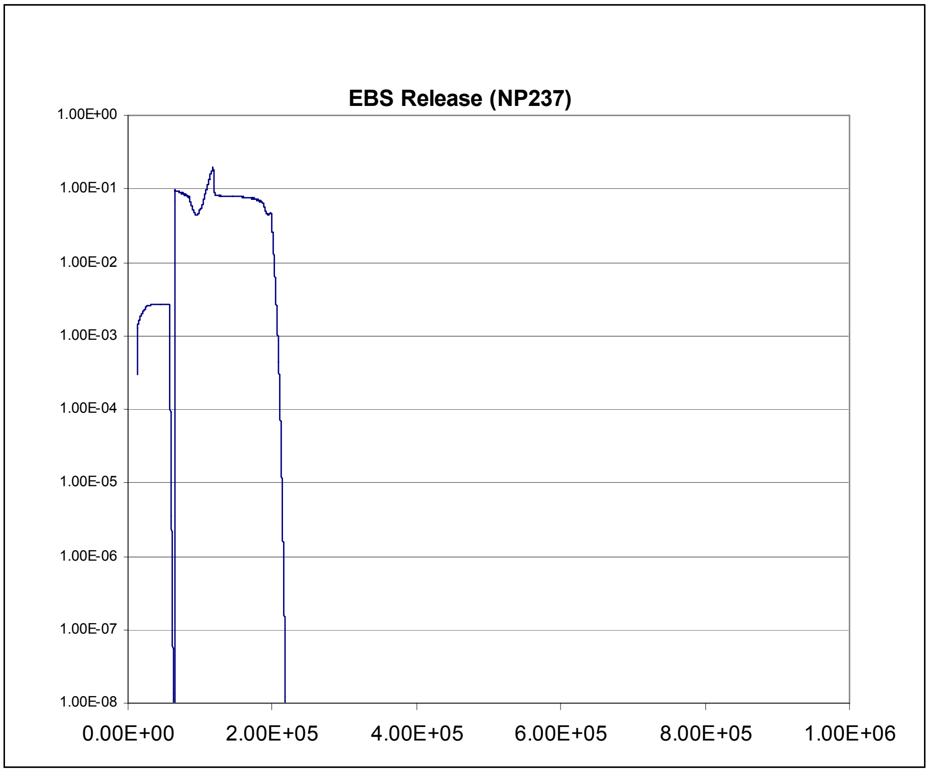


Figure 16.

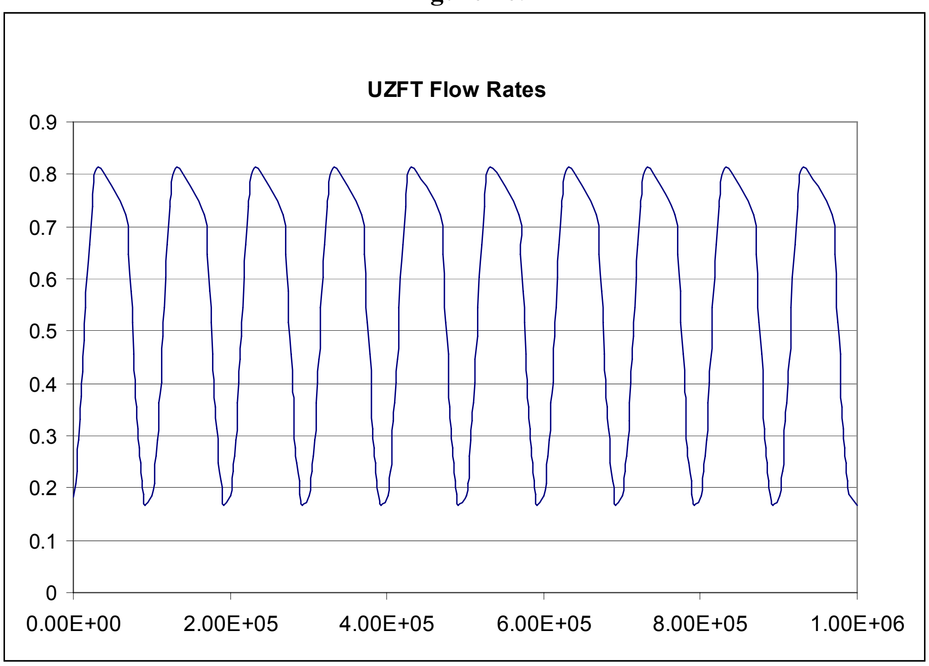


Figure 17.

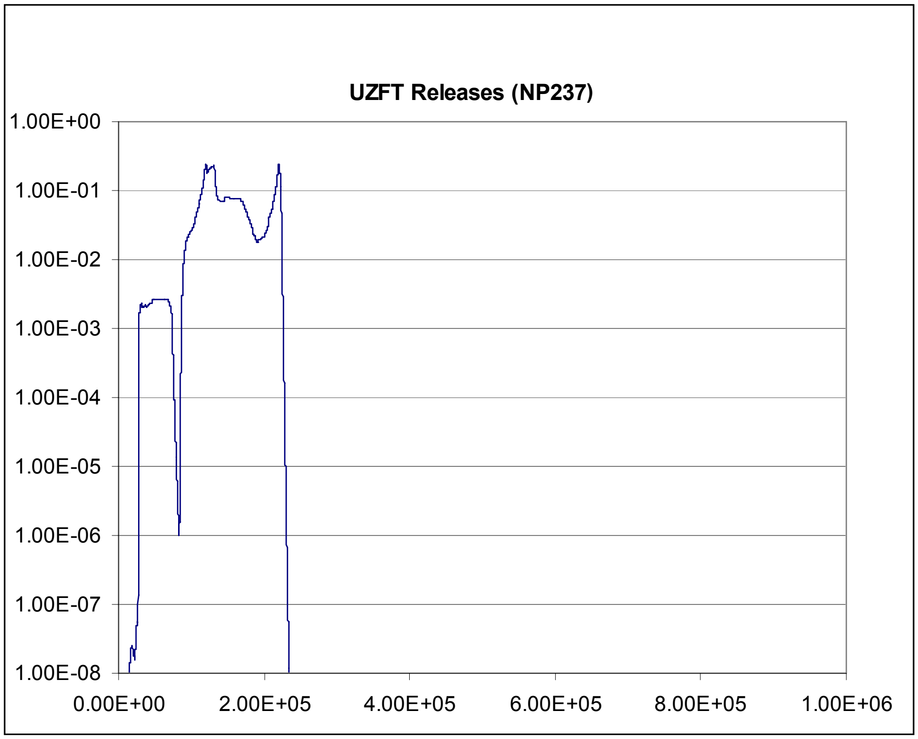


Figure 18.

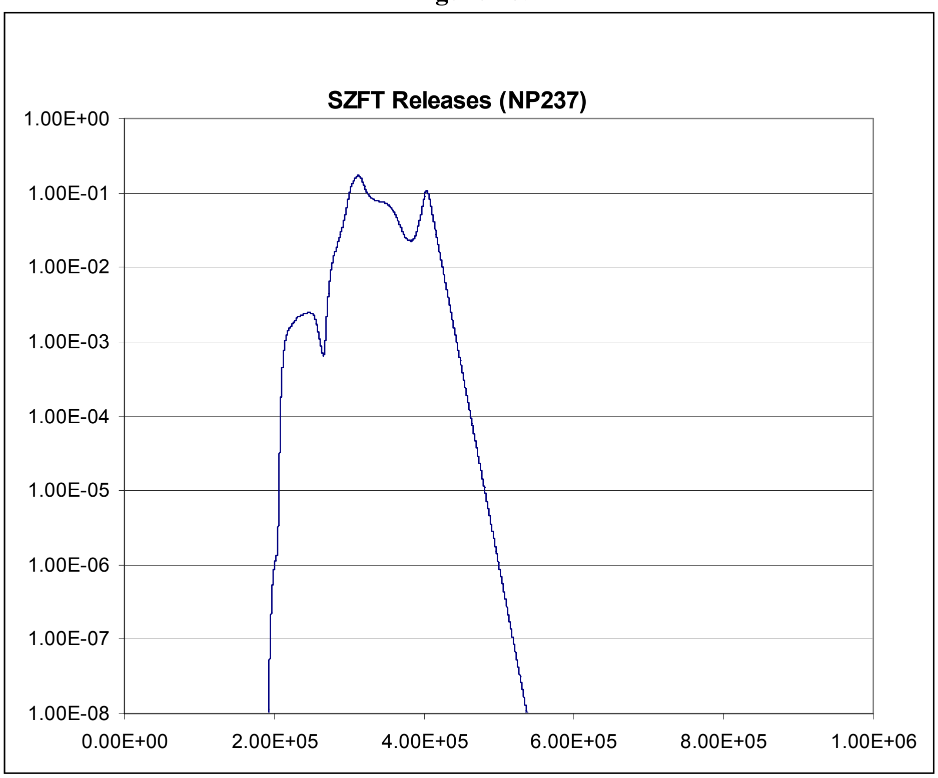


Figure 19.


Total Dose
1.00E+00
1.00E-01
1.00E-02
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
0.00E+00
2.00E+05
4.00E+05
6.00E+05
8.00E+05
1.00E+06

Figure 20.

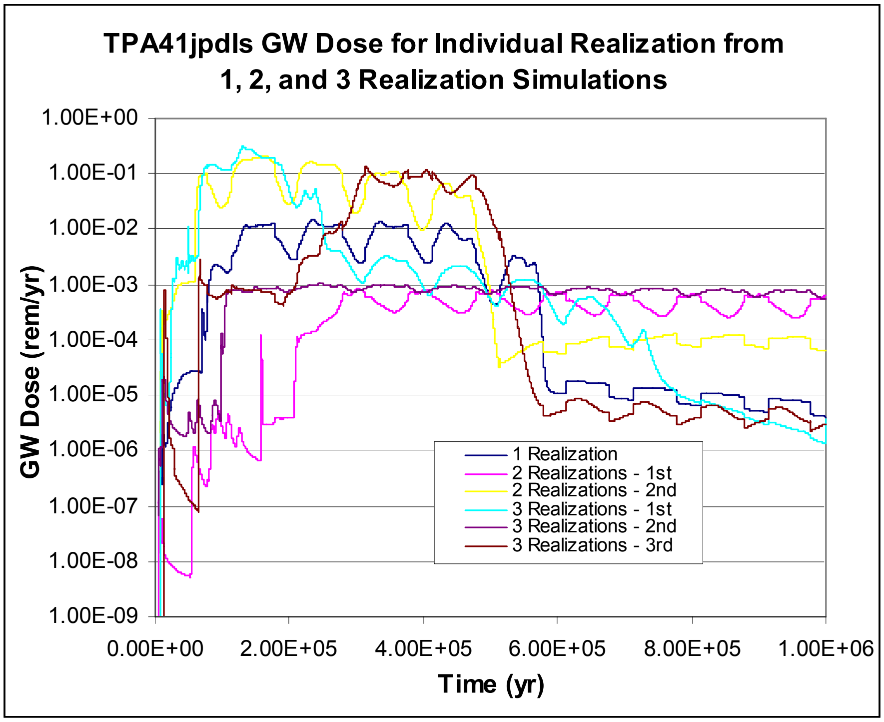


Figure 21.

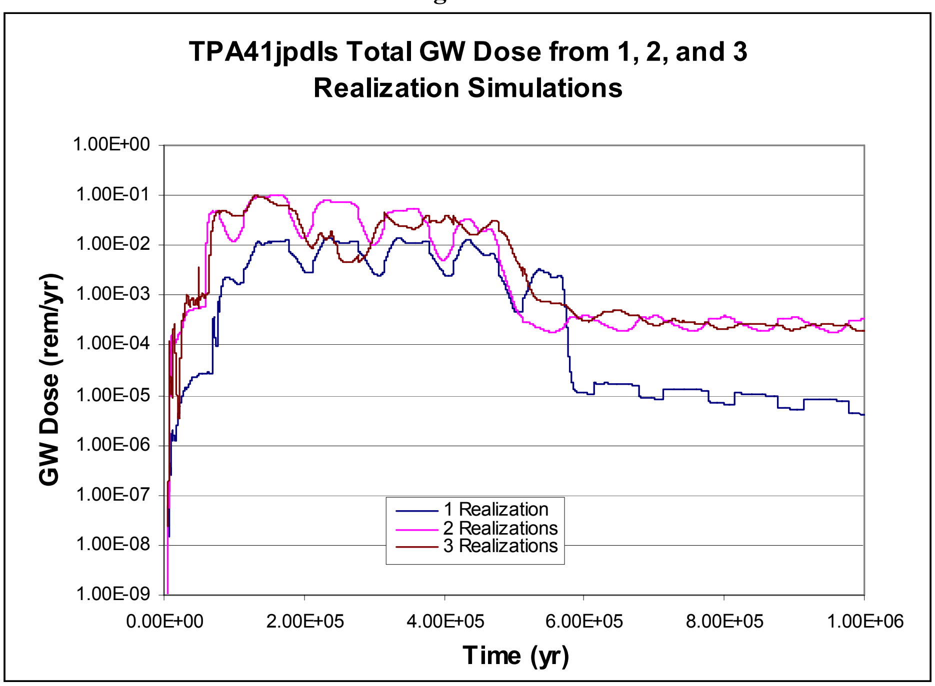


Figure 22.

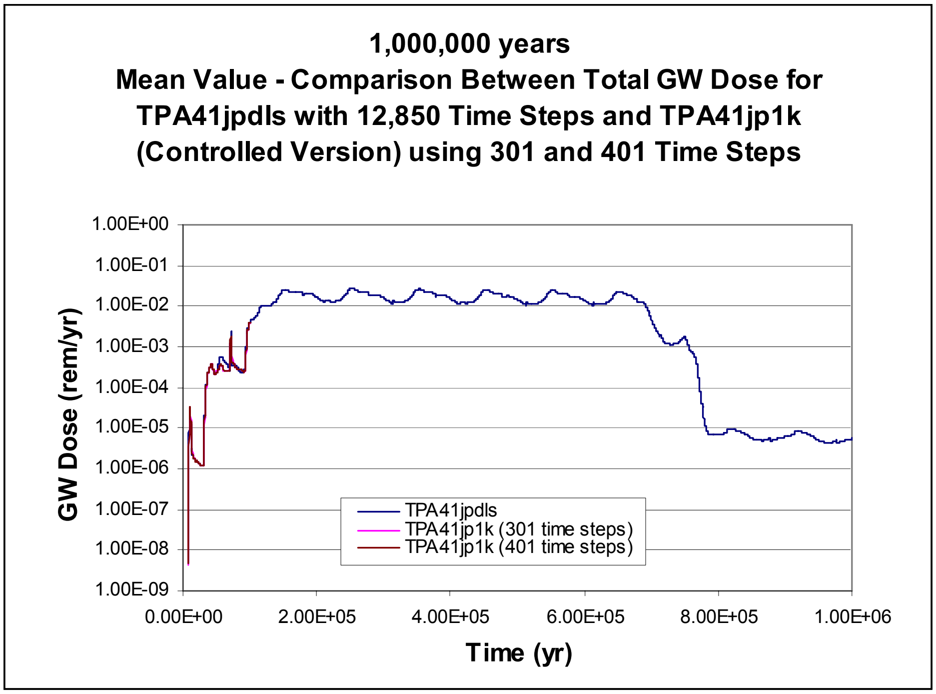


Figure 23.

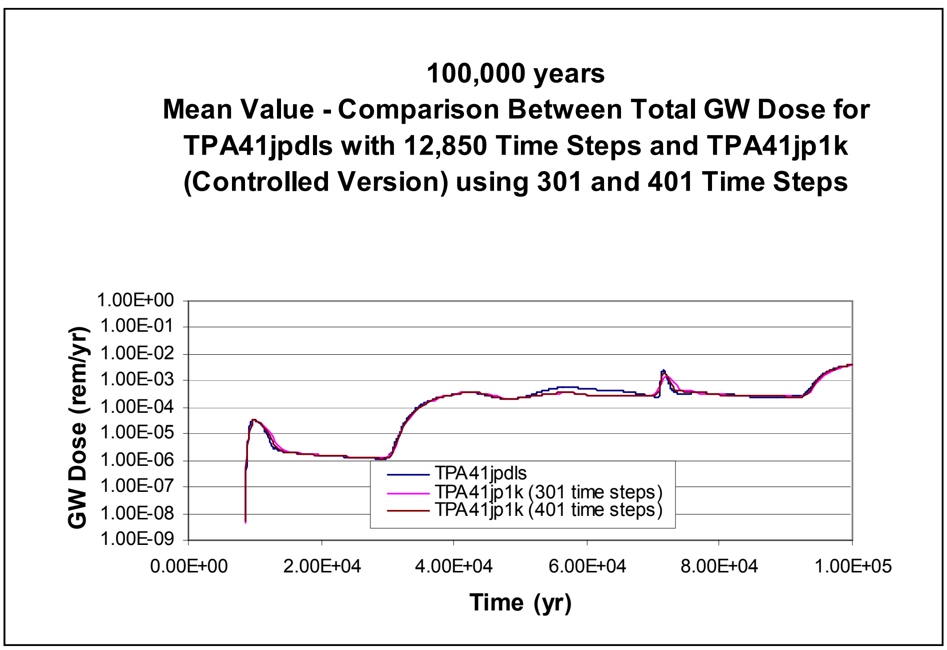


Figure 24.

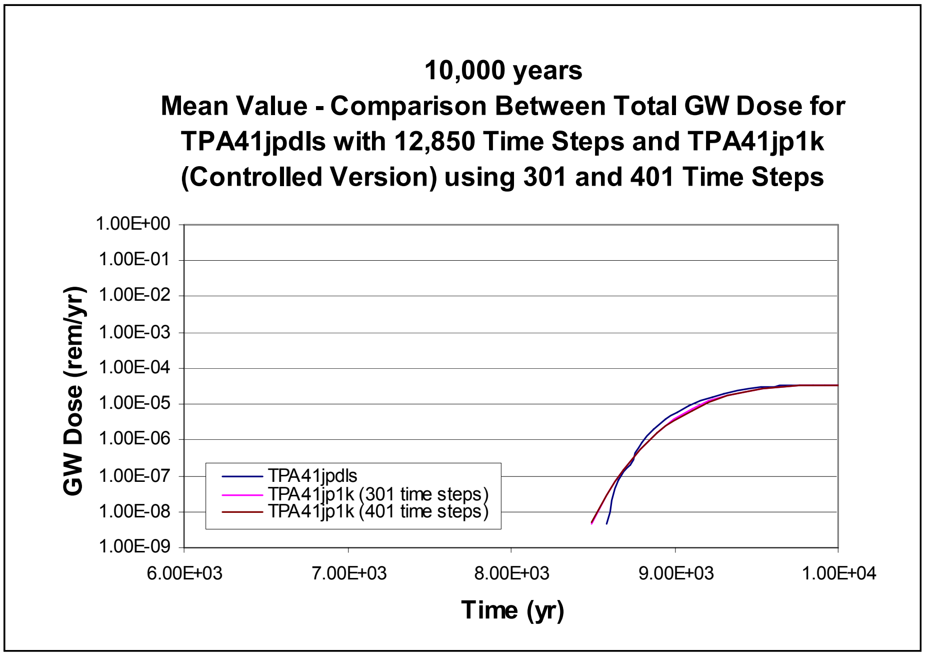


Figure 25.

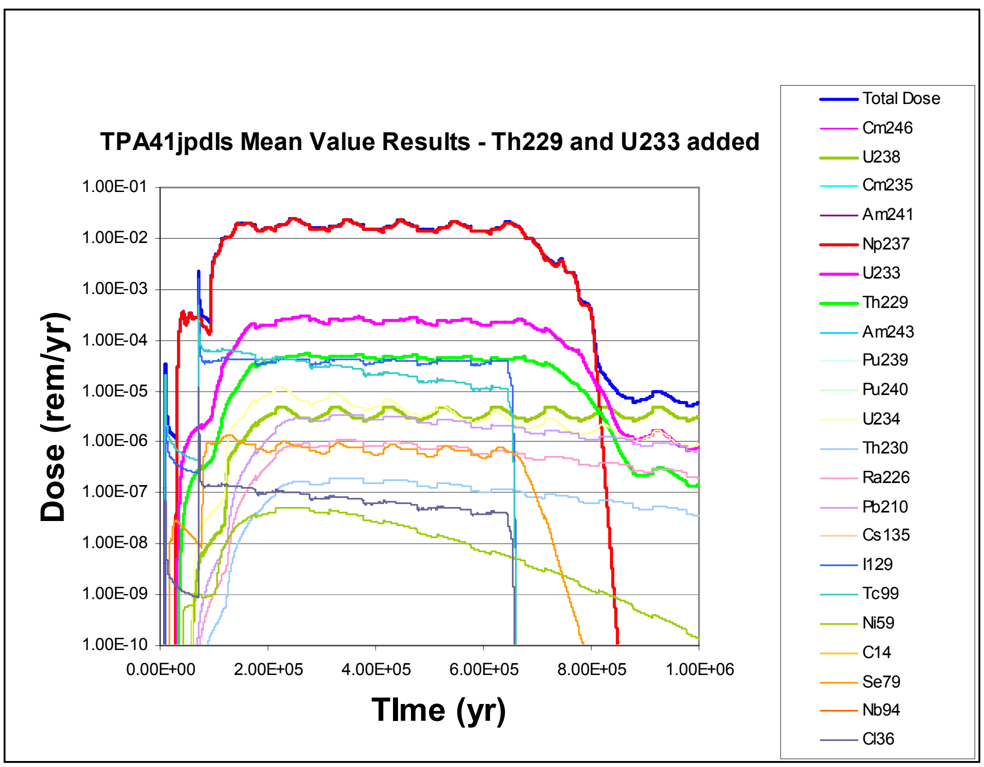


Figure 26.

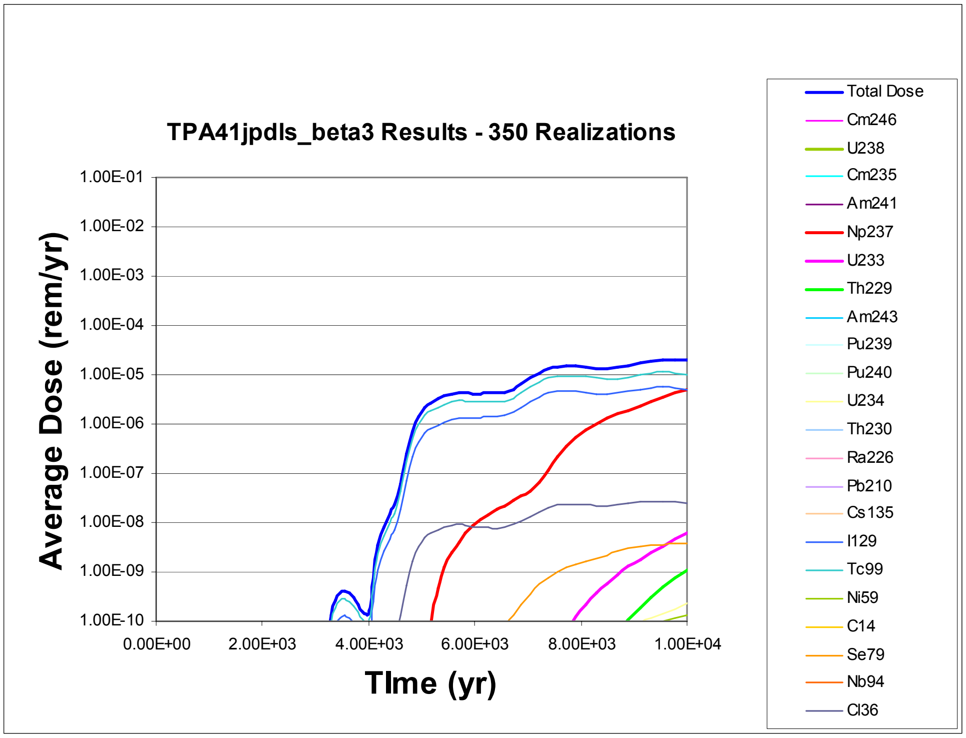


Figure 27.

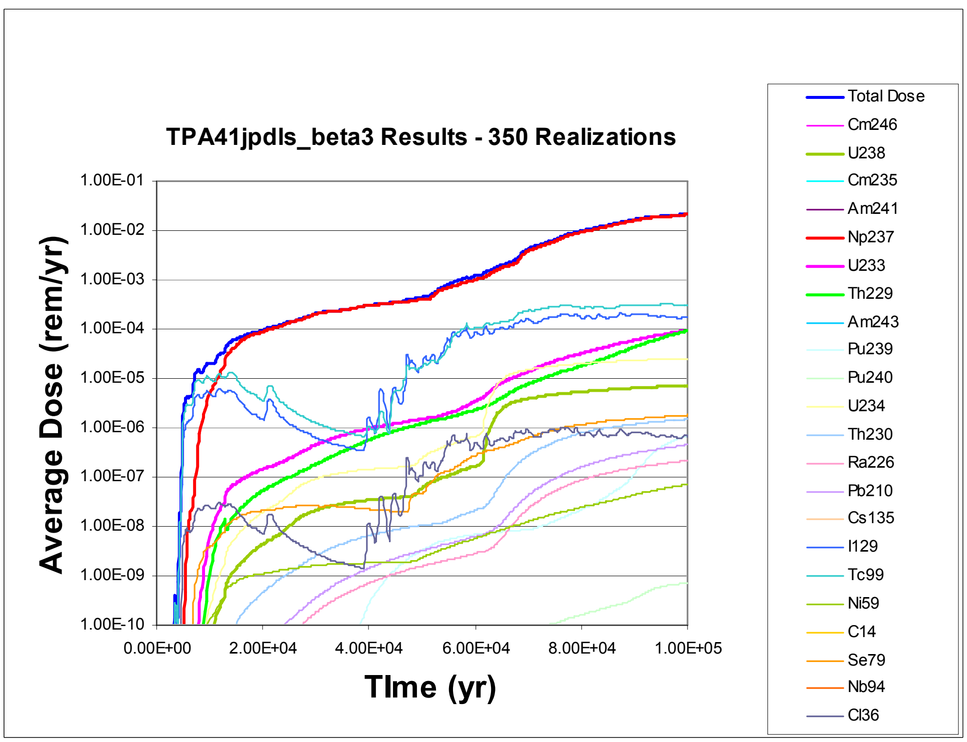


Figure 28.

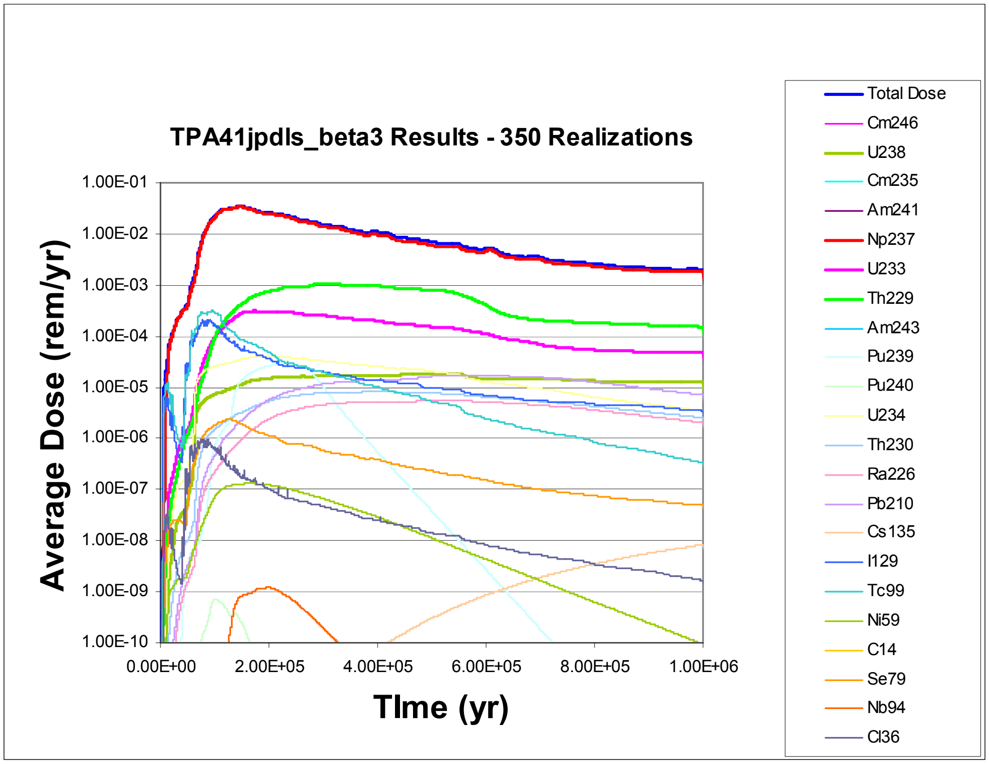

TPA41jpdls_beta3 Results - 350 Realizations
Average Dose (rem/yr)
1.00E-01
1.00E-02
1.00E-03
1.00E-04
1.00E-05
1.00E-06
1.00E-07
1.00E-08
1.00E-09
1.00E-10
0.00E+00
2.00E+05
4.00E+05
6.00E+05
8.00E+05
1.00E+06
TIme (yr)
Total Dose
Cm246
U238
Cm235
Am241
Np237
U233
Th229
Am243
Pu239
Pu240
U234
Th230
Ra226
Pb210
Cs135
I129
Tc99
Ni59
C14
Se79
Nb94
Cl36

Figure 29.

3/23/05 - Task is SCR-560 Testing. The initial SCR-560 states:

SOFTWARE CHANGE REPORT (SCR)

<table>
<tr><td>1. SCR No. (Software Developer Assigns):
PA-SCR-560</td><td>2. Software Title and Version:
TPA 5.0.0l</td><td>3. Project No:
20.06002.01.354</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td>5. Change Requested by:
S. Mohanty
Date: 2-23-05</td><td colspan="2">6. Change Authorized by (Software Developer):
R. Janetzke
Date: 2-23-05</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td>8. Implemented by:
R. Janetzke</td><td colspan="2">Date:
3-8-05</td></tr>
<tr><td colspan="3">9. Description of Acceptance Tests:</td></tr>
<tr><td>10. Tested by: R. Rice</td><td colspan="2">Date:</td></tr>
</table>

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Paramete r 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	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			

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.	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		

The following Test Plan was initially developed to this SCR.

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

Path for archive of results: \SCR560\tpa500m\SL-1 (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, repdes.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

5. Plot drift endpoints in *drifts.dat*, repository design endpoints in *repdes.dat*, and the subarea coordinates in the *tpa.inp* file
6. Use EXCEL spreadsheet to compute distance between drift endpoints and subarea boundary
7. Use EXCEL spreadsheet to compute number of WPs in each drift
8. Use EXCEL spreadsheet to compute the drift spacing from drift endpoints in *drifts.dat*
9. Use EXCEL spreadsheet to compute number of WPs in each subarea
10. Use EXCEL spreadsheet to compute drift angle

- Pass/Fail criteria: (For steps #1 - #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

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

Test Results: The EXCEL spreadsheet file (SCR560_repository_and_drift_coordinates_v002.xls) attached to this plan contains all test results. For all of these tests, the WORKSHEETS in the EXCEL file show results and that Pass/Fail Criteria listed above as passed.

- Overall test status: PASS

Test Results - The following information provides the PREVIOUS and NEW data for the repository design (*repdes.dat*) and the subarea coordinates (*tpa.inp*). Note that PREVIOUS contained 10 subareas, while NEW contains 7 subareas.

(PREVIOUS FILE) The *repdes.dat* file in the data subdirectory TPA Version 5.0.0l is listed below.

```
TITLE:  TPA 4.0 repository design and emplacement data.
**
** angle - radians
**
-.304d0
**
** rep outline vertices.
**
15
547732.82,4080960.00
548664.55,4080675.00
548588.98,4079377.55
548569.32,4078981.
548504.06,4077664.24
548479.71,4077173.06
548455.  ,4076674.51
548155.7 ,4075962.63
547897.79,4076045.46
547655.97,4076123.07
547474.7 ,4077281.6
547370.95,4077922.04
547514.88,4079310.61
547645.27,4079656.06
547732.82,4080960.00
**
** emplacement blocks
**
2
547514.88,   4079310.61, 548155.70,   4075962.63
547514.88,   4079310.61, 547732.82,   4081208.1
```

(NEW FILE) The *repdes.dat* file in the data subdirectory TPA Version 5.0.0m is listed below.

```
TITLE:  TPA 5.0.0 repository design and emplacement data.
**
** Number of repository panels
**
2
**
```

```
** Angle - radians
**
+0.304d0
**
** Panel outline vertices
**
10
547729., 4080943.
549744., 4081576.
549068., 4079690.
548606., 4079545.
548553., 4078770.
547456., 4078400.
547346., 4079145.
547390., 4080177.
547535., 4080512.
547729., 4080943.
**
** Emplacement blocks
**
1
547456., 4078400.,  549744., 4081576.
**
** Panel outline vertices
**
5
547803., 4078308.
548542., 4078549.
548430., 4076303.
547799., 4076093.
547803., 4078308.
**
** Emplacement blocks
**
1
548542., 4078549.,  547799., 4076093.
```

(PREVIOUS VALUES) The *tpa.inp* file subarea coordinates in TPA Version 5.0.0l are listed below for 10 subareas.

```
**
** Number and Location Of SubAreas[m] Based On EDA-II Design.
**
subarea
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
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
**

(NEW VALUES) The *tpa.inp* file subarea coordinates in TPA Version 5.0.0m are listed below for 7 subareas.

```
**
subarea
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.
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.
**

The following email from J. Winterle to R. Janetzke on March 8, 2005, contains updated repository subarea coordinates.

From: Ron Janetzke
To: rwrice
Cc:
Bcc:
Subject: [Fwd: TPA subareas]
Date: Thu, 24 Mar 2005 09:14:18 -0600

-------- Original Message -------- Subject: TPA subareas
Date: Tue, 08 Mar 2005 15:57:30 -0600
From: James Winterle <jwinterle@cnwra.swri.edu>
Reply-To: jwinterle@cnwra.swri.edu
Organization: CNWRA
To: 'Hans Arlt' <HDA@nrc.gov>
CC: Ronald Janetzke <rjanetzke@cnwra.swri.edu>

Hans,
There was a typographic error in the repository subarea text file I sent to you earlier. One of the points was off by 100 m. Can you delete that file and replace it with the attached one.

Jim Winterle
CNWRA
ph: 210-522-5249

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Ron Janetzke
PI, TPA Code Development
(210) 522-3318

NOTE: This file is preliminary data.

Subareas for TPA5.0 update (Coordinates in UTM, NAD-27 meters)

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

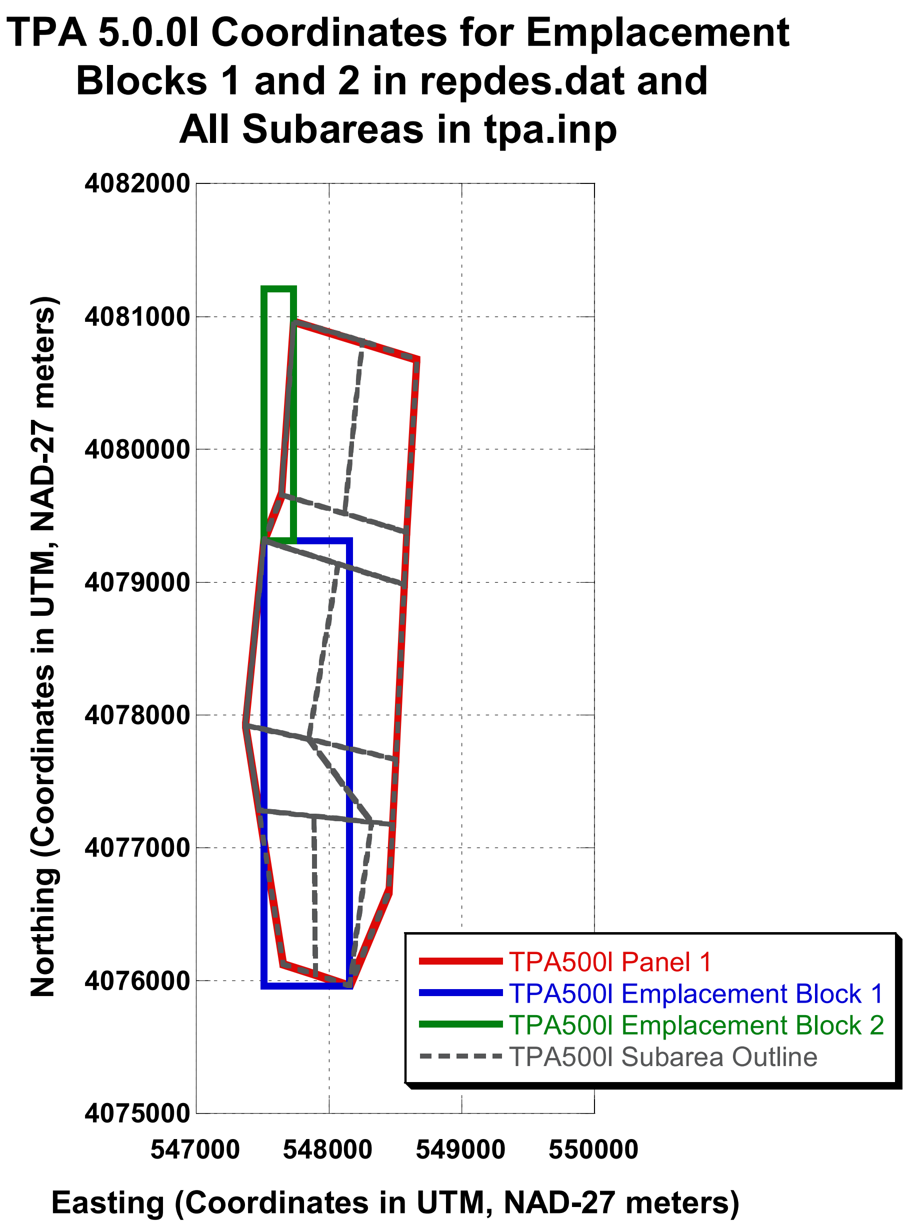
547803 4078308
548542 4078549
548523 4078132
547802 4077893
547803 4078308

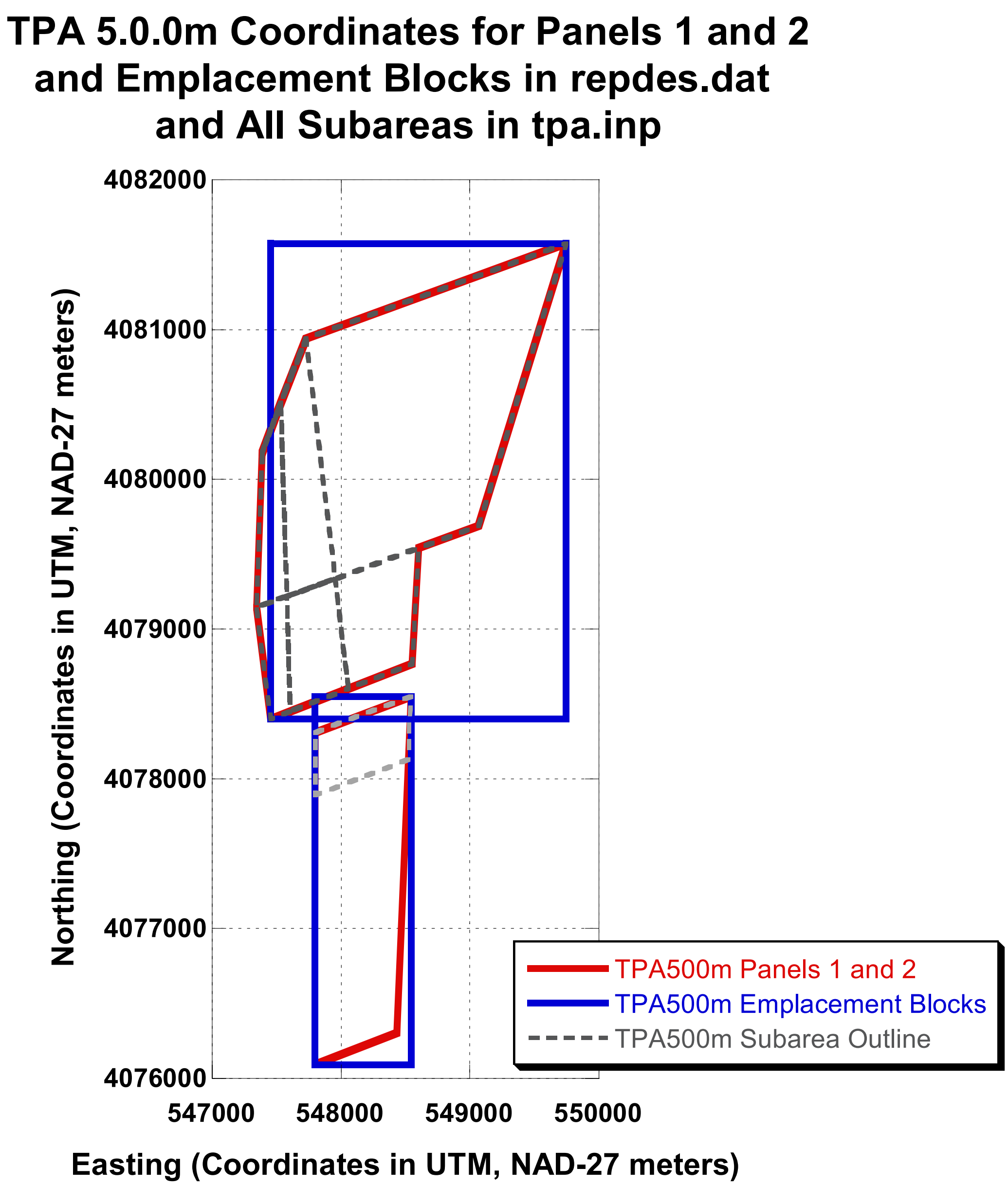
Subarea 8

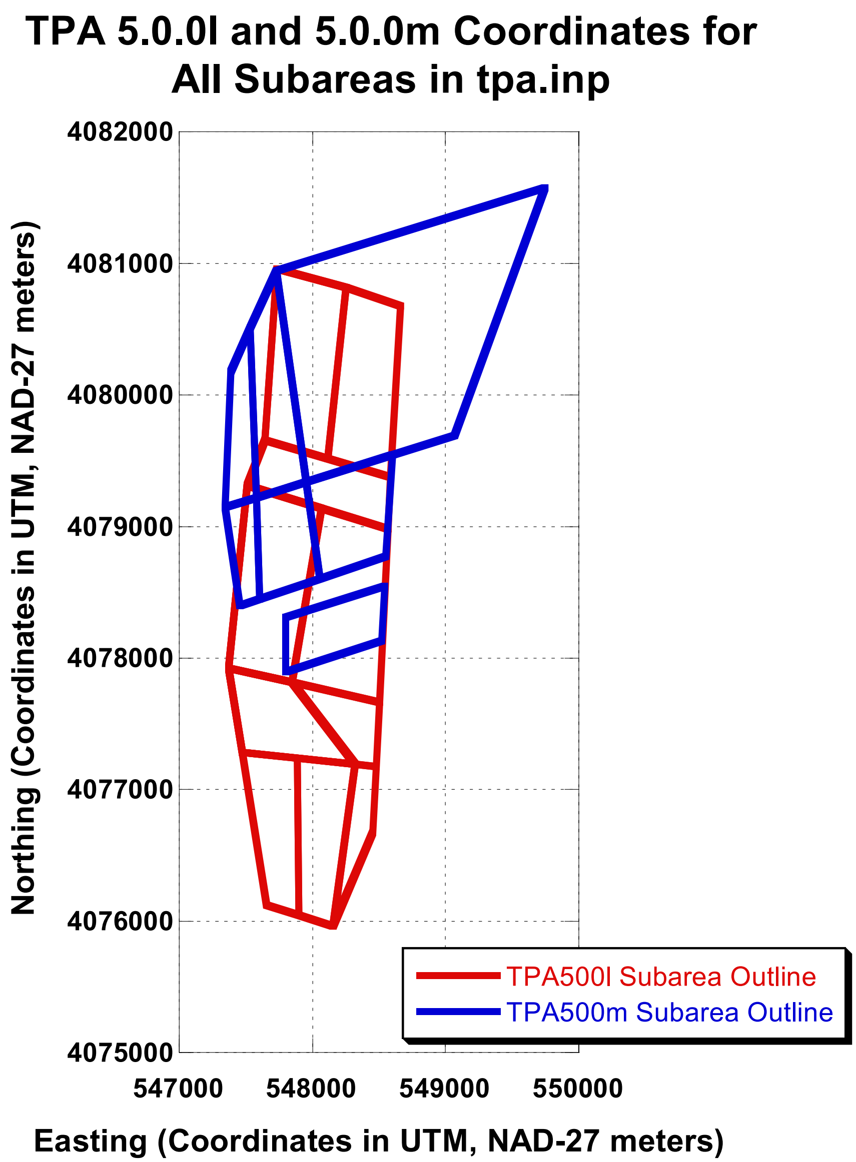
547802 4077893
548523 4078132
548430 4076303
547799 4076093
547802 4077893

In the EXCEL file SCR560_repository_and_drifts_coordinates.xls, the Workbook "Compare DOE and TPA500m" shows there are no differences between the above coordinates and the coordinates specified in the *tpa.inp* file.

Three plots are included below. In two plots, panel and emplacement block coordinates in the *repdes.dat* file and subarea coordinates in the *tpa.inp* file for TPA Version 5.0.0l and 5.0.0m codes were plotted and inspected. Additionally, one plot is provided with subarea coordinates from the *tpa.inp* file that shows the repository outline for the TPA Version 5.0.0l and 5.0.0m codes. Upon visual inspection, these plots are determined to be consistent with the expected repository outline, panels, and emplacement blocks. Detailed hand calculations using an EXCEL spreadsheet are performed to verify other parts of this test and are presented below.


TPA 5.0.0I Coordinates for Emplacement Blocks 1 and 2 in repdes.dat and All Subareas in tpa.inp
4082000
4081000
4080000
4079000
4078000
4077000
4076000
4075000
Northing (Coordinates in UTM, NAD-27 meters)
547000
548000
549000
550000
Easting (Coordinates in UTM, NAD-27 meters)
TPA500I Panel 1
TPA500I Emplacement Block 1
TPA500I Emplacement Block 2
TPA500I Subarea Outline


TPA 5.0.0m Coordinates for Panels 1 and 2
and Emplacement Blocks in repdes.dat
and All Subareas in tpa.inp
4082000
4081000
4080000
4079000
4078000
4077000
4076000
547000
548000
549000
550000
Northing (Coordinates in UTM, NAD-27 meters)
Easting (Coordinates in UTM, NAD-27 meters)
TPA500m Panels 1 and 2
TPA500m Emplacement Blocks
TPA500m Subarea Outline


TPA 5.0.0l and 5.0.0m Coordinates for
All Subareas in tpa.inp
4082000
4081000
4080000
4079000
4078000
4077000
4076000
4075000
Northing (Coordinates in UTM, NAD-27 meters)
547000
548000
549000
550000
Easting (Coordinates in UTM, NAD-27 meters)
TPA500l Subarea Outline
TPA500m Subarea Outline

Additionally, an email from J. Winterle to R. Janetzke on March 4, 2005, lists all coordinates of the repository outline (i.e., a rough outline), but also provides a smoothed outline. The text of this below is provided below, followed by a plot of the rough and smoothed repository outlines and the locations of the seven TPA 5.0.0m subarea.

From: Ron Janetzke
To: rwrice
Cc:
Bcc:
Subject: [Fwd: Repository footprint]
Date: Thu, 24 Mar 2005 09:26:18 -0600
Files:

-------- Original Message -------- Subject: Repository footprint
Date: Fri, 04 Mar 2005 14:44:19 -0600
From: James Winterle <jwinterle@cnwra.swri.edu>
Reply-To: jwinterle@cnwra.swri.edu
Organization: CNWRA
To: Ronald Janetzke <rjanetzke@cnwra.swri.edu>

Ron,
Per your request yesterday, I am sending you two outlines of the repository footprint. One file has the complete outline of the repository footprint, including the zigzaging top boundary. The other file has a footprint outline where I used a straight line across the top to eliminate the zigzaging; I tried to keep the total area about the same. In each of the files, the footprints are separated into top and bottom panel areas. If you want to see what these look like in map view compared to the design footprint, just stop by my office.

Jim Winterle
CNWRA
ph: 210-522-5249

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Ron Janetzke
PI, TPA Code Development
(210) 522-3318

Repository Footprint Coordinates

Outline points defining upper set of panels:

547759 4081013
548407 4081218
548448 4081316
549059 4081516

548902 4081130
549687 4081381
549706 4081272
549198 4080286
549070 4079710
548604 4079550
548596 4079429
548584 4079404
548552 4078773
548242 4078652
548051 4078611
547495 4078417
547433 4078487
547341 4079067
547389 4080173
547759 4081013

Outline points defining lower panel:

547803 4078308
548542 4078549
548434 4076368
548360 4076259
547902 4076106
547803 4076250
547803 4078308

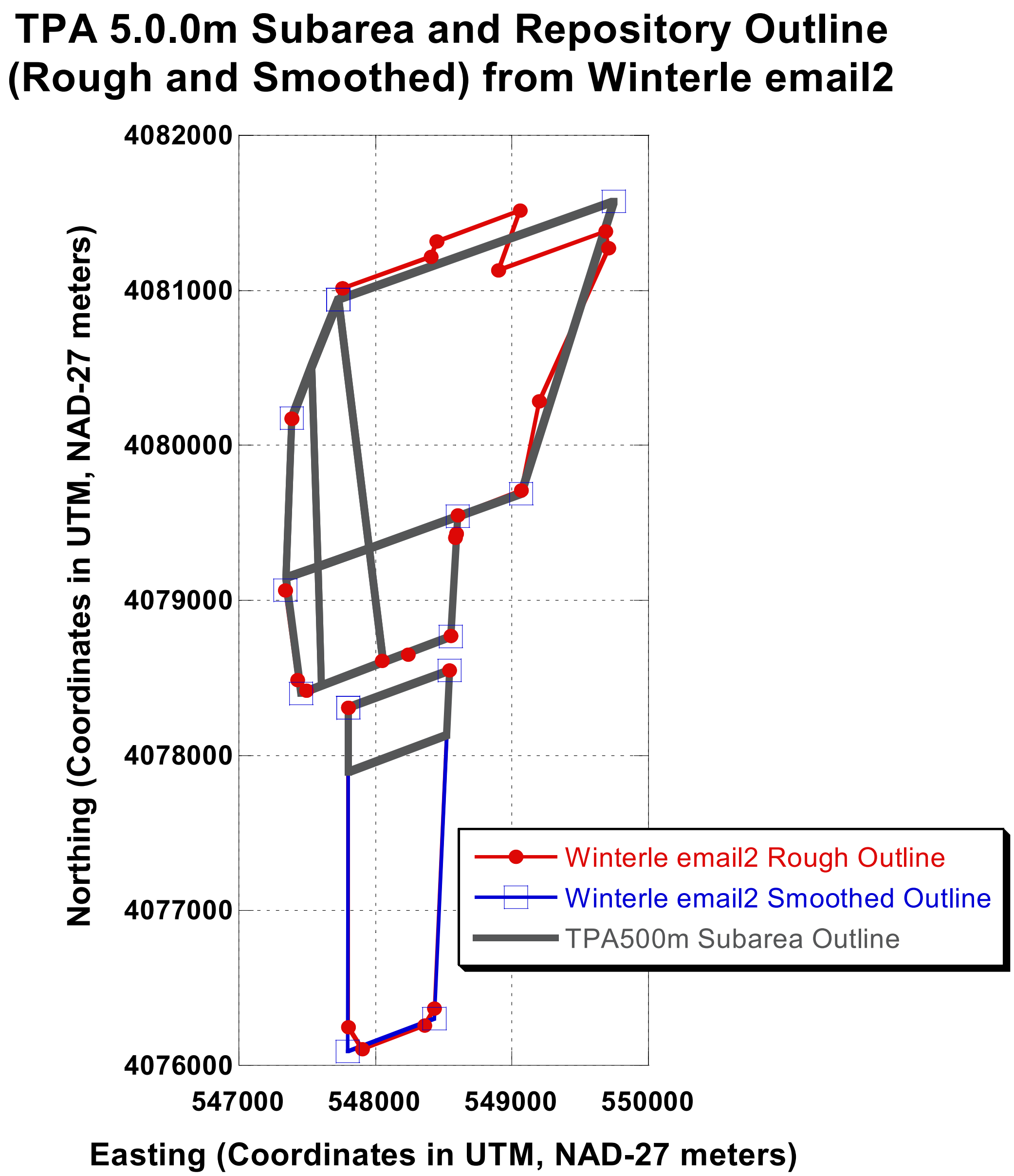
Rough repository footprint to minimize concave angles

Footprint of Upper Set of Panels

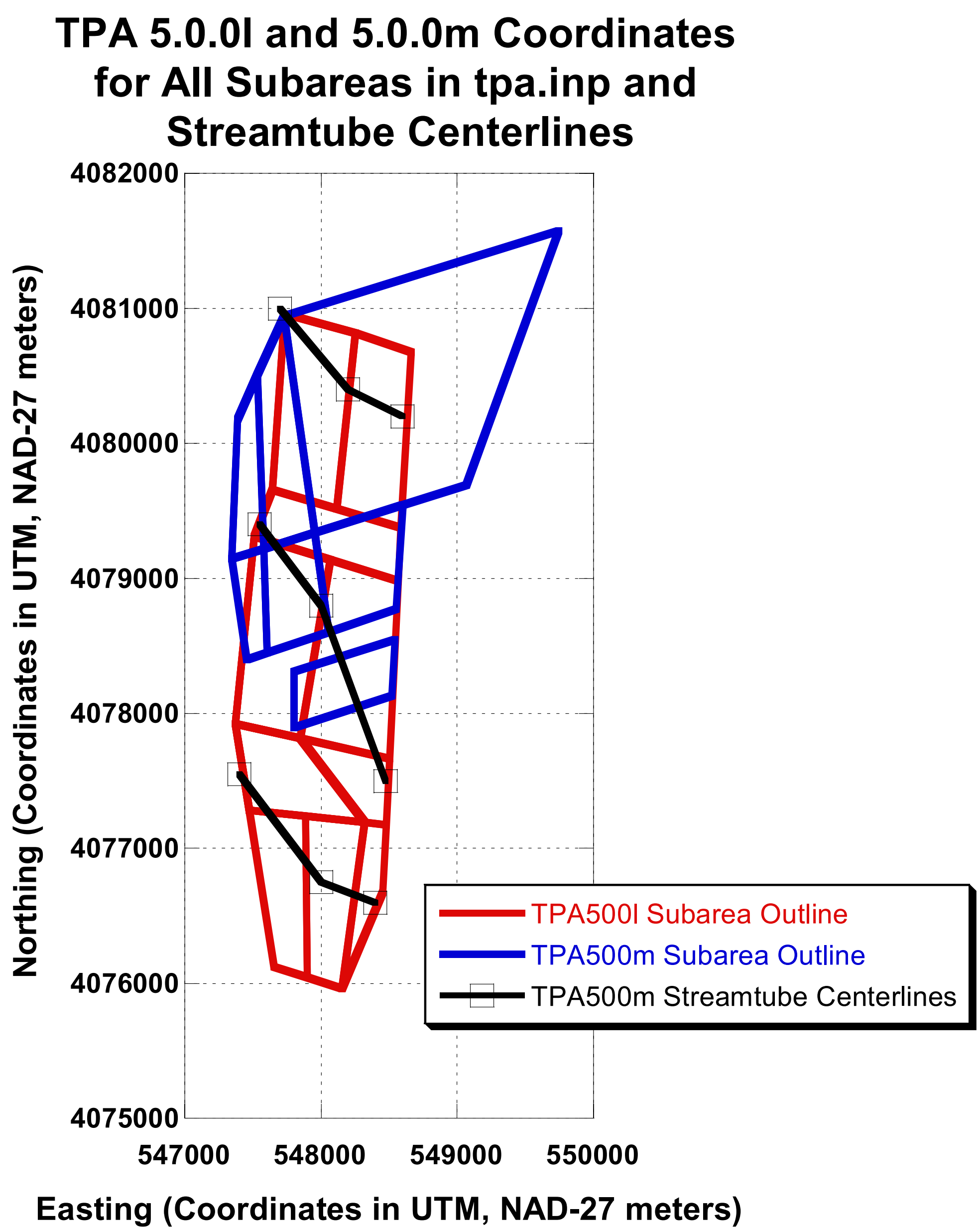
547729 4080943
549744 4081576
549068 4079690
548606 4079545
548553 4078770
547456 4078400
547341 4079067
547390 4080177
547729 4080943

Outline points defining lower panel:

547803 4078308
548542 4078549
548430 4076303
547799 4076093


TPA 5.0.0m Subarea and Repository Outline
(Rough and Smoothed) from Winterle email2
4082000
4081000
4080000
4079000
4078000
4077000
4076000
Northing (Coordinates in UTM, NAD-27 meters)
547000
548000
549000
550000
Easting (Coordinates in UTM, NAD-27 meters)
Winterle email2 Rough Outline
Winterle email2 Smoothed Outline
TPA500m Subarea Outline

Also, noted that because of the relatively large difference between the location of the subareas in the TPA Version 5.0.0l code compared with the TPA Version 5.0.0m code, it was noted that the streamtube information in *strmtube.dat* may need to be updated. A plot of subarea locations for TPA Version 5.0.0l and 5.0.0m codes with streamtube centerline locations was prepared and is presented below. From this figure, it is recommended that the information in *strmtube.dat* should be updated including streamtube centerline points and their corresponding widths and lengths, and comments in the file. Noted this to R. Janetzke, who stated this work was currently being done (3/24/05).

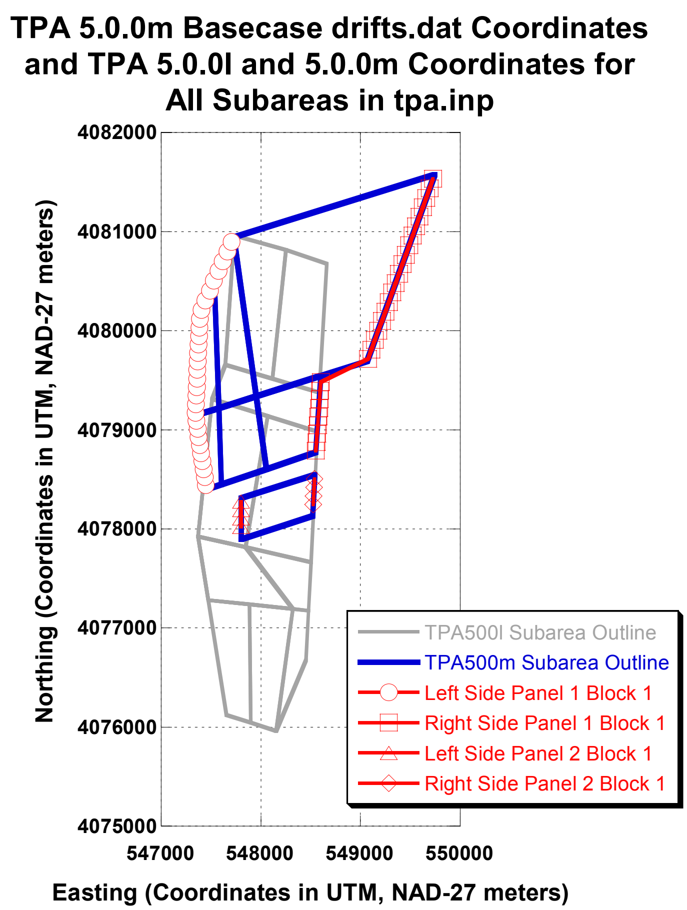

TPA 5.0.0l and 5.0.0m Coordinates for All Subareas in tpa.inp and Streamtube Centerlines
4082000
4081000
4080000
4079000
4078000
4077000
4076000
4075000
547000
548000
549000
550000
Northing (Coordinates in UTM, NAD-27 meters)
Easting (Coordinates in UTM, NAD-27 meters)
TPA500l Subarea Outline
TPA500m Subarea Outline
TPA500m Streamtube Centerlines

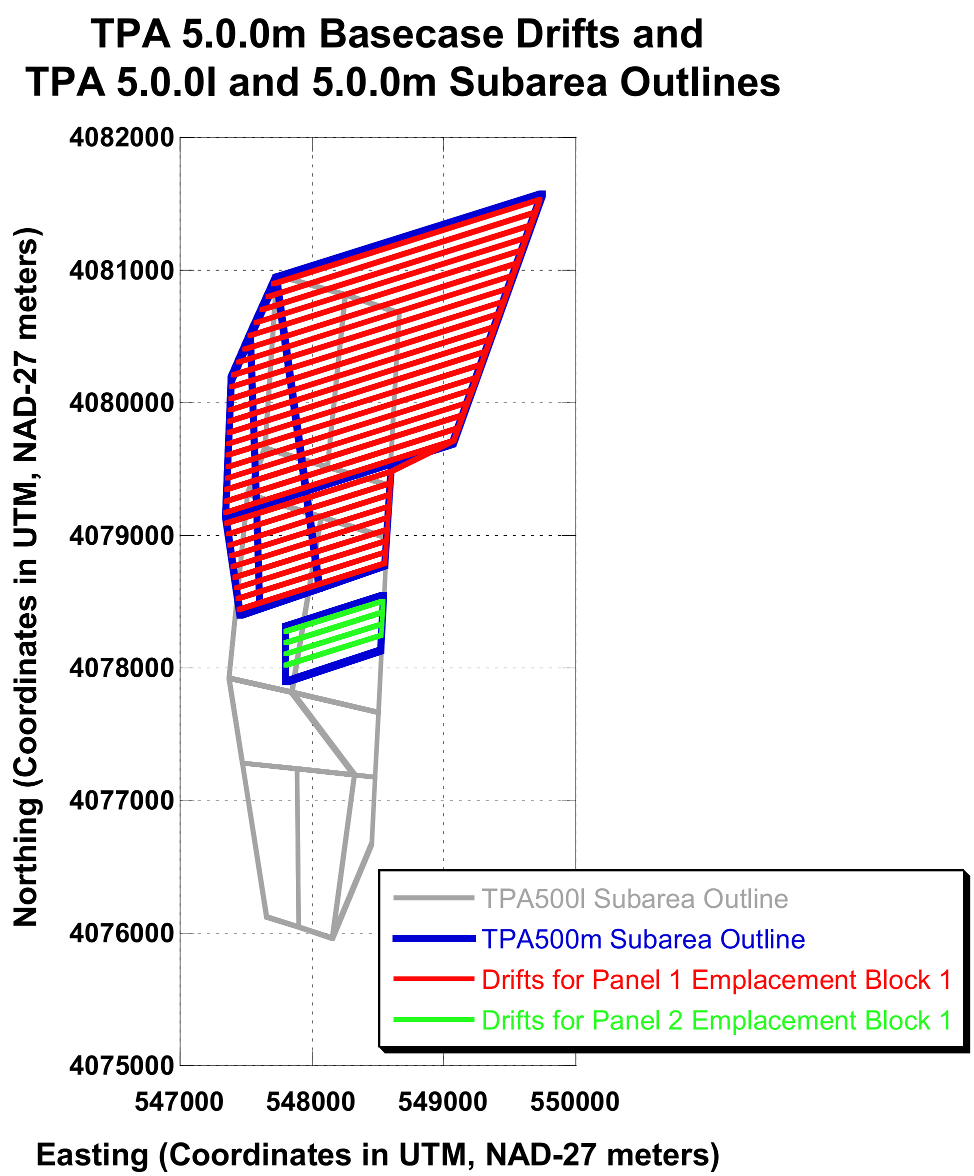
The contents of the *drifts.dat* file from a basecase TPA Version 5.0.0m code simulation is provided below.

```
TITLE:
**
**
Emplacement Block extracted from Panel
         1           1
**  Drift Endpoints
**   x1            y1            x2            y2        numWP
 5.48554160E+05 4.07878697E+06 5.47450010E+05 4.07844057E+06   188
 5.48560093E+05 4.07887372E+06 5.47438031E+05 4.07852170E+06   191
 5.48566026E+05 4.07896047E+06 5.47426051E+05 4.07860284E+06   194
 5.48571959E+05 4.07904723E+06 5.47414072E+05 4.07868397E+06   197
 5.48577892E+05 4.07913398E+06 5.47402092E+05 4.07876510E+06   200
 5.48583824E+05 4.07922074E+06 5.47390112E+05 4.07884624E+06   203
 5.48589757E+05 4.07930749E+06 5.47378133E+05 4.07892737E+06   206
 5.48595690E+05 4.07939424E+06 5.47366153E+05 4.07900851E+06   209
 5.48601623E+05 4.07948100E+06 5.47354174E+05 4.07908964E+06   212
 5.49076967E+05 4.07971502E+06 5.47347165E+05 4.07917234E+06   295
 5.49111250E+05 4.07981066E+06 5.47350834E+05 4.07925838E+06   300
 5.49145533E+05 4.07990631E+06 5.47354503E+05 4.07934442E+06   305
 5.49179816E+05 4.08000196E+06 5.47358171E+05 4.07943047E+06   310
 5.49214099E+05 4.08009761E+06 5.47361840E+05 4.07951651E+06   316
 5.49248383E+05 4.08019326E+06 5.47365508E+05 4.07960255E+06   321
 5.49282666E+05 4.08028891E+06 5.47369177E+05 4.07968860E+06   326
 5.49316949E+05 4.08038455E+06 5.47372845E+05 4.07977464E+06   331
 5.49351232E+05 4.08048020E+06 5.47376514E+05 4.07986068E+06   337
 5.49385515E+05 4.08057585E+06 5.47380182E+05 4.07994673E+06   342
 5.49419799E+05 4.08067150E+06 5.47383851E+05 4.08003277E+06   347
 5.49454082E+05 4.08076715E+06 5.47387519E+05 4.08011881E+06   352
 5.49488365E+05 4.08086279E+06 5.47403766E+05 4.08020880E+06   355
 5.49522648E+05 4.08095844E+06 5.47446284E+05 4.08030704E+06   354
 5.49556931E+05 4.08105409E+06 5.47488802E+05 4.08040527E+06   353
 5.49591215E+05 4.08114974E+06 5.47531320E+05 4.08050350E+06   351
 5.49625498E+05 4.08124539E+06 5.47575644E+05 4.08060230E+06   349
 5.49659781E+05 4.08134103E+06 5.47620139E+05 4.08070115E+06   348
 5.49694064E+05 4.08143668E+06 5.47664633E+05 4.08080000E+06   346
 5.49728347E+05 4.08153233E+06 5.47709128E+05 4.08089885E+06   344
**
Emplacement Block extracted from Panel
         2           2
**  Drift Endpoints
**   x1            y1            x2            y2        numWP
 5.48539850E+05 4.07850588E+06 5.47802940E+05 4.07827469E+06   125
 5.48535549E+05 4.07841964E+06 5.47802786E+05 4.07818975E+06   125
 5.48531249E+05 4.07833340E+06 5.47802633E+05 4.07810481E+06   124
 5.48526948E+05 4.07824715E+06 5.47802480E+05 4.07801987E+06    21
```

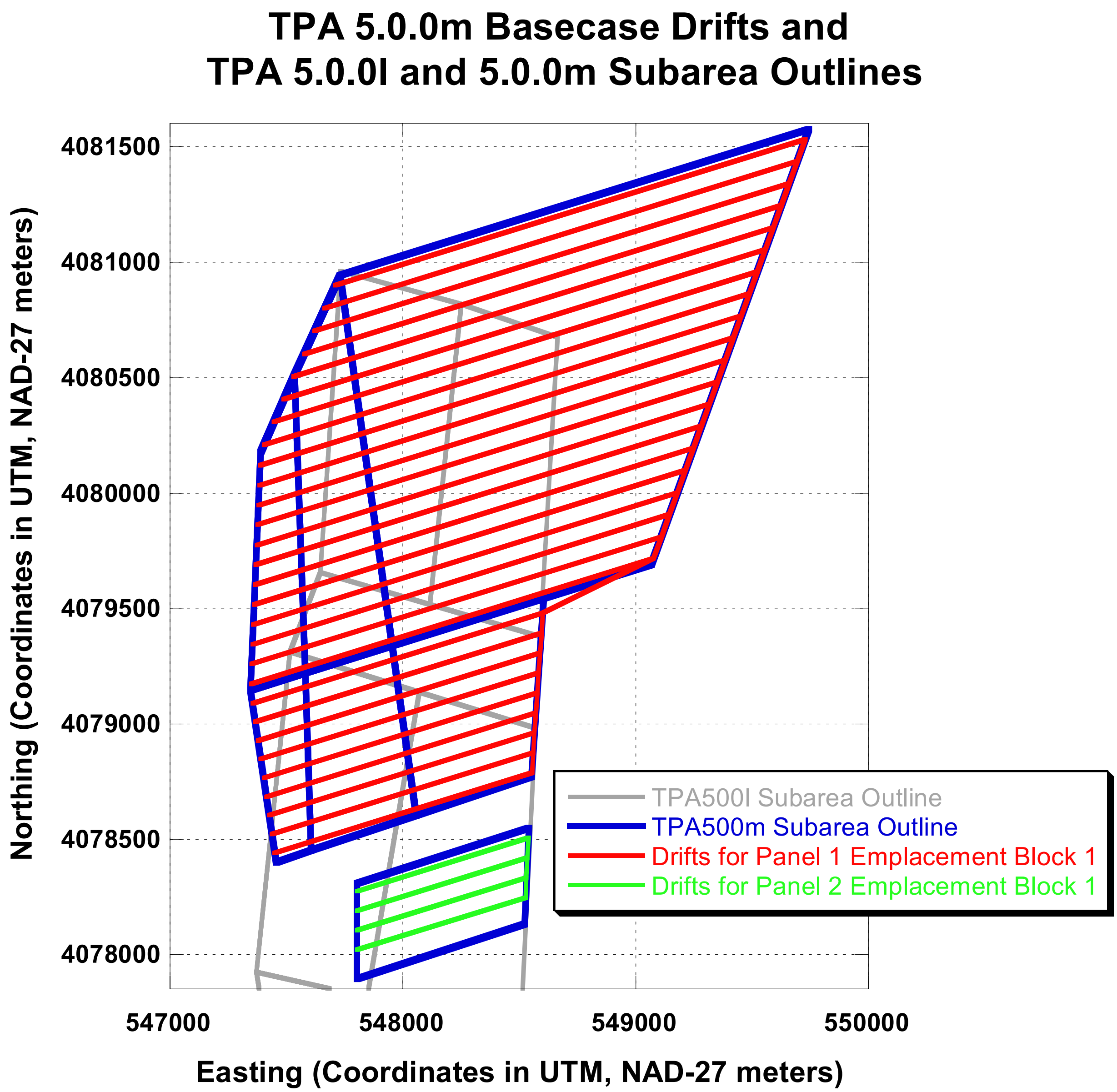
IT IS NOTED THAT THE *drift.dat* FILE DOES NOT APPEAR TO CORRECTLY PRINT THE EMPLACEMENT BLOCK NUMBER ASSOCIATED WITH THE PANEL NUMBER (i.e., probably should have Emplacement Block 1 for Panel 2). THIS DOES NOT APPEAR TO IMPACT TPA CODE CALCULATIONS, BUT IT IS MISLEADING AND IS NOTED HERE AND WILL BE PASSED ONTO TO R. JANETZKE. *AFTER CONSULTATION WITH R. JANETZKE, THE PRINTED INFORMATION IS CORRECT SINCE IT IS INTENDED TO SHOW THE CUMULATIVE EMPLACEMENT BLOCK NUMBER EVALUATED.*

By plotting the subarea coordinates and drift endpoints in *drifts.dat* for Emplacement Block 1 in Panels 1 and 2 below, it was verified that the drift endpoint coordinates in *drifts.dat* are consistent with expected locations. The plot with these coordinates is presented below. Continuing from the previous page, also plotted line segments that represent each drift in the *drifts.dat* file. Note that the right-hand side was made continuous to generate the plot.




TPA 5.0.0m Basecase Drifts and
TPA 5.0.0l and 5.0.0m Subarea Outlines
4082000
4081000
4080000
4079000
4078000
4077000
4076000
4075000
Northing (Coordinates in UTM, NAD-27 meters)
547000
548000
549000
550000
Easting (Coordinates in UTM, NAD-27 meters)
TPA500l Subarea Outline
TPA500m Subarea Outline
Drifts for Panel 1 Emplacement Block 1
Drifts for Panel 2 Emplacement Block 1

To better view the graph on the previous page, the repository region with drifts was plotted so that the drift endpoints and subarea boundaries could be highlighted. This graph is provided



below. (It is noted that Subarea 7 is not filled - this is addressed subsequently.)

From the basecase TPA Version 5.0.0m code simulation, the following information was captured.

```
==============================================================================
       exec: Welcome to TPA Version 5.0.0m
     Job started: Wed Mar 23 12:30:56 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 =      0 (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)
```

From the above screenprint and from the plot on the previous page, it was noted that Subarea 7 is not filled. After consultation with R. Janetzke, the following coordinates are recommended for Subarea 7. With these coordinates, Subarea 7 will be filled (which is consistent with Subareas 1 through 6) by moving the southern most Subarea 7 boundary northward. **The recommended new Subarea 7 coordinates, which were tested in a TPA code simulation, are provided below (the old coordinates are also listed):**

(NEW)

Subarea 7
547803., 4078308.

548542., 4078549.
548525., 4078215.
547802., 4077976.
547803., 4078308.

(OLD)

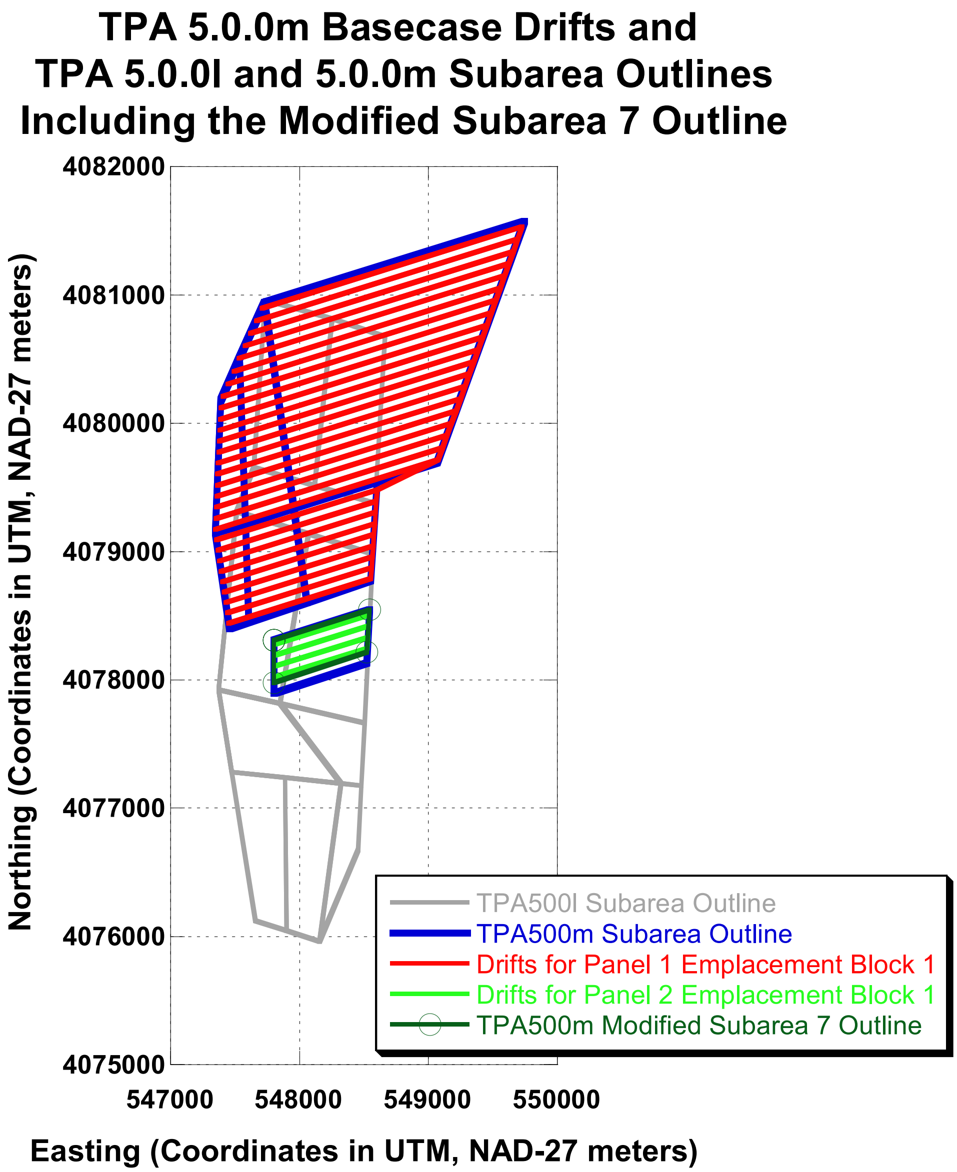
Subarea 7
547803., 4078308.
548542., 4078549.
548523., 4078132.
547802., 4077893.
547803., 4078308.

Using these new Subarea 7 coordinates, the screenprint becomes the following:

```
        ===========================================================================
      exec: Welcome to TPA Version 5.0.0m
     Job started: Thu Mar 31 15:16:03 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    241263.0    3116.5        395

Total Area [acre]        =  1096.186187299234
Total Buried Waste [MTU]  =  70039.53000000000
Repository AML [MTU/acre] =  63.89382644253370

Specified Global Parameters:

           Compliance Period =  10000.0 (yr)
       Maximum Simulation Time =  10000.0 (yr)
        Number Of Realizations =      1
           Number Of Subareas =      7
           Volcanism scenario =      0 (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)
```

Note that the number of WPs are not changed (there is 7,0040 MTUs with 7.89 MTUs/WP). However, the area of Subarea 7 decreases from 301280.0 to 241263.0 m^2, the Repository AML (MTU/acre) increases from 63.04096281984062 to 63.89382644253370, and the Total Area decreases from 1111.016184828268 to 1096.186187299234. These changes (and other information that is not changed) are expected given the decrease in the area of Subarea 7.

Additionally, the following figure shows the outline of the new Subarea 7, together with information presented on plots presented previously. (Note that Subarea 7 is now filled.)


TPA 5.0.0m Basecase Drifts and
TPA 5.0.0l and 5.0.0m Subarea Outlines
Including the Modified Subarea 7 Outline
Northing (Coordinates in UTM, NAD-27 meters)
4082000
4081000
4080000
4079000
4078000
4077000
4076000
4075000
547000
548000
549000
550000
Easting (Coordinates in UTM, NAD-27 meters)
TPA500l Subarea Outline
TPA500m Subarea Outline
Drifts for Panel 1 Emplacement Block 1
Drifts for Panel 2 Emplacement Block 1
TPA500m Modified Subarea 7 Outline

FOR A BASECASE TPA CODE SIMULATION, EXAMINATION OF EBSREL.ECH SHOWS THE NUMBER OF EXTRUSIVE WPS IS 1.2427E6 IN EACH LISTING FOR A SUBAREA. IN EXEC.F, RECOMMEND MOVING LINE #4091 ("nwpexhumed = 0") TO LINE #4057 (FOR EXAMPLE), SO THAT THIS VARIABLE WILL BE INITIALIZED.

As part of conducting SCR560 testing, the following test plan was initially developed to assess the correction of AshBulkDensity[g/cm3] parameter name. The results from the testing are presented after the test plan.

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\tpa500m\SL-2'basecase (archived on CD)
\SCR560\tpa500m\SL-2'basecase (archived on CD)

Environment variables: TPA_DATA=c:\SCR560\tpa500m
TPA_DATA=c:\SCR560\tpa500m

TPA_DATA=c:\SCR560\tpa500l
TPA_DATA=c:\SCR560\tpa500l

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:

1. 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.
2. Examine the screenprint (*tpa.out*) to verify the problem in the AshBulkDensity[g/cm3] name in Version 5.0.0l
3. 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 successful 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 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 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: PASS

4/8/05 The following provides results from testing SCR-560. Note that one test is passed and two tests fail.

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:

11. Plot drift endpoints in *drifts.dat*, repository design endpoints in *repdes.dat*, and the subarea coordinates in the *tpa.inp* file
12. Use EXCEL spreadsheet to compute distance between drift endpoints and subarea boundary
13. Use EXCEL spreadsheet to compute number of WPs in each drift
14. Use EXCEL spreadsheet to compute the drift spacing from drift endpoints in *drifts.dat*
15. Use EXCEL spreadsheet to compute number of WPs in each subarea
16. 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

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: FAIL (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 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 =      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 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 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 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 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 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 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: <u>FAIL</u> (SCR #570 addresses this test failure)

The final SCR, which contains test results, follows.

SOFTWARE CHANGE REPORT (SCR)

<table>
<tr><td>1. SCR No. (Software Developer Assigns):
PA-SCR-560</td><td>2. Software Title and Version:
TPA 5.0.0l</td><td>3. Project No:
20.06002.01.354</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td>5. Change Requested by:
S. Mohanty
Date: 2-23-05</td><td colspan="2">6. Change Authorized by (Software Developer):
R. Janetzke
Date: 2-23-05</td></tr>
<tr><td colspan="3">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.</td></tr>
</table>

8. Implemented by: R. Janetzke	**Date:** 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

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Paramete r 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	N/A		

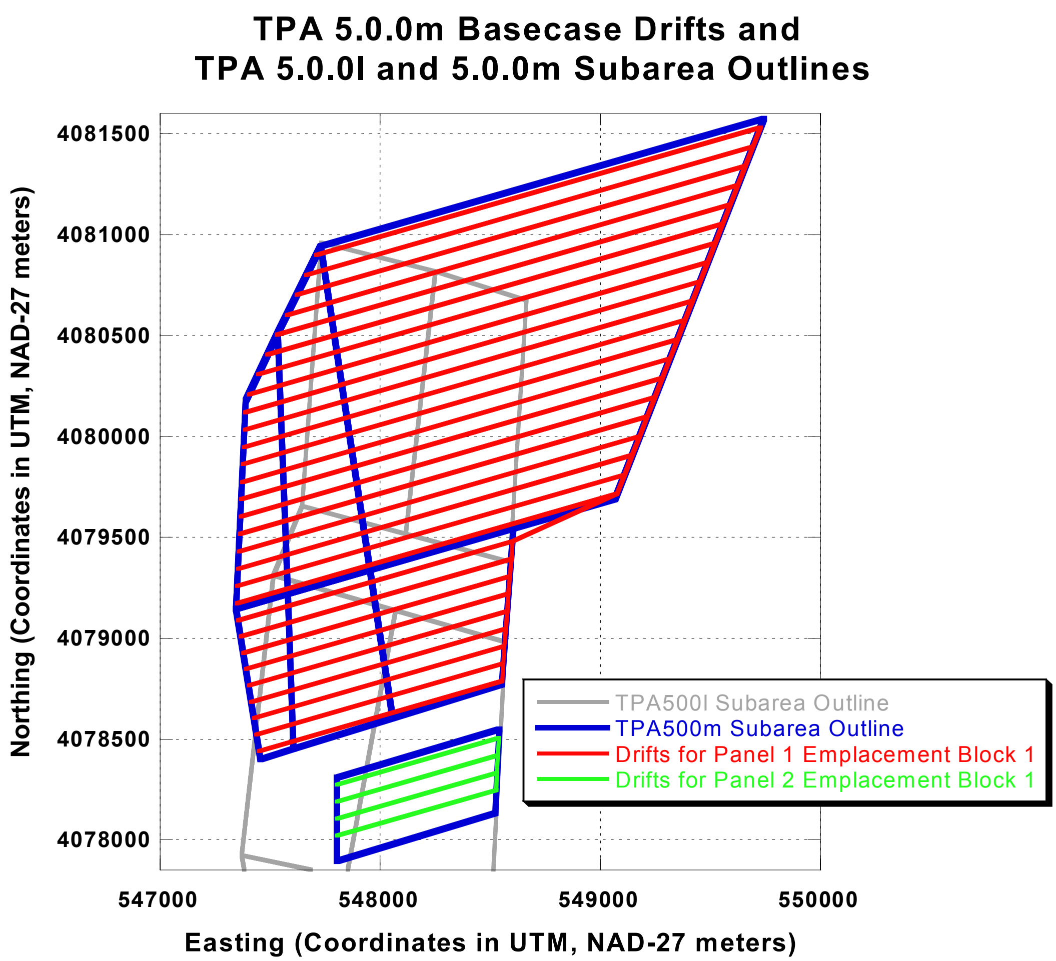
				edaii 6-cw 547887.3,4077238.1 548322.7,4077192.2 548155.7,4075962.63 547897.79,4076045.46 547887.3,4077238.1 edaii 7-cw 548322.7,4077192.2 548479.71,4077173.06 548455,4076674.51 548155.7,4075962.63 548322.7,4077192.2 edaii 8-cw 547645.27,4079656.06 548588.98,4079377.55 548569.32,4078981 547514.88,4079310.61 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			

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.	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	SubareaOfVolcanicEvent[]	Subarea in which the conduit is considered.	Iuniform	1, 10		
Modify To	Volcano	SubareaOfVolcanicEvent[]	Subarea in which the conduit is considered.	Iuniform	1, 7		

4/18/05 From the testing activity reported earlier in this notebook for SCR #560, the following information was emailed to R. Janetzke to recommend changes to the *tpa.inp* (subarea 7 coordinates) and exec.f (involving initializing the number of exhumed WPs) files.

To better view the graph on the previous page, the repository region with drifts was plotted so that the drift endpoints and subarea boundaries could be highlighted. This graph is provided below. (It is noted that Subarea 7 is not filled - this is addressed subsequently.)



From the basecase TPA Version 5.0.0m code simulation, the following information was captured.

```
==========================================================================
        exec: Welcome to TPA Version 5.0.0m
      Job started: Wed Mar 23 12:30:56 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 =      0 (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)
```

From the above screenprint and from the plot on the previous page, it was noted that Subarea 7 is not filled. After consultation with R. Janetzke, the following coordinates are recommended for Subarea 7. With these coordinates, Subarea 7 will be filled (which is consistent with Subareas 1 through 6) by moving the southern most Subarea 7 boundary northward. **The recommended new Subarea 7 coordinates, which were tested in a TPA code simulation, are provided below (the old coordinates are also listed):**

(NEW)

Subarea 7
547803., 4078308.
548542., 4078549.
548525., 4078215.
547802., 4077976.

547803., 4078308.

(OLD)

Subarea 7
547803., 4078308.
548542., 4078549.
548523., 4078132.
547802., 4077893.
547803., 4078308.

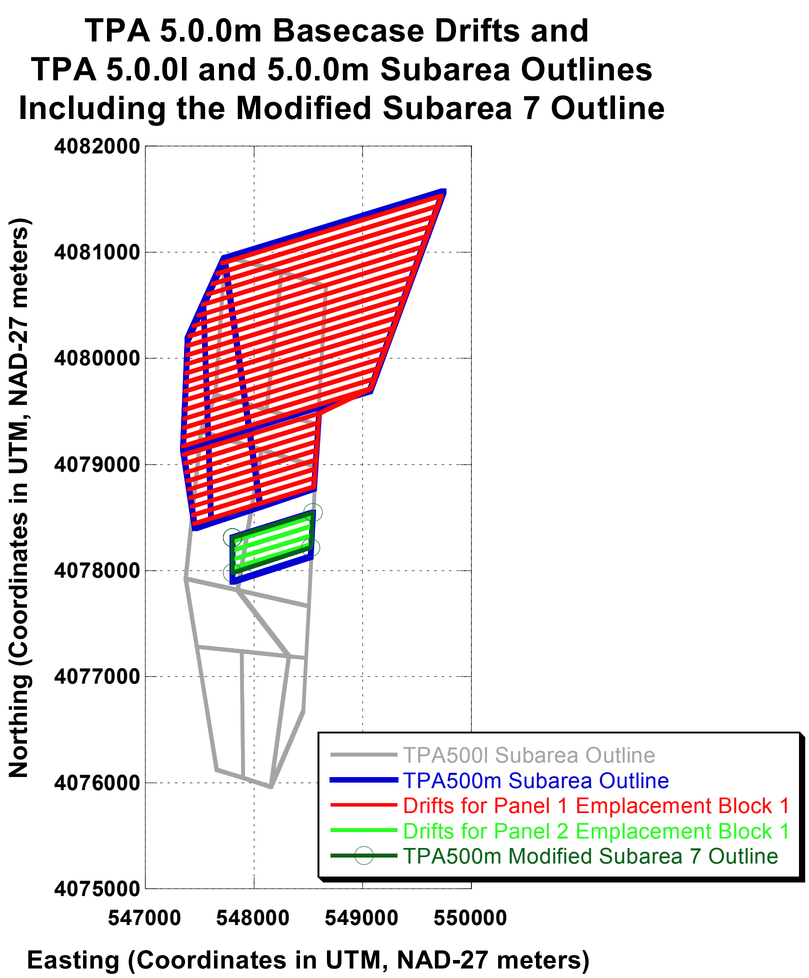
Using these new Subarea 7 coordinates, the screenprint becomes the following:

```
    ===========================================================================
       exec: Welcome to TPA Version 5.0.0m
      Job started: Thu Mar 31 15:16:03 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    241263.0    3116.5       395

Total Area [acre]        =  1096.186187299234
Total Buried Waste [MTU]  =  70039.53000000000
Repository AML [MTU/acre] =  63.89382644253370

Specified Global Parameters:

          Compliance Period =  10000.0 (yr)
      Maximum Simulation Time =  10000.0 (yr)
       Number Of Realizations =      1
          Number Of Subareas =      7
          Volcanism scenario =      0 (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)
```

Note that the number of WPs are not changed (there is 7,0040 MTUs with 7.89 MTUs/WP). However, the area of Subarea 7 decreases from 301280.0 to 241263.0 m^2, the Repository AML (MTU/acre) increases from 63.04096281984062 to 63.89382644253370, and the Total Area decreases from 1111.016184828268 to 1096.186187299234. These changes (and other information that is not changed) are expected given the decrease in the area of Subarea 7.

Additionally, the following figure shows the outline of the new Subarea 7, together with information presented on plots presented previously. (Note that Subarea 7 is now filled.)

FOR A BASECASE TPA CODE SIMULATION, EXAMINATION OF EBSREL.ECH SHOWS THE NUMBER OF EXTRUSIVE WPS IS 1.2427E6 IN EACH LISTING FOR A SUBAREA. IN EXEC.F, RECOMMEND MOVING LINE #4091 ("nwpexhumed = 0") TO LINE #4057 (FOR EXAMPLE), SO THAT THIS VARIABLE WILL BE INITIALIZED.



Also, noted the following during compiling and sent these recommendations onto to R. Janetzke on 4/19/05 as suggested changes to avoid these compile warnings

```
Note 1:
*******
in invent.f (lines 1615 and 1616)
     double precision yearofburnupdata
     double precision yearofemplacement

these are already defined in inventi.i
(suggest deleting these two lines from invent.f)


Note 2:
*******
suggest defining "aseed1" using the following
somewhere around line 1712 in sampler.f

     double precision aseed1
```

Additionally, noted that it is recommended that the variable "maxseismicevents" in the *seisadj.i* file be increased from 7100 to 10000 (for example) since during 1,000,000 years simulations this maximum is being exceeded and TPA code execution is stopped. The contents of the *seisadj.i* file is listed below for the TPA Version 5.0.0o code.

```
c      seisadj.i
c      Include file for exec and mechfail to define the maximum number of
c      seismic events.
c
c      GADAMS PA-SCR-415 11-12-02: File added as part of this SCR to eliminate
c      automatic arrays from the TPA code.
c
      INTEGER maxseismicevents
cc rwr 2-4-05; SCR 530
cc modified for long TPA simulations
cc     PARAMETER (maxseismicevents = 1500)
      PARAMETER (maxseismicevents = 7100)
```

Note: this recommendation was presented to R. Janetzke.

As part of preliminary work associated with SCR569 intended to identify changes needed to remove calculation for dry oxidation from the TPA Version 5.0.0o code, modified source code and tested those changes. The 4 modified files were: *failt.f*, *ebsfail.f*, *tpa.inp*, and *tpanames.dbs*. The file comparison ("fc") for each of these 4 modified files follow.

For *failt.f*:

```
Comparing files failt.f and FAILT.F.ORIGINAL
***** failt.f
          tyears = tstop - tstart

cc rwr 4-15-05  SCR569 - do not call -
cc              modified since corrosion by dry oxidation is neglігle
cc            call dryoxdwp(i, tyears, temp2, grainr, nseries, gbthick,
cc     &                   constant1, pntd)
cc            pnt = pnt + pntd
          pntd = 0.0

          pnt = pnt + pntd
***** FAILT.F.ORIGINAL
          tyears = tstop - tstart
          call dryoxdwp(i, tyears, temp2, grainr, nseries, gbthick,
     &                   constant1, pntd)
          pnt = pnt + pntd
*****

***** failt.f
c          Dry air oxidation
cc rwr 4-15-05  SCR569 - there is no dry oxidation -
cc              modified since corrosion by dry oxidation is negligle
cc            mode = 'dry oxd'
          mode = 'dry air'
          ecrit = 0.0D0
***** FAILT.F.ORIGINAL
c          Dry air oxidation
          mode = 'dry oxd'
          ecrit = 0.0D0
*****

***** failt.f

cc rwr 4-15-05  SCR569 - there is no dry oxidation -
cc              modified since corrosion by dry oxidation is negligle
cc         write (*, '(a42,1pe15.3)') 'penetration by dry oxidation [m]:',
cc     &         pntf
        write (*, '(a42,1pe15.3)')
     &         'penetration by humid air oxidation [m]:',pntf
        write (*, '(a42,6x,a)') 'echoed input data in:', 'echo_fail.dat'
***** FAILT.F.ORIGINAL

        write (*, '(a42,1pe15.3)') 'penetration by dry oxidation [m]:',
     &         pntf
        write (*, '(a42,6x,a)') 'echoed input data in:', 'echo_fail.dat'
*****

***** failt.f
```

```
cc rwr 4-15-05  SCR569 - subroutine not called -
cc            modified since corrosion by dry oxidation is negligle
cc c==========================================================================
cc        subroutine dryoxdwp(ipr, tyears, tempc, grainr, nseries,
cc     &                    gbthick, constant1, penetd)
cc c==========================================================================
cc c      Purpose: Calculates the corrosion penetration depth
cc c               returned in the last argument.
cc c
cc c--------------------------------------------------------------------
cc c      nomenclature:
cc c      pi:           the constant pi
cc c      tempc:        temperature in celcius
cc c      temp1:        tempc in kelvin
cc c      dfsvtym:      matrix diffusivity
cc c      dfsvtygb      grain boundary diffusivity
cc c      constant1:    a constant relating matrix and grain  boundary
cc c                    oxygen diffusivity in metal
cc c      grainr:       grain radius [micrometer]
cc c      gbthick:      grain bundary thickness [micrometer]
cc c      tyears:       time in years
cc c      thour:        tyears in hours
cc c      nseries:      number if terms in infinite series for wp oxidation
cc c                    boundary diffusivities
cc c--------------------------------------------------------------------
cc c      note:
cc c      dg:    dm/constant1
cc c      rgas1:  universal gas constant
cc c            = 1.987 (cal)/(g mol)(k)
cc c            = 4.184e-3*1.987 (kj)/(g mol)(k)
cc c
cc
c==========================================================================
=
cc        implicit none
cc
cc        DOUBLE PRECISION constant1, ddd1, ddd2, dfsvtygb, dfsvtym,
cc     &        gbthick,grainr, penetd, pi, rgas1, sum, temp1, tempc,
cc     &        timehr, tyears, xxx1
cc        integer ipr, nnn, nseries
cc
cc        pi = 4.*atan(1.)
cc        rgas1 = 1.987
cc
cc        temp1 = 273. + tempc
cc        xxx1 = 169./(4.184e-3*rgas1*temp1)
cc
cc        if ( xxx1.gt.65. ) then
cc          xxx1 = 65.
cc        end if
```

```
cc
cc        dfsvtym = 575.e-6 * exp( - xxx1)
cc        dfsvtym = dfsvtym * 1.e12 * 60 * 60
cc        dfsvtygb = dfsvtym / constant1
cc        ddd1 = 4. * dfsvtym / (grainr * gbthick * dfsvtygb)
cc
cc        timehr = tyears * 365. * 24.
cc        sum = 0.
cc
cc        do 100 nnn = 1, nseries
cc          ddd2 = dfsvtym * nnn**2 * pi**2 * timehr / grainr**2
cc          if ( ddd2.gt.65. ) then
cc            ddd2 = 65.
cc          end if
cc          sum = sum + exp( - ddd2)
cc
cc   100   continue
cc
cc        penetd = 1. / sqrt(ddd1 * sum)
cc
cc c       convert from micrometer to meter:
cc
cc        penetd = penetd / 1.e6
cc
cc        return
cc        end
```

***** FAILT.F.ORIGINAL

```
c=====================================================================
      subroutine dryoxdwp(ipr, tyears, tempc, grainr, nseries,
    &                    gbthick, constant1, penetd)
c=====================================================================
c      Purpose: Calculates the corrosion penetration depth
c               returned in the last argument.
c
c-------------------------------------------------------------------
c      nomenclature:
c      pi:            the constant pi
c      tempc:         temperature in celcius
c      temp1:         tempc in kelvin
c      dfsvtym:       matrix diffusivity
c      dfsvtygb       grain boundary diffusivity
c      constant1:     a constant relating matrix and grain  boundary
c                     oxygen diffusivity in metal
c      grainr:        grain radius [micrometer]
c      gbthick:       grain bundary thickness [micrometer]
c      tyears:        time in years
c      thour:         tyears in hours
c      nseries:       number if terms in infinite series for wp oxidation
```

```
c                   boundary diffusivities
c--------------------------------------------------------------------
c      note:
c      dg:     dm/constant1
c      rgas1:  universal gas constant
c              = 1.987 (cal)/(g mol)(k)
c              = 4.184e-3*1.987 (kj)/(g mol)(k)
c
c==============================================================================
=
       implicit none

       DOUBLE PRECISION constant1, ddd1, ddd2, dfsvtygb, dfsvtym,
     &        gbthick,grainr, penetd, pi, rgas1, sum, temp1, tempc,
     &        timehr, tyears, xxx1
       integer ipr, nnn, nseries

       pi = 4.*atan(1.)
       rgas1 = 1.987

       temp1 = 273. + tempc
       xxx1 = 169./(4.184e-3*rgas1*temp1)

       if ( xxx1.gt.65. ) then
         xxx1 = 65.
       end if

       dfsvtym = 575.e-6 * exp( - xxx1)
       dfsvtym = dfsvtym * 1.e12 * 60 * 60
       dfsvtygb = dfsvtym / constant1
       ddd1 = 4. * dfsvtym / (grainr * gbthick * dfsvtygb)

       timehr = tyears * 365. * 24.
       sum = 0.

       do 100 nnn = 1, nseries
         ddd2 = dfsvtym * nnn**2 * pi**2 * timehr / grainr**2
         if ( ddd2.gt.65. ) then
           ddd2 = 65.
         end if
         sum = sum + exp( - ddd2)

  100  continue

       penetd = 1. / sqrt(ddd1 * sum)

c      convert from micrometer to meter:

       penetd = penetd / 1.e6
```

```
      return
      end

*****
```

For *ebsfail.f*:

```
Comparing files ebsfail.f and EBSFAIL.F.ORIGINAL
***** ebsfail.f
c    command       =

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc            modified since corrosion by dry oxidation is negligle
cc c    constant1      =

c    corrpar1      = common
***** EBSFAIL.F.ORIGINAL
c    command       =
c    constant1      =
c    corrpar1      = common
*****

***** ebsfail.f
c    garb          =

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc            modified since corrosion by dry oxidation is negligle
cc c    gbthick        =

c    ghy1          =
c    ghy2          =
***** EBSFAIL.F.ORIGINAL
c    garb          =
c    gbthick        =
c    ghy1          =
c    ghy2          =
*****

***** ebsfail.f
c    gox2          =

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc            modified since corrosion by dry oxidation is negligle
cc c    grainr         =

c    humd          =
***** EBSFAIL.F.ORIGINAL
c    gox2          =
c    grainr        =
c    humd          =
```

```
*****

***** ebsfail.f
c     iclcrit2       =

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc c     iconstant1      =

c     icratehac      =
***** EBSFAIL.F.ORIGINAL
c     iclcrit2       =
c     iconstant1      =
c     icratehac      =
*****

***** ebsfail.f
c     iflag          =

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc c     igbthick        =

c     ighy1          =
c     ighy2          =
***** EBSFAIL.F.ORIGINAL
c     iflag          =
c     igbthick        =
c     ighy1          =
c     ighy2          =
*****

***** ebsfail.f
c     igox2          =

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc c     igrainr         =

c     ihumdc1        =
c     ihumdc2        =
***** EBSFAIL.F.ORIGINAL
c     igox2          =
c     igrainr        =
c     ihumdc1        =
c     ihumdc2        =
*****

***** ebsfail.f
      integer iclcrit2
```

```
cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc      integer iconstant1

      integer icratehac
***** EBSFAIL.F.ORIGINAL
      integer iclcrit2
      integer iconstant1
      integer icratehac
*****

***** ebsfail.f
      integer iflag

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc       integer igbthick

      integer ighy1
***** EBSFAIL.F.ORIGINAL
      integer iflag
      integer igbthick
      integer ighy1
*****

***** ebsfail.f
c      integer igox2

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc      integer igrainr

      integer ihumdc1
***** EBSFAIL.F.ORIGINAL
c      integer igox2
      integer igrainr
      integer ihumdc1
*****

***** ebsfail.f
      double precision clcrit2

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc       double precision constant1

      double precision cpass
***** EBSFAIL.F.ORIGINAL
      double precision clcrit2
      double precision constant1
```

```
      double precision cpass
*****

***** ebsfail.f
      double precision garb

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc             modified since corrosion by dry oxidation is negligle
cc       double precision gbthick

      double precision ghy1
***** EBSFAIL.F.ORIGINAL
      double precision garb
      double precision gbthick
      double precision ghy1
*****

***** ebsfail.f
      double precision ghy2

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc             modified since corrosion by dry oxidation is negligle
cc       double precision grainr

      double precision humd
***** EBSFAIL.F.ORIGINAL
      double precision ghy2
      double precision grainr
      double precision humd
*****

***** ebsfail.f

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc             modified since corrosion by dry oxidation is negligle
cc       common / ebsfail4a / iwplen, iwpdia, icthick1, icthick2,
cc      &  igrainr, igbthick, iconstant1, ihumdc1,ihumdc2, ifilmthk,
      common / ebsfail4a / iwplen, iwpdia, icthick1, icthick2,
     &  ihumdc1,ihumdc2, ifilmthk,
     &  iclcritw, iinhToClw,   ideltaEcInhW,
***** EBSFAIL.F.ORIGINAL

      common / ebsfail4a / iwplen, iwpdia, icthick1, icthick2,
     &  igrainr, igbthick, iconstant1, ihumdc1,ihumdc2, ifilmthk,
     &  iclcritw, iinhToClw,   ideltaEcInhW,
*****

***** ebsfail.f

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
```

```
cc            modified since corrosion by dry oxidation is negligle
cc
cc        call clearchar( 60, name )
cc        name = 'MetalGrainRadius[micrometer]'
cc        igrainr =  ispquery( name )
cc
cc        call clearchar( 60, name )
cc        name = 'GrainBoundaryThickness[micrometer]'
cc        igbthick = ispquery(  name )
cc
cc        call clearchar( 60, name )
cc        name = 'DryOxidationConstant'
cc        iconstant1 = ispquery(  name )

***** EBSFAIL.F.ORIGINAL

      call clearchar( 60, name )
      name = 'MetalGrainRadius[micrometer]'
      igrainr =  ispquery( name )

      call clearchar( 60, name )
      name = 'GrainBoundaryThickness[micrometer]'
      igbthick = ispquery(  name )

      call clearchar( 60, name )
      name = 'DryOxidationConstant'
      iconstant1 = ispquery(  name )

***** ebsfail.f

cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc            modified since corrosion by dry oxidation is negligle
cc      grainr = valuesp( igrainr )
cc      gbthick = valuesp( igbthick )
cc      constant1 = valuesp( iconstant1)
      humdc1 = valuesp( ihumdc1 )
***** EBSFAIL.F.ORIGINAL

      grainr = valuesp( igrainr )
      gbthick = valuesp( igbthick )
      constant1 = valuesp( iconstant1)
      humdc1 = valuesp( ihumdc1 )
*****

***** ebsfail.f
      read(iebsfailtmp,100)aline
cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc            modified since corrosion by dry oxidation is negligle
cc      write(aline(1:11),fmt='(e11.4)') grainr
      write(iebsfailinp,100) aline
```

```
***** EBSFAIL.F.ORIGINAL
      read(iebsfailtmp,100)aline
      write(aline(1:11),fmt='(e11.4)') grainr
      write(iebsfailinp,100) aline
*****

***** ebsfail.f
      read(iebsfailtmp,100)aline
cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc       write(aline(1:11),fmt='(e11.4)') gbthick
      write(iebsfailinp,100) aline
***** EBSFAIL.F.ORIGINAL
      read(iebsfailtmp,100)aline
      write(aline(1:11),fmt='(e11.4)') gbthick
      write(iebsfailinp,100) aline
*****

***** ebsfail.f
      read(iebsfailtmp,100)aline
cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
cc              modified since corrosion by dry oxidation is negligle
cc       write(aline(1:11),fmt='(e11.4)') constant1
      write(iebsfailinp,100) aline
***** EBSFAIL.F.ORIGINAL
      read(iebsfailtmp,100)aline
      write(aline(1:11),fmt='(e11.4)') constant1
      write(iebsfailinp,100) aline
*****
```

For *tpanames.dbs*:

```
Comparing files tpanames.dbs and TPANAMES.DBS.ORIGINAL
***** tpanames.dbs
InnerWPThickness[m]                              WP-IWThk
CriticalRelativeHumidityHumidAirCorrosion                CrtRHHAC
***** TPANAMES.DBS.ORIGINAL
InnerWPThickness[m]                              WP-IWThk
MetalGrainRadius[micrometer]                        MtlGrnRd
GrainBoundaryThickness[micrometer]                       GrnBndrT
DryOxidationConstant                             DryOxdtC
CriticalRelativeHumidityHumidAirCorrosion                CrtRHHAC
*****
```

For *tpa.inp*:

```
Comparing files tpa.inp and TPA.INP.ORIGINAL
***** tpa.inp
**
** cc rwr 4-15-05  SCR569 - do not need dry oxidation parameters -
** cc              modified since corrosion by dry oxidation is negligle
```

```
** cc
** cc constant
** cc MetalGrainRadius[micrometer]
** cc 13.75
** cc **
** cc constant
** cc GrainBoundaryThickness[micrometer]
** cc 7.0e-4
**
** cc constant
** cc DryOxidationConstant
** cc 9999.0
**
***** TPA.INP.ORIGINAL
**
constant
MetalGrainRadius[micrometer]
13.75
**
constant
GrainBoundaryThickness[micrometer]
7.0e-4
**
constant
DryOxidationConstant
9999.0
**
```

Transmitted via email these file comparisons together with the original files from TPA Version 5.0.0o and the modified file on to R. Janetzke on 4/19/05. The text of that email follows.

From: Rwrice
To: rjanetzke@cnwra.swri.edu
Cc: Rwrice
Bcc:
Subject: SCR569_preliminary Testing/Coding - Remove Dry Oxidation
Date: Tue, 19 Apr 2005 18:57:59 -0400
Files: FILE_COMPARISON_all_modified_files.wpd (35K)

Ron,

Attached please find a WordPerfect file with
modifications I made (file comparisons) to
tpa.inp, ebsfail.f, tpanames.dbs, and failt.f
to remove dry oxidation calculations from the
TPA Version 5.0.0o code as part of preliminary
work for SCR569.

This removal was recommended by Osvaldo

since dry oxidation is negligible (it was a problem
because the high temperatures [above 370 deg C or so]
were causing WP failures at times around 100 years).

It is Osvaldo's position that temperatures this
high will not be possible (since cladding failure occurs
at 360 deg C). Maybe Randy, Osvaldo, and/or George
should be involved in this SCR (which can be both
removing dry oxidation and not allowing temperatures
to be above 300 deg C)?

For all of the original files, modified files, and file comparisons,
please goto the scratch drive in SMohanty/Rob/SCR569_preliminary.

Please contact me if you have any questions.

Thanks,

Rob

As a result of SCR560 testing, it was recommended that the TPA source code be modified to fill subareas that are outside of the emplacement block with a number of WPs that are in the emplacement block as listed in the *drifts.dat* file, and not to extend the endpoints of the drifts to the subarea boundaries (see SCR560 testing documented earlier in this scientific notebook). To follow-up on this recommendation, the *reader.f* and *subarea.f* files were modified as shown below in the file comparison. Preliminary testing was conducted to determine whether these modifications correctly assigned WPs to subareas. The tests were passed.

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*:

```
Comparing files reader.f.modified and READER.F.ORIGINAL
***** reader.f.modified
      dimension b(2)

cc rwr 4-19-05 SCR570 - add these lines to define integer variables as a
cc`                 part of making sure when a subarea
cc                  is larger than the emplacement block, the drift
cc                  endpoints are not extended to the subarea boundaries
      integer iflagahit
      integer iflagbhit

c
***** READER.F.ORIGINAL
      dimension b(2)
c
*****

***** reader.f.modified


cc rwr 4-19-05 SCR570 - determine whether points a and b are in  subarea isa
          call qphitsa(a,isa,iflagahit)
          call qphitsa(b,isa,iflagbhit)

c         If each WP is its own drift, skip these computations.
***** READER.F.ORIGINAL

c         If each WP is its own drift, skip these computations.
*****

***** reader.f.modified

cc rwr 4-19-05 SCR570 - make a(i) on left (east) and b(i) on right (west)
cc            a(1) = xw
cc            a(2) = yw
cc            b(1) = xe
cc            b(2) = ye
            a(1) = xe
            a(2) = ye
            b(1) = xw
            b(2) = yw

          endif
***** READER.F.ORIGINAL

            a(1) = xw
            a(2) = yw
            b(1) = xe
            b(2) = ye
```

```
           endif
*****

***** reader.f.modified

cc rwr 4-19-05 SCR570 - add these lines to make sure the when a subarea
cc                    is larger than the emplacement block, the drift
cc                    endpoints are not extended to the subarea boundaries
cc           call qlhitsa( a, b, isa, iflaglhit, alengthinsa )
           if (iflagahit .eq. 1 .and. iflagbhit .eq. 1) then
             alengthinsa = driftlength
             iflaglhit = 1
           elseif (iflagahit .eq. 1 .and. iflagbhit .eq. 0) then
             a(1) = drxy1(1,idrift,iempblk)
             a(2) = drxy1(2,idrift,iempblk)
             call qlhitsa( a, b, isa, iflaglhit, alengthinsa )
           elseif (iflagahit .eq. 0 .and. iflagbhit .eq. 1) then
             b(1) = drxy2(1,idrift,iempblk)
             b(2) = drxy2(2,idrift,iempblk)
             call qlhitsa( a, b, isa, iflaglhit, alengthinsa )
           else
             call qlhitsa( a, b, isa, iflaglhit, alengthinsa )
           endif

           if (iflaglhit .eq. 1) then
***** READER.F.ORIGINAL

           call qlhitsa( a, b, isa, iflaglhit, alengthinsa )
           if (iflaglhit .eq. 1) then
*****
```

For this SCR570 preliminary work, original files, modified files, and file comparisons were placed on the scratch drive and an email sent to R. Janetzke with a file attachment that provides the text of the file comparison. The text of that email follows.

From: Rwrice
To: rjanetzke@cnwra.swri.edu
Cc: Rwrice
Bcc:
Subject: SCR570_preliminary Testing/Coding - Do Not Overfill SA With A Smaller Emplacement Block
Date: Wed, 20 Apr 2005 19:03:57 -0400
Files: SCR570_FILE_COMPARISON_all_modified_files.wpd (14K)

Ron,

As we discussed previously, this is part of
preliminary work for SCR570.

Attached please find a WordPerfect file with
modifications I made (file comparisons) to
reader.f and subarea.f to avoid the situation
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.

I noted the need for this modification during my testing
associated with SCR560, in which there was a failed test.

For all of the original files, modified files, and file comparisons,
please goto the scratch drive in SMohanty/Rob/SCR570_preliminary.

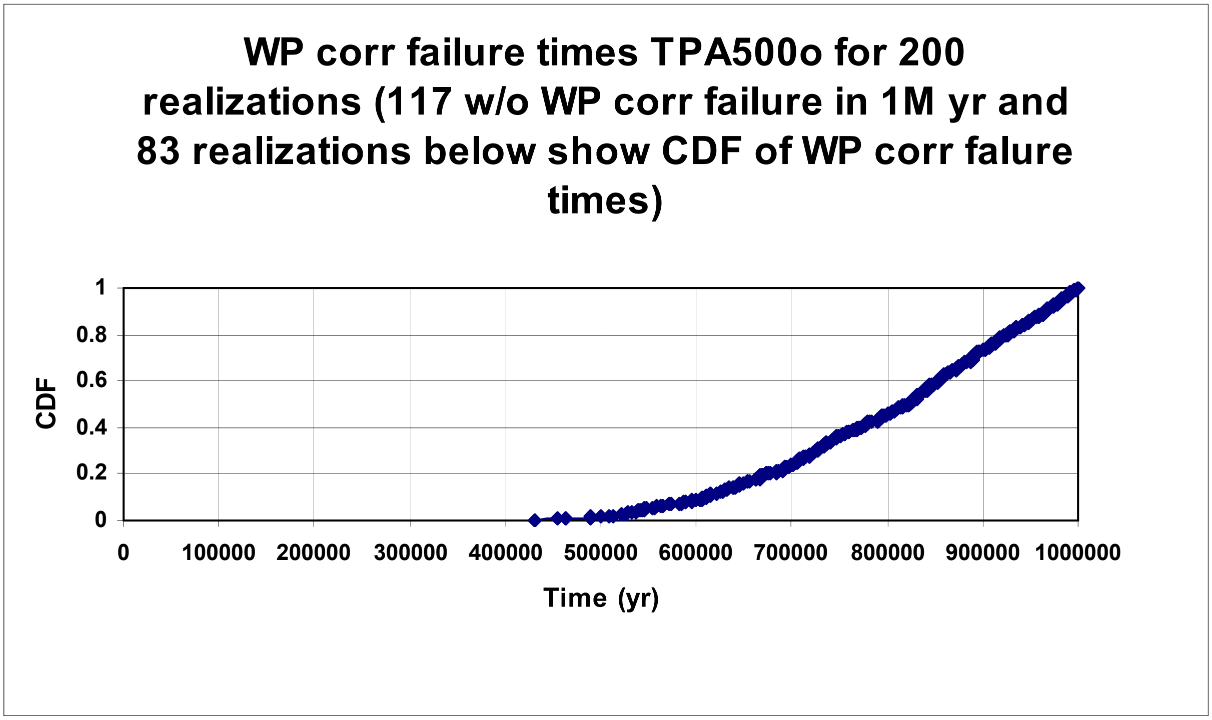
Please contact me if you have any questions.

Thanks,

Rob

April 26, 2005 - Examined output from TPA500o for WP corrosion failure times from a mean value run for SA7 and plotted the results below. Note about 60% of realizations do not have corrosion failure with failure times beginning at about 430,000 years. This plot will be reviewed to determine if this results are reasonable.

Also, plotted results from the above TPA simulation for *climato2.dat*, *ebsflo.dat*, and *NEFIIUZ.VEL* because of a concern that the inputs to UZFT at consistently cyclical, however the NEFTRAN input flow velocities seem to exhibit local maxima during the 100kyr cycles (i.e., the 100kyr peaks are not consistent). See the plot below. Again, this plot will also be reviewed to determine if this results are reasonable.


WP corr failure times TPA500o for 200 realizations (117 w/o WP corr failure in 1M yr and 83 realizations below show CDF of WP corr falure times)
CDF
1
0.8
0.6
0.4
0.2
0
0
100000
200000
300000
400000
500000
600000
700000
800000
900000
1000000
Time (yr)

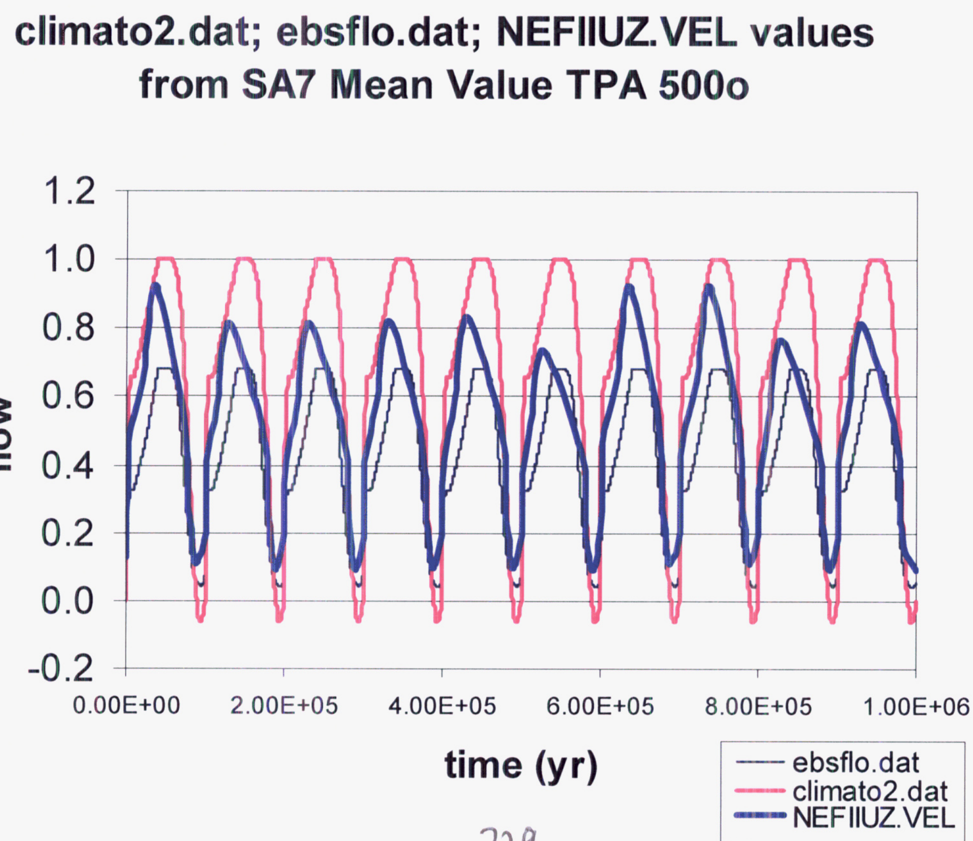
In addition to concerns about WP corrosion failure times and inconsistent peaks in NEFTRAN UZ input flow rates, there are concerns about hardcoding the end of the reflux period at 20kyr (instead of 210kyr) in *nfenv.f* and that NEFTRAN UZ execution stops with TPA500o (for example) because of the U234 chain (note that if either just U234 is removed or the U234 chain of 4 members, U234 to Th230 to Ra226 to Pb210, is entirely removed from the *tpa.inp* file, the TPA code execution does not stop - reasons for this behavior are believed to be tied to Kds which are hardcoded using Turner's routine in *uzft.f*. Again, this information will also be reviewed to determine if this results are reasonable.

April 27, 2005 - During this work, identified the following questions that were passed on to R. Janetzke. Plots and text file were presented.

Questions About TPA Code 500o Results

prepared by R. Rice (4/27/05)

1. End of the reflux period is hardcoded at 20,000 yr. The "long simulation" changes involved modifying this value from 10,000 yr. Note that if the end of the reflux period is not specified, previous TPA code results have shown there are about 1 of 20 realizations f o r 1



page # obscured by Figure JRW 1/29/10

M yr that have no releases because there is no flow onto the waste package. Therefore, a value of 20,000 yr was selected and specified.

2. NEFTRAN UZ execution stops after 5-7 realizations because of array out of bounds troubles. The U234-Th230-Ra226-Pb210 chain is involved. Note that either removing U234 or removing the entire chain results in successful TPA code execution.

3. The NEFTRAN UZ velocity values, written in UZFT to the *nefii.vel* file, show instabilities in the maximum values over the 100,000 yr climato cycles.

4. The WP corrosion failure times from a 200 realization TPA code simulation show about 60% of the realizations do not exhibit corrosion failures; the quickest WP corrosion failure time is about 430,000 yr; about 4% of the WP corrosion failures are before 60,000 yr; about 16% of the WP corrosion failures are before 80,000 yr; and about 8% of the WP corrosion failures are after 90,000 yr.

5. The FAILT model is showing 500 yr failure times when large time steps are used (i.e., 23 or fewer time steps in the 10,000 yr compliance period - which corresponds to time steps of about 500 yrs). Additionally, there appears to be a convergence problem with FAILT in TPA 4.1 and more recent versions compared with TPA 3.

5/5/5

During testing for SCR546, found that the files *relcum.out* and *ebsrel.rlt* contained information in "Fraction Left" this was no longer needed now that the TPA code has been extended beyond 100,000 yr. After consultation with R. Janetzke, decided to modify RELEASET.F to remove printing "Fraction Left" and the variable "pleft" to the *relcum.out* file. Note that this also fixes the information in the *ebsrel.rlt* file, since this file is written by *exec.f* by reading in lines from *relcum.out* and then writing out those lines to *ebsrel.rlt*. Note that negative numbers and very small negative numbers were in these files for simulation times greater than 100,000 years. See the examples below for these files from 10kyr, 100kyr, and 1,000kyr TPA code simulations using version 500o.

From "ebsrel.rlt" and "relcum.out"
(for 10kyr using TPA500o for real 1 of 500; sa1)

```
  Radionuclide Halflife[yr]    xnoloss[ci]       amwp[ci]      xmass[ci]
Fraction Left
     CM246      4.7310E+03     6.6484E-01     1.5355E-03     1.8326E-01
  7.2435E-01
     U238       4.4680E+09     4.6605E+00     1.2927E+00     2.7032E-03
  9.9942E-01
     CM245      8.4990E+03     3.7268E+00     8.6074E-03     1.0273E+00
  7.2435E-01
```

AM241	4.3220E+02	3.9322E+00	9.0818E-03	1.0839E+00	7.2435E-01
NP237	2.1400E+06	1.6484E+01	3.8073E-02	4.5439E+00	7.2435E-01
U233	1.5850E+05	6.7935E-01	9.4534E-02	9.4298E-02	8.6119E-01
TH229	7.3390E+03	2.3490E-01	1.3983E-03	6.3893E-02	7.2799E-01
AM243	7.3800E+03	1.7621E+02	4.0698E-01	4.8573E+01	7.2435E-01
PU239	2.4060E+04	3.6402E+03	9.9637E+02	1.5466E+01	9.9575E-01
PU240	6.5370E+03	2.8738E+03	7.9273E+02	6.0821E+00	9.9788E-01
U234	2.4450E+05	1.9373E+01	5.3738E+00	1.1236E-02	9.9942E-01
TH230	7.7000E+04	1.6974E+00	8.6743E-03	4.6313E-01	7.2715E-01
RA226	1.6000E+03	1.3251E+00	3.2563E-03	3.6506E-01	7.2450E-01
PB210	2.2300E+01	1.3199E+00	3.1963E-03	3.6368E-01	7.2446E-01
CS135	2.3000E+06	1.2080E+01	2.7124E-02	3.5733E+00	7.0420E-01
I129	1.5700E+07	5.4447E-01	1.1955E-03	1.6953E-01	6.8863E-01
TC99	2.1300E+05	2.2014E+02	5.0775E-01	6.0897E+01	7.2337E-01
NI59	8.0000E+04	5.8191E+01	1.3440E-01	1.6040E+01	7.2435E-01
C14	5.7290E+03	3.1821E+00	6.6145E-03	1.1076E+00	6.5192E-01
SE79	1.1000E+06	1.5068E+00	3.4179E-03	4.3485E-01	7.1141E-01
NB94	2.0300E+04	1.4570E+01	3.3651E-02	4.0162E+00	7.2435E-01
CL36	3.0100E+05	2.3598E-01	4.3586E-04	9.9286E-02	5.7926E-01

From “ebsrel.rlt” and “relcum.out”
(for 100kyr using TPA500o for real 1 of 500; sa1)

Radionuclide	Halflife[yr]	xnoloss[ci]	amwp[ci]	xmass[ci]	Fraction Left
CM246	4.7310E+03	1.2476E-06	4.4451E-09	1.0125E-06	1.8847E-01
U238	4.4680E+09	4.6605E+00	3.7573E+00	4.1409E-02	9.9111E-01
CM245	8.4990E+03	2.4187E-03	8.6175E-06	1.9629E-03	1.8847E-01
AM241	4.3220E+02	2.5483E-03	9.0792E-06	2.0680E-03	1.8847E-01
NP237	2.1400E+06	1.6026E+01	5.7098E-02	1.3006E+01	1.8847E-01
U233	1.5850E+05	5.7437E+00	1.1190E+00	3.5627E+00	3.7973E-01
TH229	7.3390E+03	5.2419E+00	1.6115E-01	4.1115E+00	2.1565E-01

AM243	7.3800E+03	3.7578E-02	1.3389E-04	3.0496E-02	1.8847E-01
PU239	2.4060E+04	2.7814E+02	1.8398E+02	4.2725E+01	8.4639E-01
PU240	6.5370E+03	2.0604E-01	1.3821E-01	2.9728E-02	8.5572E-01
U234	2.4450E+05	1.5011E+01	1.2102E+01	1.3337E-01	9.9111E-01
TH230	7.7000E+04	1.0088E+01	2.0810E-01	8.0144E+00	2.0553E-01
RA226	1.6000E+03	9.9812E+00	1.0798E-01	8.0277E+00	1.9572E-01
PB210	2.2300E+01	9.9797E+00	1.0698E-01	8.0275E+00	1.9562E-01
CS135	2.3000E+06	1.1757E+01	4.0722E-02	9.6028E+00	1.8322E-01
I129	1.5700E+07	5.4231E-01	1.8369E-03	4.4514E-01	1.7917E-01
TC99	2.1300E+05	1.6425E+02	5.8440E-01	1.3334E+02	1.8821E-01
NI59	8.0000E+04	2.6681E+01	9.5058E-02	2.1652E+01	1.8847E-01
C14	5.7290E+03	5.9384E-05	1.9042E-07	4.9311E-05	1.6962E-01
SE79	1.1000E+06	1.4237E+00	4.9819E-03	1.1602E+00	1.8510E-01
NB94	2.0300E+04	6.7429E-01	2.4024E-03	5.4721E-01	1.8847E-01
CL36	3.0100E+05	1.9181E-01	5.4650E-04	1.6290E-01	1.5072E-01

From "ebsrel.rlt" and "relcum.out"
(for 1000kyr using TPA500o for real 1 of 500; sa1)

Radionuclide	Halflife[yr]	xnoloss[ci]	amwp[ci]	xmass[ci]	Fraction Left
CM246	4.7310E+03	1.6977E-28	0.0000E+00	1.8821E-15	-1.1086E+13
U238	4.4680E+09	4.6598E+00	4.5516E+00	4.1701E-01	9.1051E-01
CM245	8.4990E+03	4.9704E-28	0.0000E+00	3.8200E-15	-7.6857E+12
AM241	4.3220E+02	3.1151E-24	0.0000E+00	5.2858E-15	-1.6968E+09
NP237	2.1400E+06	1.1974E+01	3.0462E-05	1.2767E+01	-6.6272E-02
U233	1.5850E+05	1.2705E+01	1.2382E-01	1.3424E+01	-5.6529E-02
TH229	7.3390E+03	1.2739E+01	1.6488E-02	1.3567E+01	-6.4980E-02
AM243	7.3800E+03	2.6595E-26	0.0000E+00	3.2374E-15	-1.2173E+11
PU239	2.4060E+04	1.5269E-09	3.7240E-15	1.6281E-09	-6.6272E-02
PU240	6.5370E+03	4.8958E-25	1.0512E-30	6.6417E-30	9.9999E-01
U234	2.4450E+05	1.1703E+00	1.1432E+00	1.0473E-01	9.1051E-01

```
     TH230        7.7000E+04      1.7048E+00      1.6561E-02      1.8012E+00
 -5.6560E-02
     RA226        1.6000E+03      1.7159E+00      7.0523E-03      1.8226E+00
 -6.2164E-02
     PB210        2.2300E+01      1.7161E+00      6.9224E-03      1.8229E+00
 -6.2240E-02
     CS135        2.3000E+06      8.9640E+00      2.2171E-05      9.5415E+00
 -6.4428E-02
     I129         1.5700E+07      5.2118E-01      1.2606E-06      5.5402E-01
 -6.3004E-02
     TC99         2.1300E+05      8.7810E+00      2.2310E-05      9.3622E+00
 -6.6182E-02
     NI59         8.0000E+04      1.0955E-02      2.7871E-08      1.1681E-02
 -6.6272E-02
     C14          5.7290E+03      6.2954E-28      0.0000E+00      4.1042E-14
 -6.5193E+13
     SE79         1.1000E+06      8.0747E-01      2.0176E-06      8.6003E-01
 -6.5087E-02
     NB94         2.0300E+04      3.0387E-14      0.0000E+00      5.3792E-14
 -7.7022E-01
     CL36         3.0100E+05      2.4142E-02      4.9118E-08      2.5422E-02
 -5.2997E-02
```

5/10/05 - Began testing for SCR546. The WordPerfect file with this SCR has been inserted below:

SOFTWARE CHANGE REPORT (SCR)

<table>
<tr><td>1. SCR No. (Software Developer Assigns):
PA-SCR-546</td><td>2. Software Title and Version:
TPA 5.0.0g</td><td>3. Project No:
20.06002.01.354</td></tr>
<tr><td colspan="3">4. Affected Software Module(s), Description of Problem(s): releaset.f

Releaset has long run times for long simulation times.</td></tr>
<tr><td>5. Change Requested by:
R. Codell
Date: 2-2-2005</td><td colspan="2">6. Change Authorized by (Software Developer):
R. Janetzke
Date: 2-4-2005</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td>8. Implemented by:
R. Codell</td><td colspan="2">Date:
2-12-05</td></tr>
<tr><td colspan="3">9. Description of Acceptance Tests:</td></tr>
<tr><td>10. Tested by:
O. Osidele</td><td colspan="2">Date:</td></tr>
</table>

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)

```
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
        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
```

While examining initial output found the following in *ebsrel.rlt*:

Release information taken from RELCUM.OUT

1.00000E+04 Simulation Time

Type#	Failed	Fail Time[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	2	1.1026E+03	2.1619E+02	1.1307E+03	1.3469E+03
2	0	1.1026E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.1026E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.1026E+03	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

Noted that the "Fail Time" shown above for Type #1 (initial failures) is not "0.00". This was passed on to R. Janetzke so that RELEASET could be modified to print a time of "0.00" for initial failures. Suggested modifying the RELEASET code which writes this information to *relcum.out* by determining whether itype=1 - if so, write out a value of 0.00 for the variable tfail. Note that there are no incorrect release rates calculated. See the following comparison of information in the *ebsrel.ech* and *ebsrel.rlt* files.

ebsrel.ech

Input file tpa.inp as supplied with TPA Version 5.0.0o Code.
Base case.
TPA 5.0.0o, Job started: Thu May 05 14:07:13 2005
Echo of EBSREL Input Values

type of event	number wps failed	time of event
INITIAL	2.0000E+00	0.0000E+00
FAULTING	0.0000E+00	0.0000E+00
VOLCANO	0.0000E+00	0.0000E+00
SEISMO 1	0.0000E+00	9.9639E+02
SEISMO 2	0.0000E+00	3.4659E+03
SEISMO 3	0.0000E+00	7.3763E+03
SEISMO 4	0.0000E+00	5.0500E+05
CORROSION	0.0000E+00	1.0000E+06
EXTRUSIVE	2.0316E+06	0.0000E+00

ebsrel.rlt

Input file tpa.inp as supplied with TPA Version 5.0.0o Code.
Base case.
TPA 5.0.0o, Job started: Thu May 05 14:22:54 2005
EBSREL Results

with the output mode specified in "tpa.inp"

Release information taken from RELCUM.OUT

1.00000E+04 Simulation Time

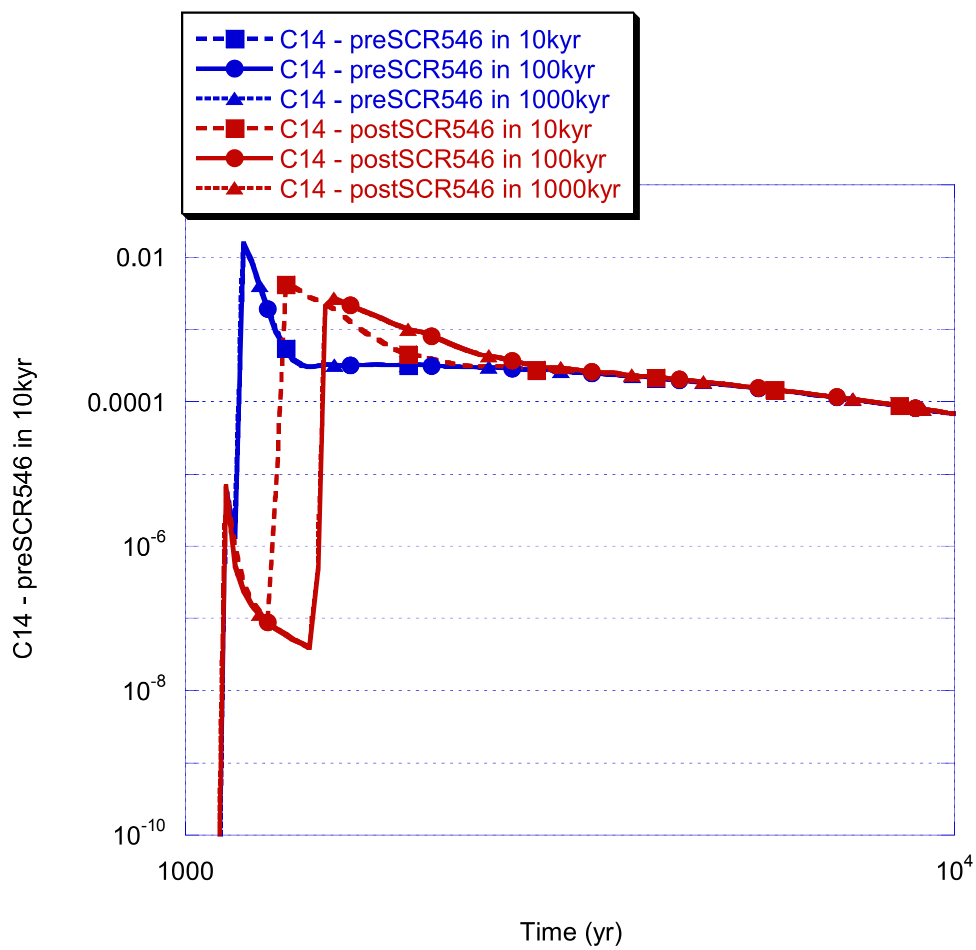
Type#	Failed	Fail Time[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	2	1.1026E+03	2.1619E+02	1.1307E+03	1.3469E+03
2	0	1.1026E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.1026E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.1026E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	3.4659E+03	0.0000E+00	0.0000E+00	0.0000E+00

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

Recommended to R. Janetzke that "Fail Time[yr]" be changed to "Start SF Wet[yr]". Also noted the "EXTRUSIVE" number is incorrect.

During a run of the TPA Version 500o code at the beginning of testing for SCR546, plotted the following results for an indicator radionuclide (C14) for 10kyr, 100kyr, and 1000kyr simulations using RELEASET with and without the changes introduced in SCR546.

Noted in the above plot that preSCR546 release rates exhibit an earlier and higher peak than the postSCR546 release rates for all simulation times. Examination of the *ebsrel.rlt* file from the pre- and post-SCR546 runs showed a later WP fill time. See the following lines from pre- and post-SCR546 runs from the *ebsrel.rlt* file.



From pre-SCR546

Type#	Failed	Fail Time[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	2	1.1026E+03	5.8238E+01	1.1307E+03	1.1890E+03

From post-SCR546

Type#	Failed	Fail Time[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	2	1.1026E+03	2.1619E+02	1.1307E+03	1.3469E+03

The increased fill time explains the difference in the peak and the time of the peak release shown in the previous figure. However, it is currently unclear why there are releases prior to the filling of the WP with water, unless these releases are from diffusion.

Need to note that I talked to R. Codell who recommended a switch in *releaset.f* for different min volume for long simulations. After consultation with R. Janetzke, sent R. Codell an email asking him for recommendations to modify *releaset.f* and add a switch.

Examined output from a TPA Version 500o run for 500 realizations, 1e6 yrs, the max. num. seismic events increased to 10,000, the U234 chain removed, and the dry oxidation constant set at 1e20 (i.e., this removes dry oxidation). In realization 3 of 500 and subarea 3 of 7, noted that there was WP corrosion failure at about 2,200 years - this early failure is not expected since WP corrosion failure times should be at about 500,000 years or beyond. Also, the WP failed from localized corrosion, which is not expected to occur in this version of the code. See below for *failt.f* input (*ebsrel.inp*) and output (*failt.out*) files that show this condition. After talking with R. Janetzke, decided to test whether this condition still exists in the modified *failt.f* (which will be available for testing within approximately one week).

From *ebsrel.inp*

```
\Default input file for ebsfail
|
\simulation time
1000000.00                    ! tend: simulation time leng
\
\Geometry
 5.1650  1.6590               ! wplen,wpdia: wp length and
 0.2000E-01  0.5000E-01       ! cthick1,cthick2: wp layers
 3.5000E-02                   ! thickness: weld alloy thic
|
\Dry oxidation of wp outer overpack
 0.1375E+02                   ! grainr: metal grain radius
25                            ! nseries: terms in infinite
```

```
 0.7000E-03              ! gbthick: bundary thickness
 0.1000E+21              ! constant1: constant relati
|
\evaporation-condensation
 0.2000E+00   0.3000E+00       ! humdc1, humdc2: crit. rel.
 0.0000E+00              ! filmthk: thickness of wate
|
\ Weld Area parameters
 1.0093E+03              ! ErpInt: Erp Intercept [mVS
-1.0000E+01              ! TErpInt: Temp Coef Erp Int
-5.8420E+02              ! ErpSlope: Erp Slope [mVSHE
 3.7000E+00              ! TErpSlope: Temp Coeff of E
 0.4319E-02              ! clcritw: minimum chloride
 0.3000E+00              ! inhToClw: critical inhibit
 0.8000E+03              ! deltaEcInhWeld: Increase i
 0.0000E+00              ! frac_weld_surf, weld surfa
|
\Critical Potential Parameters(Ep: pitting potential [mVshe]
-0.5848E+03              ! xipto: outer overpack Ep i
 0.3920E+01              ! pttemo: temp. coef. of out
-0.2450E+02              ! slpto: outer overpack Ep s
-0.1100E+01              ! slpttemo: temp. coef. of o
 0.1598E+04              ! xirpo: outer overpack Erp
-0.1310E+02              ! rptemo: temp. coef. of out
-0.3627E+03              ! slrpo: outer overpack Erp
 0.2300E+01              ! slrptemo: temp. coef. of o
-0.2000E+03              ! xipti: inner overpack Ep i
 0.0000E+00              ! pttemi: temp. coef. of inn
-0.2400E+03              ! slpti: inner overpack Ep s
 0.0000E+00              ! slpttemi: temp. coef. of i
-0.1000E+05              ! xirpi: inner overpack Erp
 0.0000E+00              ! rptemi: temp. coef. of inn
 0.0000E+00              ! slrpi: inner overpack Erp
 0.1000E+01              ! slrptemi: temp. coef. of i
|
\Corrosion potential parameters (hi: high pH parameter, lo:
 0.6000E+01              ! pHtran: transition pH betw
 0.5510E+10   0.7570E+10       ! ire1hi,ire1lo, C/(m^2 yr),
 0.2480E-01  0.1287E-01       ! beta1hi, beta1lo, effectiv
 0.5000E+00              ! betahy1: transfer coeffici
\
 0.5510E+10  0.7570E+10       ! ire2hi,ire2lo, C/(m^2 yr),
 0.2480E-01  0.1287E-01       ! beta2hi, beta2lo, effectiv
 0.5000E+00              ! betahy2: transfer coeffici
\
 0.0000E+00              ! rkhy1 [Coul/(m^2 yr)], rat
 0.4000E+05  0.4000E+05       ! g1hi, g1lo [J/mol], activa
 0.2500E+05              ! ghy1 [J/mol], activation e
 0.1897E-01  0.2560E-01       ! npH1hi, npH1lo, pH reactio
0.0248 0.01287                ! nO1hi, nO1lo, oxygen react
```

```
\
 0.0000E+00                  ! rkhy2 [Coul/(m^2 yr)], rat
 0.4000E+05  0.4000E+05        ! g2hi, g1lo [J/mol], activa
 0.2500E+05                  ! ghy2 [J/mol], activation e
 0.1897E-01  0.2560E-01        ! npH2hi, npH2lo, pH reactio
0.0248   0.01287               ! nO2hi, nO2lo, oxygen react
\
 0.1305E+04  0.0  0.0          ! aa(1,1) [C/m2/yr], aa(1,2)
 0.1000E+11  0.0  0.0          ! aa(2,1) [C/m2/yr], aa(2,2)
 0.4470E+05                  ! g1anod [J/mol], act. energ
 0.4470E+05                  ! g2anod [J/mol], act. energ
 0.3680E+03                  ! refTanod [K], temperature
\
 0.0000E+00                  ! eexpt: measured galvanic c
 0.2500E-03                  ! rcoef: coef. for loc. corr
 0.1000E+01                  ! rexpont: exponent for loc.
 0.1000E+01                  ! rcoef2: coef. for loc. cor
 0.1000E+01                  ! rexpont2: exponent for loc
 0.2500E-07                  ! cratehac: humd.air corr.rt
 0.0000E+00                  ! xcouple, efficiency of gal
 0.0000E+00                  ! xread: factor for defining
 0.5000E+00                  ! clcrit1: min. chloride con
 0.1000E-09                  ! clcrit2: min. chloride con
 0.1000E+00                  ! inhToCl1: critical inhibit
 0.1000E+11                  ! inhToCl2: critical inhibit
 0.8000E+03                  ! deltaEcInh1: Incr in crit
 0.0000E+00                  ! deltaEcInh2: Incr in crit
 0.1000E+01                  ! cfactor: factor for changi
 0.2100E+00                  ! xgas: oxygen partial press
 0.0000E+00  0.1000E+01  0.1000E+01 althk: scale thick;taus:
 0.1000E+01                  ! cfactor2: factor for chang
|
\ Drip shield failure parameters
 1.0000000000E+04              ! ds_time_mark: Time mark fo
 7.5000E-01  3.8849452894E+02   ! fraction_failed_first, fai
 1.0000E+00                  ! fraction_failed_mark: frac
 1.0000E+00                  ! fraction_failed_end_sim: f
|
\ Radiolysis parameters
 0.0000E+00   0.7000E-04       !deltaEo, lamb: Radiolysis p
0.869000E+04 0.798000E+04 0.259700E-01 0.249400E-01  wtmol1
|
\Mechanical failure data
 0.3103E+03  0.1000E+01           ! yieldstr: yield strengt
 0.3040E+03                    ! dkic: fracture toughnes
|
\Runge-kutta control parameters
 0.1000E-02  0.1000E+01        ! dtini, dtmax
 0.1000E-01  0.1000E-29        ! errrel (same as eps), erra
|
```

\end

From *failt.out* (i..e, the *failt.f* screenprint)

```
ebspac (engineering barrier system performance assessment code)
this is the part of the code that computes wp failure time
version= 1.0
Thu May 12 08:40:49 2005
nhist3= 5001
nhist= 5001

**Calculation of Weld Failure Time**
 Case II: RH transitioned to aqueous
 Localized corrosion intitiated at   2235.22   years
Weld failure time =   2364.57  yr
**End of Weld Failure Calculation**

          calculation of waste package failure time
=============================================================================
===========
             end of simulation time [yr]:    1000000.
     no. of rows of data to pass to release.f:        5001
----------------------------------------------------------------------------------
ilayer  tstop     tcan     ecrit     ecorr   chloride   rthick     mode
      [yr]      [C]      [vshe]     [vshe]    flag       [m]
=============================================================================
===========
1      2.31     59.73    0.0000     0.0000    0    7.0000000E-02  dry oxd
1      4.67     65.86    0.0000     0.0000    0    7.0000000E-02  dry oxd
1      7.09     68.36    0.0000     0.0000    0    7.0000000E-02  dry oxd
1      9.57     69.56    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     12.10     70.21    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     14.70     70.54    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     17.35     70.65    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     20.07     70.60    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     22.85     70.44    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     25.69     70.14    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     28.61     69.48    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     31.59     68.71    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     34.63     67.90    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     37.76     67.08    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     40.95     66.26    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     44.22     65.45    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     47.56     64.66    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     50.99    146.38    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     54.49    188.34    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     58.08    198.75    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     61.75    202.63    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     65.50    204.06    0.0000     0.0000    0    7.0000000E-02  dry oxd
1     69.35    204.23    0.0000     0.0000    0    7.0000000E-02  dry oxd
```

1	73.28	203.65	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	77.31	202.64	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	81.43	201.38	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	85.64	199.92	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	89.96	198.33	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	94.37	196.65	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	98.89	194.92	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	103.52	193.15	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	108.25	191.37	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	113.10	189.58	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	118.06	206.89	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	123.13	345.03	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	128.32	389.13	0.0000	0.0000	0	6.9872276E-02	dry oxd
1	133.64	407.84	0.0000	0.0000	0	6.9744553E-02	dry oxd
1	139.08	416.05	0.0000	0.0000	0	6.9616829E-02	dry oxd
1	144.64	418.92	0.0000	0.0000	0	6.9489106E-02	dry oxd
1	150.34	418.75	0.0000	0.0000	0	6.9361382E-02	dry oxd
1	156.17	411.93	0.0000	0.0000	0	6.9233659E-02	dry oxd
1	162.13	404.07	0.0000	0.0000	0	6.9105935E-02	dry oxd
1	168.24	396.45	0.0000	0.0000	0	6.8978211E-02	dry oxd
1	174.49	389.05	0.0000	0.0000	0	6.8850488E-02	dry oxd
1	180.88	383.59	0.0000	0.0000	0	6.8722764E-02	dry oxd
1	187.43	378.53	0.0000	0.0000	0	6.8595041E-02	dry oxd
1	194.13	373.60	0.0000	0.0000	0	6.8467317E-02	dry oxd
1	200.98	368.81	0.0000	0.0000	0	6.8339594E-02	dry oxd
1	208.00	364.14	0.0000	0.0000	0	6.8211870E-02	dry oxd
1	215.18	359.58	0.0000	0.0000	0	6.8084147E-02	dry oxd
1	222.52	355.13	0.0000	0.0000	0	6.8005265E-02	dry oxd
1	230.04	350.77	0.0000	0.0000	0	6.8004909E-02	dry oxd
1	237.74	346.52	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	245.62	342.36	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	253.68	338.29	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	261.93	334.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	270.37	330.43	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	279.01	326.63	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	287.85	322.94	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	296.90	319.34	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	306.16	315.80	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	315.64	312.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	325.34	308.93	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	335.26	305.61	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	345.42	302.35	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	355.82	299.16	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	366.46	296.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	377.35	292.95	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	388.49	289.95	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	399.90	287.00	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	411.57	284.10	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	423.52	281.26	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	435.74	278.47	0.0000	0.0000	0	6.8004905E-02	dry oxd

1	448.25	275.72	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	461.06	273.05	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	474.16	270.42	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	487.57	267.17	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	501.30	263.91	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	515.35	260.70	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	529.72	257.54	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	544.43	254.44	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	559.49	251.39	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	574.90	248.42	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	590.67	245.49	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	606.80	242.63	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	623.32	239.81	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	640.22	237.04	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	657.52	234.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	675.23	231.66	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	693.34	229.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	711.89	226.44	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	730.86	223.91	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	750.28	221.43	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	770.16	218.99	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	790.50	216.59	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	811.32	214.24	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	832.62	211.92	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	854.42	209.64	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	876.74	207.38	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	899.57	205.16	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	922.94	202.98	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	946.86	200.83	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	971.34	198.71	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	996.39	196.34	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1022.03	193.95	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1048.26	191.60	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1075.12	189.30	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1102.60	187.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1130.72	184.78	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1159.50	182.56	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1188.96	180.36	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1219.10	178.18	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1249.95	176.04	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1281.53	173.92	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1313.84	171.83	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1346.91	169.76	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1380.75	167.72	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1415.39	165.70	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1450.83	163.68	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1487.11	161.69	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1524.23	159.72	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1562.23	157.77	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1601.11	155.84	0.0000	0.0000	0	6.8004905E-02	dry oxd

```
1    1640.91    153.94    0.0000    0.0000    0    6.8004905E-02  dry oxd
1    1681.63    152.06    0.0000    0.0000    0    6.8004905E-02  dry oxd
1    1723.31    150.20    0.0000    0.0000    0    6.8004905E-02  dry oxd
1    1765.97    148.36    0.0000    0.0000    0    6.8004905E-02  dry oxd
1    1809.62    146.51    0.0000    0.0000    0    6.8003814E-02  hmd oxd
1    1854.30    144.67    0.0000    0.0000    0    6.8002697E-02  hmd oxd
1    1900.02    142.85    0.0000    0.0000    0    6.8001554E-02  hmd oxd
1    1946.81    141.05    0.0000    0.0000    0    6.8000384E-02  hmd oxd
1    1994.70    139.45    0.0000    0.0000    0    6.7999187E-02  hmd oxd
1    2043.71    138.18    0.0000    0.0000    0    6.7997961E-02  hmd oxd
1    2093.87    136.92    0.0000    0.0000    0    6.7996708E-02  hmd oxd
1    2145.20    135.68    0.0000    0.0000    0    6.7995424E-02  hmd oxd
1    2197.73    134.46    0.0000    0.0000    0    6.7994111E-02  hmd oxd
failt: Outer overpack LC initiated at 2251.489900000000  years
failt: Outer overpack LC initiated at 2217.888650000000  years
failt: Outer overpack LC initiated at 2214.528525000000  years
failt: Outer overpack LC initiated at 2212.848462500001  years
failt: Outer overpack LC initiated at 2212.008431250000  years
1    2251.49    133.24    0.2730    0.4099    1    5.7841544E-02  local
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    2306.51    132.06    -9.9599   -10.3811    1   -6.9455288E+01  general
==========================================================================
===========
              wp wetting time [yr]:       2198.
              wp failure time [yr]:       2251.
     penetration by dry oxidation [m]:      2.006E-03
              echoed input data in:      echo_fail.dat
          output data are in files:      ebstrh.dat and corrode.out
==========================================================================
===========
```

5/12/05 - The following files for SCR546 and the SCR546 Test Plan were completed and submitted to R. Janetzke.

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: R. Codell Date: 2-2-2005	**6. Change Authorized by** (*Software Developer*): 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: R. Codell	**Date:** 2-12-05	
9. Description of Acceptance Tests: See attachment for description of acceptance tests.		
10. Tested by: ~~O. Osidele~~ R. Rice	**Date:** 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
         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
```

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:

6. Examine the peak mean dose and the time of the peak mean dose from these runs in the screenprint
7. Compare the values in #1 from corresponding TPA Versions 5.0.0g and 5.0.0h code runs
8. 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: PASS

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 *ebsrel.rlt*

- **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: PASS

It is important to note that the RELEASET code did not exhibit the 20 times faster performance stated in the SCR. Instead, performance was affected as shown in the previous table. This is thought to be attributable to differences between TPA Versions 4.1 and 5.0, since the code developer for this SCR (R. Codell) modified, tested, and submitted modifications to the TPA Version 4.1 code RELEASET source code. Those modifications were then incorporated into the TPA Version 500g code. However, as stated in the SCR, release rates were impacted as early times, but the later release rates were not different at longer simulation times.

5/19/05

The TPA Version 5.0.1beta code was made available for validation testing. Using this version of the TPA code on GRYPHON, the following observations were made and communicated to R. Janetzke (told S. Mohanty about these observations and will inform him when he lets me know he is available). (Note that (1) these runs were conducted by modifying the maximum simulation time from 1e4 to 1e6 yrs and increasing the number of time steps to 4800 from the end of the compliance period to the maximum time and (2) the complete 500 realization runs were accomplished by removing all colloids and also leaving only I129 and Tc99 as aqueousnuclides.)

1. In 500 realizations, 99+% of each of the subarea loop calculations have no WP failures in 1e6 yr (this is from a 500 realization, basecase run). For the remaining subarea/realization calculations, there are two cases of failures beyond 2,000 yrs (sa4real12 at 282,000 yrs and sa5real75 at 680,000 yr) which have LC that doesn't completely fail the outer overpack and then a few 100,000 yrs are required to failure the outer overpack and the remaining 21 cases have WP failure complete outer overpack corrosion by LC prior to 2,000 (sa2real75 at 770yrs; sa3real89 at 1,400 yrs; sa3real89 at 1,400 yrs; sa2real123 at811 yrs; sa3eral123 at 1,130 yrs; sa5real123 at 730 yrs; sa2real147 at 1,641 yrs; sa3real147 at 1,766 yrs; sa5real147 at 1,562 yrs; sa6real147 at 1,641 yrs; sa1real222 at 922 yrs; sa2real222 at 1,313 yrs; sa3real222 at 1,601 yrs; sa4real222 at 1,048 yrs; sa5real222 at 1,130 yrs; sa6real222 at 1,415 yrs; sa4real392 at 832 yrs; saq5real392 at 876 yrs; sa2real408 at 1,219 yrs; sa3real408 at 1,313 yrs; sa5real408 at 1,250 yrs; and sa6real408 at 1,219 yrs.

2. In 500 realizations, the statement in the screenprint about exceeding the fracture permeability and needing to set the saturation at 1.00 occurred in 9 out of 3,000 (0.3%) of the subarea/realization calculations. These were sa2real287, sa5real287, sa1real322, sa2real322, sa3real322, sa5real322, sa6real322, sa2real434, and sa5real434.

3. Implications of #1 above appear to be that average WP lifetime is about 4 or 5 million years.

4. TPA code execution stopped in sa4real1 with basecase 1e6 yrs, 4800 time steps *tpa.inp* file run because of UZ NEFTRAN array out of bounds for the Cm245->Am241->etc chain.

5. In 350 realizations, TPA code execution stopped in sa4real2 with basecase 1e6 yrs, 4800 time steps *tpa.inp* file run because of UZ NEFTRAN array out of bounds for the Cm245->Am241->etc chain (this is similar to #4 above).

6. In 500 realizations, TPA code execution stopped in sa2real1 with basecase 1e6 yrs, 4800 time steps *tpa.inp* file run because of UZ NEFTRAN array out of bounds for the U234->Th230->etc. chain (this is a different chain than #4 and #5 above).

7. Maximum WP temperature now appears to be about 170 deg C (compared to TPA Version 500o which had maximum WP temperatures over 400 deg C).

8. There are many WP failures now form SEISMIC events (maybe about 40-50% of subarea/realization calculations), including subarea/realization calculations with multiple SEISMIC event failures (R. Janetzke mentioned there was a new SEISMIC hazardcurve)

9. For the bathtub model, still observing releases from the WP before it is filled with water (releases begin when water starts contacting the WP). See the file *ebsthr.dat* for failure times and the *relcum.out* file for startfill time, stopfill time, etc. information.

5/20/05

After meeting with R. Janetzke and C. Scherer yesterday, prepared the following initial list of tests for Task ID 11 (Checkpoint/restart; system tests) for TPA 5.0.1 Module Validation. This initial list of tests includes verifying the correct functioning/specification of the following:

1. Checkpoint/restart for times beyond 100,000 yrs

2. WP counting (i.e., intrusive VOLCANO, INITIAL, FAULTING, SEISMIC, and CORROSION) for the number of WPs in a subarea - note that extrusive VOLCANO WP failures are intended to be double counted with the GW pathway WP failures

3. With VOLCANO activated, use a switch to select (i) the new ASHREMOB model and (ii) the previous model to compute GS dose; perform simulations with and without the DirectReleaseOnly switch activated

4. Determine consistency in output and convergence of results based on the number of time steps and the maximum simulation time (i..e, up to 5,001 time steps and a maximum

simulation time of 1,000,000 yrs); run with a Compliance Period different than 10,000 yrs; and run with 1 large subarea with the about the same area that covers roughly the same region as subareas 1 through 6

5. Consistency in subarea coordinates in the *tpa.inp* file; repository outline, panels, and emplacement blocks in the *repdes.dat* file; and drift endpoints in the *drifts.dat* file - also, consistency in the number of WPs assigned to each subarea based on the information in these 3 files; perform tests using *tpa.inp* subarea coordinates and *repdes.dat* information with known outcomes

6. Select 1 subarea, divide that subarea (i.e., into 4 pieces), and examine TPA code output for the two cases

7. Activate the switch to run SZFT NEFTRAN twice using separate TUFF and ALLUVIUM legs and compare with the switch not activated (i.e., one SZFT NEFTRAN execution with two legs)

8. Functioning of the *tpa.inp* file flags (perform using one-on and all-others-off approach)

9. Failure to execute any of the TPA code standalone code results in stopped execution of the TPA code

10. Using a data code modification for calculating RDs, the values in the *tpa.inp* file are used in TPA code calculations

(Related to #10 - Note: call Paul to ask about the information in the data file *coefkdeq.dat* to calculate RDs and whether this has been tested and is a part of the RARI Progress Report - or whether these values have been updated since then - this will determine the extent of needed testing for these values - I think, by looking at the comments, this information is included in the Progress Report and has been tested a lot already)

- the above is a preliminary/initial list of tests that will be refined and added to, as needed.

5/25/05

Talked with R. Janetzke and S. Painter and learned the following about reversible and irreversible colloids.

The flag in the *tpa.inp* file for the "IrreversibleColloidModel[0=no,1=yes]" parameter is used to specify whether colloids (i.e., J-species) are tracked (= 1) or whether they are set equal to zero (

= 0). This parameter could be named something like “HaveJ-SpeciesColloids[0=1,1=yes]”. Basecase is =1 (i.e., track colloids)

For the non-J-species (or reversibles), the TPA code has the capability to adjust RD/KD and mass transfer values in the NEFTRAN input file *nefii.inp* using “concentration” parameters for each UZ and SZ layer in the *tpa.inp* file. The TPA code modifies RD/KD and mass transfer values based in *nefii.inp* based on these values. Note that, in contrast to the irreversible case (i.e., colloids) which tracks 2 separate species/phases, the reversible case lumps both species/phases together. Reversibles are part of the basecase since the “concentration” are non-zero. Reversibles can be removed by setting these “concentrations” equal to zero.

5/31/05

Completed testing for SCR571. The completed SCR and Test Plan follow. Both the SCR and Test Plan were forwarded onto R. Janetzke in an email attachment. A CD containing all files from this test and the Test Plan was delivered by hand to R. Janetzke.

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 Test Plan that is attached to and follows this SCR		
10. Tested by: R. Rice	**Date:** 5/31/05	

CNWRA Form TOP-5 (05/2000)

SCR571 UPDATE REQUIREMENTS for TPA.INP

Status (ADD, DELETE, MODIFY TO, MODIFY FROM)	**Module**	**Paramete r 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 ',
***************
```

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_TPA_Runs\tpa500w\test_0_basecase and \SCR571_TPA_Runs\tpa500x\test_0_basecase (archived on a CD)

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_TPA_Runs\tpa500w\test_1 and
\SCR571_TPA_Runs\tpa500x\test_1 (archived on a CD)

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_TPA_Runs\tpa500w\test_2 and
\SCR571_TPA_Runs\tpa500x\test_2 (archived on a CD)

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-579</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-579.

Prepared test plans for TPA 501 Validation Testing - Tasks 2 (INVENT), 8 (EBSREL/RELEASET), and 12 (NUMRECIP). Submitted these test plans as *.WPD files to R. Janetzke via three emails in three separate attachments. Note that C. Scherer is preparing the test plan for Task 11 (Checkpoint/restart and system-level).

The contents of these three test plans are listed below.

SOFTWARE VALIDATION TEST REPORT (SVTR)

SVTR#: *Task ID - 2*	**Project#: 20.06002.01.352**
Software Name: TPA	**Version: 5.0.1betaA**
Test ID: *INVENT*	**Test Series Name: (none)**

Test Method

x code inspection	x spreadsheet
x output inspection	x graphical
x hand calculation	□ comparison with external code results

Test Objective: Verify implementation of new data in *burnup.dat* and consistency in using the year for emplacement in *burnup.dat* and *tpa.inp* files. Confirm the addition of new radionuclides to *nuclides.dat* (colloids added) and their participation in release calculations in the EBS, UZ, SZ, and dose computations.

Test Environment Setup

Hardware (platform, peripherals): P-IV Toshiba Laptop, AMD Athlon Desktop, and SUN PC system

Software (OS, compiler, libraries, auxiliary codes or scripts): XP Professional, LF95 FORTRAN

Input Data (files, data base, mode settings): Execute the basecase TPA 5.0.1betaA code for a single subarea and one realization; aqueousnuclide and colloid chains will be modified in *tpa.inp* and the time for waste emplacement in *burnup.dat* and *tpa.inp* will be modified to values that are anticipated to yield expected results in the nuclides tracked in calculations and in the initial inventory used in release calculations.

Assumptions, constraints, and/or scope of test: Execute the TPA 5.0.1betaA code using both basecase and modified values in the *burnup.dat* and *tpa.inp* files.

Test Procedure: See the information following this SVTR.	
Test Results **Location: See the attached CD.** **Test Criterion or Expected Results: See "Expected Results" on the Test Procedure following this SVTR.** **Test Evaluation (Pass/Fail):**	
Notes: (none)	
Tester: R. Rice	**Date: 7/1/05**

6/2/05

TEST PROCEDURE

TPA 5.0.1 Module Validation - Task ID 2

Task Title: "invent" - Verify implementation of new data in *burnup.dat* and consistency in using the year for emplacement in *burnup.dat* and *tpa.inp* files. Confirm the addition of new radionuclides to *nuclides.dat* (colloids added) and their participation in release calculations in the EBS, UZ, and SZ and dose computations.

Point of Contact: Rob Rice

Other team member(s): Oleg Povetko

Suggested Reviewer: Lane Howard (*burnup.dat* and *tpa.inp*); Rasvan Nes (*nuclides.dat*)

Test Suite: See below

Files to be modified: *burnup.dat*, *tpa.inp*

Output files: *ebstrhc.inp* (NFENV output), *trelease.out* (RELEASET output), *ebspac.nuc* (RELEASET input), *nefiiuz.out* (UZ NEFTRAN output), *nefiisz.out* (SZ NEFTRAN output), *rgwnr.tpa*, and screenprint

Test methodology: **<u>TPA CODE EXECUTION</u>**

<u>BURNUP</u>

– Execute the TPA Version 5.0.1betaA code using the basecase *tpa.inp* file for one realization and subarea 1 with maximum simulation times of 10kyr, 100kyr, and 1000kyr. Use the TPA Version 5.0.1betaA code *burnup.dat* file and the TPA Versions 5.0.0g and 5.0.0o code *burnup.dat* file since these files show different levels of burnup . **Expected Results:** Plotting the temperatures and *burnup.dat* values should show that the highest temperatures are associated with highest burnup; likewise, the lowest temperatures are associated with lowest burnup.

<u>YEAR OF EMPLACEMENT</u>

– Execute the TPA Version 5.0.1betaA code using the basecase *tpa.inp* file with VOLCANO activated for one realization and subarea 1 with maximum simulation times of 10kyr, 100kyr, and 1000kyr. Then, modify the year of emplacement in the *tpa.inp* and *burnup.dat* file to 2133 (i.e., one hundred years later).
Expected Results: Using spreadsheet/hand calculations, the inventories in *ebspac.nuc* (for GW) and in the screenprint for the GS should be decayed 100 years. Note: evaluate selected radionuclides.

<u>NUCLIDES.DAT</u>

– Execute the TPA Version 5.0.1betaA code using the basecase *tpa.inp* file for one realization and subarea 1 with maximum simulation times of 10kyr, 100kyr, and 1000kyr. Then, add the new radionuclides in *nuclides.dat* to the *tpa.inp* file. Note: other parameters will also need to be added to the *tpa.inp* file that are radionuclide-specific, like gap fractions and solubilities.
Expected Results: Inspecting *ebspac.nuc*, *nefiiuz.inp*, and *nefiisz.inp* should show these radionuclide releases in TPA code EBS, UZ, SZ, and dose calculations.

SOFTWARE VALIDATION TEST REPORT (SVTR)

SVTR#: *Task ID - 8*	**Project#: 20.06002.01.352**
Software Name: TPA	**Version: 5.0.1betaA**
Test ID: *EBSREL/RELEASET*	**Test Series Name: (none)**

Test Method

- □ code inspection
- x output inspection
- □ hand calculation
- x spreadsheet
- x graphical
- □ comparison with external code results

Test Objective: Evaluate the use of the time-dependent parameter *fwet*, the drip shield factor, and the weld factor in the RELEASET standalone code calculations for determining the flow of water onto the waste package. The *fwet* parameter is from the *wpflow.def* file and is written to the RELEASET input file *ebsflo.dat*; whereas the drip shield factor and the weld factor are computed in RELEASET using information from the RELEASET input file *ebstrh.dat*. Also, examine the functionality of RELEASET gap fraction and cladding.

Test Environment Setup

Hardware (platform, peripherals): P-IV Toshiba Laptop, AMD Athlon Desktop, and SUN PC system

Software (OS, compiler, libraries, auxiliary codes or scripts): XP Professional, LF95 FORTRAN

Input Data (files, data base, mode settings): Execute the basecase TPA 5.0.1betaA code for a single subarea and one realization; *wpflow.def* will be modified to values that are anticipated to yield expected results; and screenprints will be added to RELEASET following calculation of *qin()* to show all of the factors used. Values for gap fraction and cladding in the *tpa.inp* file be modified one at a time.

Assumptions, constraints, and/or scope of test: Execute the TPA 5.0.1betaA code and then use the RELEASET input files generated from this run in RELEASET standalone tests.

Test Procedure: See the information following this SVTR.

Test Results

Location: See the attached CD.

Test Criterion or Expected Results: See “Expected Results” in the Test Procedure following this SVTR.

Test Evaluation (Pass/Fail):

Notes: (none)	
Tester: R. Rice	Date: 7/1/05

TEST PROCEDURE

TPA 5.0.1 Module Validation - Task ID 8

Task Title: "ebsrel/releaset" - determining flow in RELEASET using *fwet* and the drip shield factor and the weld factor; examine functionality of RELEASET gap fraction and cladding

Point of Contact: Rob Rice

Other team member(s): Osvaldo Pensado

Suggested Reviewer: Dick Codell

Test Suite: See below

Files to be modified: *wpflow.def*, *ebsflo.dat*, *ebstrh.dat, releaset.f*,

Output files: *ebsflo.dat* (*ebsrel.f* output), *ebsnef.dat* (TPA code RELEASET output), *trelease.out* (RELEASET output), and RELEASET screenprint

Test methodology: **1. TPA CODE EXECUTION**

– Execute the TPA Version 5.0.1betaA code using the basecase *tpa.inp* file for one realization and subarea 1 with maximum simulation times of 10kyr, 100kyr, and 1000kyr. **Expected Results:** The "fwet" values in the *wpflow.def* file should be correctly transferred and mapped to TPA code times in the RELEASET input file *ebsflo.dat*.

– Execute the TPA Version 5.0.1betaA code using the basecase *tpa.inp* file for one realization and subarea 1 with maximum simulation times of 10kyr, 100kyr, and 1000kyr. Modify parameters, one at a time, for gap fractions and cladding in the *tpa.inp* file (specifically, GapFractionFor[***element]***, CladdingCorrectionFactor, CladdingVelocityEnhancementFactor[], FuelRodHalfLength[m], and FuelRadiusInRod[m]) and execute the TPA code again.
Expected Results: The release rates in the RELEASET output file *ebsnef.dat* should be either increased or decreased according to the change in these parameters (i.e.,

increasing gap fraction, cladding correct factor, velocity, length, and radius should increase the release rates).

2. RELEASET STANDALONE EXECUTION

- Use the RELEASET input files generated from the TPA code execution described above for 1000kyr.
- Modify RELEASET to screenprint values for *qin()* and all of the factors used to
- Modify values for "fwet" in the *ebsflo.dat* file to zero and execute RELEASET.

  Expected Results: There should be zero release in *trelease.out*.
- Modify values for fwet" in the *ebsflo.dat* file to 1.0 and 5.0 for all times and execute RELEASET twice.

  Expected Results: the releases in *trelease.out* should increase by a factor of 5.0 for solubility-limited releases indicated in last column of *trelease.out*.
- Modify the WP corrosion failure time, the drip shield failure time, and the weld failure time in the *ebstrh.dat* file for all six possible arrangements for the timing of these events and for situations when these event occur concurrently. Execute RELEASET for each of these situations.

  Expected Results: In the screenprint, the correct values for the weld factor and the drip shield factor, which are based on the WP corrosion, the drip shield, and the weld failure times, should be used to compute *qin()* in RELEASET. (Note the drip shield factor should be zero prior to drip shield failure; the weld factor should be zero prior to occurrence of either weld failure or WP corrosion failure; if WP corrosion failure occurs before weld failure, the weld factor should be equal to one; and if weld failure is before WP corrosion failure, the weld factor should be equal to area of spent fuel exposed from weld failure and then once WP corrosion failure occurs this weld factor should be equal to one.)

SOFTWARE VALIDATION TEST REPORT (SVTR)

SVTR#: *Task ID - 12*	**Project#: 20.06002.01.352**
Software Name: TPA	**Version: 5.0.1betaA**
Test ID: *NUMRECIP*	**Test Series Name: (none)**

Test Method

□ code inspection	x spreadsheet
x output inspection	x graphical
x hand calculation	x comparison with external code results

Test Objective: Determine whether the four new *numrecip.f* subroutines correctly determine roots within the specified intervals and tolerance using (i) the TPA code and (ii) a test driver

Test Environment Setup

Hardware (platform, peripherals): P-IV Toshiba Laptop and AMD Athlon Desktop

Software (OS, compiler, libraries, auxiliary codes or scripts): XP Professional, LF95 FORTRAN, test driver

Input Data (files, data base, mode settings): basecase *tpa.inp* file with 10 kyr, 100 kyr, and 1,000 kyr maximum times; also, driver with test cases for each of the four *numrecip.f* subroutines: zbrent, zbrent1, zbrak, zbrak1

Assumptions, constraints, and/or scope of test: TPA code and test driver execution

Test Procedure: See the information following this SVTR.

Test Results

Location: See the attached CD.

Test Criterion or Expected Results: Results should be equal to analytical solutions and within the specified interval and tolerance

Test Evaluation (Pass/Fail):

Notes: (none)

Tester: R. Rice	**Date: 7/1/05**

TPA 5.0.1 Module Validation - Task ID 12

Task Title: "numrecip" - New subroutine

Point of Contact:	Rob Rice
Other team member(s):	Ron Janetzke
Suggested Reviewer:	Gordon Wittmeyer (agreed to this review task)
Test Suite:	See below
Subroutines to be tested:	zbrent, zbrent1, zbrak, zbrak1

Test methodology:

1. TPA CODE IMPLEMENTATION

- modify the source code for these 4 subroutines in the *numrecip.f* file to screenprint the input and output for each subroutine
- execute the TPA Version 5.0.1betaA code using the basecase *tpa.inp* file for 10kyr, 100kyr, and 1,000 kyr with the 4,800 time steps for the 1,000 kyr case
- for each of the four subroutines, use spreadsheet calculations/plt values to determine the roots of the functions; verify that these routines are computing the correct roots during TPA code execution (given the intervals and tolerances in those instances)

2. TEST DRIVER

- write a driver with test cases that calls these four subroutines
- test cases will contain 0^{th}, 1^{st}, 2^{nd}, 3^{rd}, and 4^{th} order polynominals with known zeros
- interval testing (single and multiple intervals) will include specifications less than, within and greater than the known solutions for the polynominals
- range of tolerances (high, medium, and low values) will be investigated to determine the correctness of the subroutine results
- the correct "errorflag" value will be checked for a correct value (i.e., the lack of convergence to a known root after 30,000 iterations)

6/30/05

Performed test runs on the "TPA" machine, which is now loaded with the 64-bit OS instead of the 32-bit OS (XP Professional). For a 1,024 realization basecase TPA501betaC simulation, found the run times increased slightly with the 64-bit OS (4h to 4h23m for 1 simulation; 4.75h to 5h for 2 simulations; 7h to 7h20m for 3 simulations; and 9.3h to 9h38m for 4 simulations). Also, found screenprint error messages for the 2, 3, and 4 simulation case with the 32-bit and 64-bit Oss. There are a difference in TPA code results in one of the 4 simulations - all other cases and outputs were not affected in the 64-bit OS runs (note that results were different in the 32-bit OS runs when there was a screenprint message for the 2, 3, and 4 simulation cases).

The following contains the 64-bit OS screenprints for 4 simulations (note the 4 simulation cases were repeated once - see "try2"). Below, there are also results from the file comparisons between the *tpa.out* files.

TPA 501betaC - Basecase with 10,000 years, 1024 realizations, run on "TPA"

FIRST RUN

```
d:\rrice\tpa501betaC\4runs_1user\run1>..\..\tpa.exe > tpa.out
The file exists (CreateFile, errno=80, unit= 6).
The file exists (CreateFile, errno=80, unit=30).
The file exists (CreateFile, errno=80, unit= 6).

d:\rrice\tpa501betaC\4runs_1user\run2>..\..\tpa.exe > tpa.out


d:\rrice\tpa501betaC\4runs_1user\run3>..\..\tpa.exe > tpa.out
The file exists (CreateFile, errno=80, unit= 7).
 Error occurs at or near line 81 of _redflt_
 Called from or near line 110 of _MAIN__

d:\rrice\tpa501betaC\4runs_1user\run4>..\..\tpa.exe > tpa.out
The file exists (CreateFile, errno=80, unit= 6).
```

SECOND RUN

```
d:\rrice\tpa501betaC\4runs_1user\run1\try2>..\..\..\tpa.exe > tpa.out
The file exists (CreateFile, errno=80, unit=23).
 Error occurs at or near line 1170 of _MAIN__
The file exists (CreateFile, errno=80, unit= 6).
The file exists (CreateFile, errno=80, unit= 4).

d:\rrice\tpa501betaC\4runs_1user\run2\try2>..\..\..\tpa.exe > tpa.out

d:\rrice\tpa501betaC\4runs_1user\run3\try2>..\..\..\tpa.exe > tpa.out
The file exists (CreateFile, errno=80, unit=30).
```

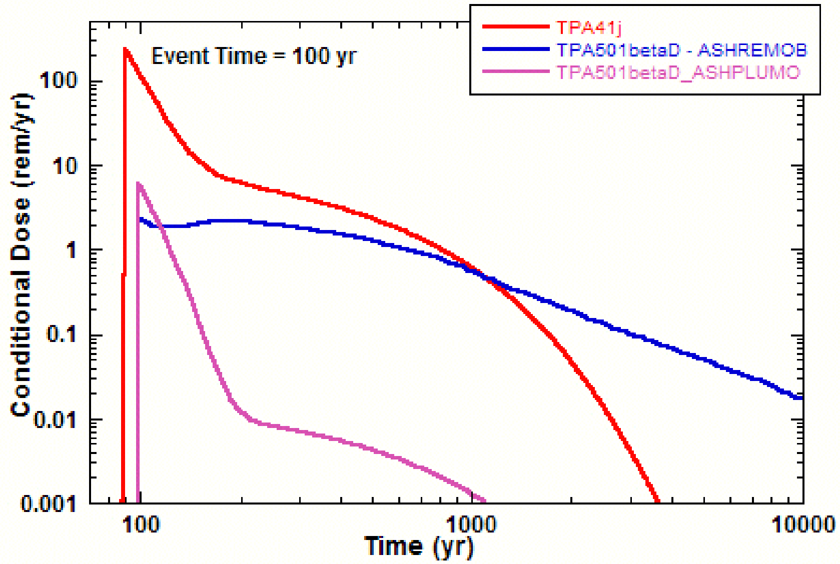
```
The file exists (CreateFile, errno=80, unit= 6).
The file exists (CreateFile, errno=80, unit=30).

d:\rrice\tpa501betaC\4runs_1user\run4\try2>..\..\..\tpa.exe > tpa.out
The file exists (CreateFile, errno=80, unit=30).
The file exists (CreateFile, errno=80, unit= 7).
 Error occurs at or near line 81 of _redflt_
 Called from or near line 110 of _MAIN__
The file exists (CreateFile, errno=80, unit= 6).
The file exists (CreateFile, errno=80, unit=30).
The file exists (CreateFile, errno=80, unit= 6).
The file exists (CreateFile, errno=80, unit= 6).
```

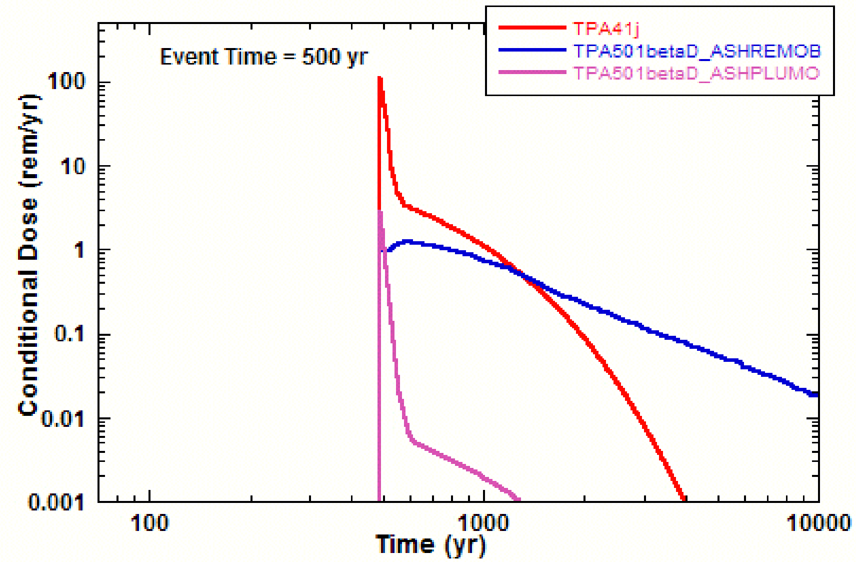
ALL SHOW NO DIFFERENCES, EXCEPT FOR START TIME OF THE RUN AND THE FOLLOWING:

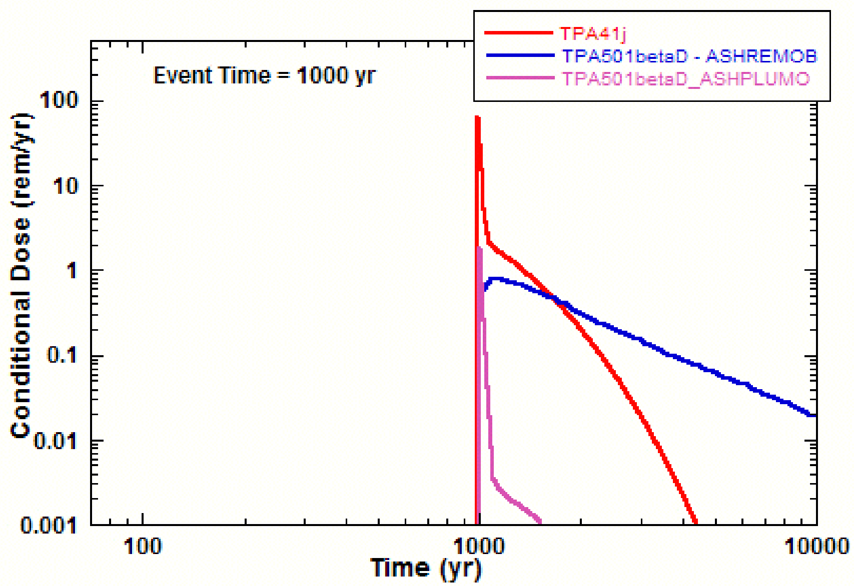
```
d:\rrice\tpa501betaC\4runs_1user\run4\try2>fc tpa.out ..\tpa.out
Comparing files tpa.out and ..\TPA.OUT
***** tpa.out
        exec: Welcome to TPA Version 5.0.1betaC
      Job started: Thu Jun 30 18:20:27 2005
===============================================================
***** ..\TPA.OUT
        exec: Welcome to TPA Version 5.0.1betaC
      Job started: Thu Jun 30 08:24:22 2005
===============================================================
*****

***** tpa.out
            I129    1.0966E-02 [mrem/yr]  at  2.363E+03 yr
            Tc99    3.4337E-03 [mrem/yr]  at  1.995E+03 yr
            Cl36    6.2777E-04 [mrem/yr]  at  1.995E+03 yr
            Se79    2.4237E-04 [mrem/yr]  at  2.863E+03 yr
***** ..\TPA.OUT
            I129    1.0966E-02 [mrem/yr]  at  2.363E+03 yr
            Tc99    6.7448E-04 [mrem/yr]  at  2.363E+03 yr
            Cl36    3.8173E-04 [mrem/yr]  at  2.363E+03 yr
            Se79    2.4237E-04 [mrem/yr]  at  2.863E+03 yr
*****

d:\rrice\tpa501betaC\4runs_1user\run4\try2>
```

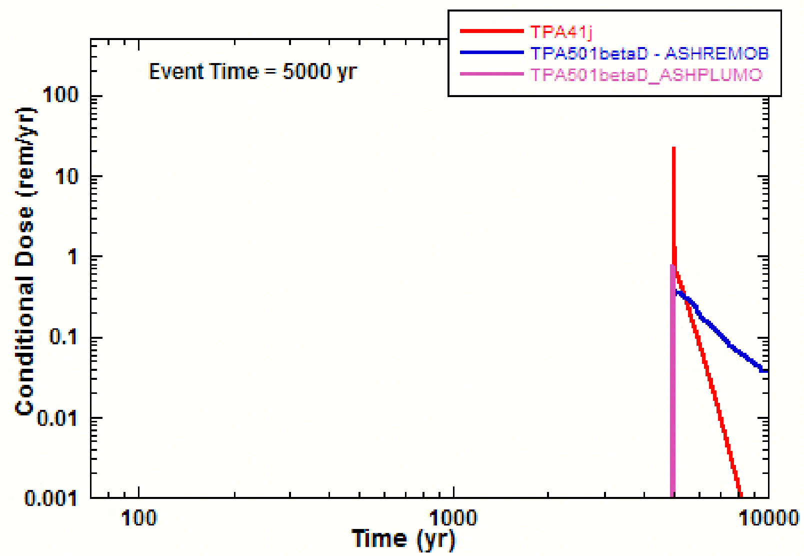
In summary, the 32-bit and 64-bit OS performance appears to be equivalent on the “TPA” machine.

July 14, 2005 - prepared plots of results with the ASHREMOB model and without that model. Those plots are provided below.


Event Time = 100 yr
TPA41j
TPA501betaD - ASHREMOB
TPA501betaD_ASHPLUMO
Conditional Dose (rem/yr)
100
10
1
0.1
0.01
0.001
100
1000
10000
Time (yr)


Event Time = 500 yr
TPA41j
TPA501betaD_ASHREMOB
TPA501betaD_ASHPLUMO
Conditional Dose (rem/yr)
100
10
1
0.1
0.01
0.001
100
1000
10000
Time (yr)


Event Time = 1000 yr
TPA41j
TPA501betaD - ASHREMOB
TPA501betaD_ASHPLUMO
Conditional Dose (rem/yr)
100
10
1
0.1
0.01
0.001
100
1000
10000
Time (yr)


Event Time = 5000 yr
TPA41j
TPA501betaD - ASHREMOB
TPA501betaD_ASHPLUMO
Conditional Dose (rem/yr)
100
10
1
0.1
0.01
0.001
100
1000
10000
Time (yr)

July 20, 2005 - the following information summarizes a discussion of the impacts of including glass with spent fuel in the TPA code. Emailed this information to the participants in the meeting.

Summary of Telephone Discussion
Individuals - S. Mohanty, R. Janetzke, O. Pensado, R. Rice
TPA Version 501betaE

Topic - Impacts of Adding Glass on the Heat Load

1. S. Mohanty wanted to know how glass was modeled in betaE - including its physical distribution and heat load.

2. R. Rice had told S. Mohanty that the number of WPs increased from 8,876 to 12,176 with the addition of glass. Also, with the additional of glass, Subarea 3 became completely filled (from 5,318 to 6,148 WPs); Subarea 7 became completely filled (from 0 to 723 WPs); and Subarea 8 became filled with 1,747 equivalent WPs (from 0 to 1,747 WPs).

3. R. Janetzke noted that an equivalent WP was used to determine the emplacement of WPs in each subarea. The equivalent WP contained about 5.5 MTU/WP, instead of 7.89 MTU/WP for SF and about 0.25 for glass (as specified in the tpa.inp file). The TPA code drift calculator fills each subarea in TPA 501betaE with these equivalent WPs. For temperature calculations, equivalent WPs are used (i.e., the burnup.dat file was adjusted to account for glass). For release calculations, those equivalent WPs are partitioned between SF and glass according to the fraction of glass in the repository (this is a tpa.inp) parameter. Then, RELEASET is executed twice - once for SF failed WPs and once for glass failed WPs. The release rates are summed and then that release is partitioned into colloids.

4. O. Pensado stated the burnup.dat file was modified to maintain 1.45 kW/m in the drift. S. Mohanty noted that by adding glass inventory, the Repository AML would decrease to less than 60 MTU/acre which is a design criterion. (From TPA code results, by adding glass, the AML decreases from about 67 to 54 in TPA Versions betaD to betaE). O. Pensado said the 1.45 kW/m was also a design criterion and that DOE Technical Basis documents referred to this value and not the AML of 60 MTU/acre. O. Pensado said that in the TPA code, the AML and linear heat loading design criteria cannot both be satisfied. Since DOE documents referred to the linear heat load, his approach was to meet that design criterion and not the AML.

July 20, 2005 - the following information was prepared to show the difference in results between TPA code 4.1jpd and the 5.0.1beta versions.

	TPA 4.1j	**TPA 5.0.1betaD**
Peak Expected Dose	0.021 mrem/yr at 9,769 yr (basecase, 350 realizations, 10,000 yr)	106 mrem/yr at 9,543 yr (basecase, 1024 realizations, 10,000 yr)

% Peak Expected Dose

TPA 4.1j		TPA 5.0.1betaD	
Tc-99	**51.90%**	**Pu-239**	**50.20%**
I-129	**25.43%**	**Pu-240**	**38.67%**
Np-237	**20.43%**	**Am-243**	**8.63%**
Cl-36	0.13%	Tc-99	0.99%
Se-79	0.02%	I-129	0.80%
		Cm-245	0.19%
		Am-241	0.18%
		U-234	0.10%
		Th-230	0.06%
		Np-237	0.05%
		Cm-246	0.03%
		Se-79	0.02%
		U-238	0.02%
		Cl-36	0.01%
		U-233	0.01%

Simulation Time Effect on Peak Expected Dose

TPA 4.1j	TPA 5.0.1betaD
10,000 yrs: 0.021 mrem/yr at 9,769 yr 100,000 yr: 9.9 mrem/yr at 100,000 yr	available results: 10,000 yr; 100,000 yr; and 1,000,000 yr simulations give similar results (i.e., ~100 mrem/yr at ~10,000 yr)

WP failures

TPA 4.1j	TPA 5.0.1betaD	
only initial defective WPs in 10,000 yr (average = 0.5% of all WPs) WP corrosion failures 40,000 - 100,000 yr	initial, seismic, corrosion (localized), weld	
	initial: average =	0.5% of all WPs
	seismic: average =	12.5% of all WPs at 762 yrs (325 to 1,562 yr)
	corrosion: average =	5.7% of all WPs at 1,092 yrs (515 to 3,227 yr)
	weld: average = calculations	26% of subarea at 1,153 yrs (475 to 6,040 yrs)

In addition to the 5.7% corrosion failures

For 1,000,000 yr/350 realizations:

0.1% realizations (all subareas in 1 realization) have WP corrosion failure from 47,000 to 57,000 yr; and 0.1% of subareas (6 subareas) have WP corrosion failure from 640,000 to 900,000 yr. There are no corrosion failures in all other cases for 1,000,000 yrs.

WP Failure Effect on Peak Expected Dose

no effect (only initial defective WP failures in 10,000 yr)

basecase: 106 mrem/yr at 9,107 yr
w/o irrev*: 3.1 mrem/yr at 2,863 yr (34x less)
w/o corr*: 51.2 mrem/yr at 10,000 yr (52% decrease)
w/o seis*: 79.3 mrem/yr at 9,543 yr (25% decrease)
w/o weld*: 91.7 mrem/yr at 8,896 yr (13% decrease)

Also,
only initial*: 0.052 mrem/yr at 2,796 yr
(i.e., w/o irrev/corr/seis/weld) (2,040x less)
Note: I129 (65%); Tc99 (33%); Cl36 (1%) contribute to this peak. (matches TPA4.1j)

only initial/irrev*: 2.6 mrem/yr at 10,000 yr
(i.e., w/o corr/seis/weld) (50x more)

w/o irrev/corr*: same as w/o irrev

w/o seis/weld*: 63.8 mrem/yr at 9,322 yr

(* = all other settings are basecase)

Individual Realization Effect on Peak Expected Dose

1% of realizations (10/1,024) constitute 90% of Peak Expected Dose (1 realization contributes to 50% o Peak Expected Dose at ~50 rem/yr)

Drip Shield Failure Time

sampled parameter (lognormal distribution)	calculated with "dsfail"
mean = 7,422 yr (2,700 to 20,400 yr)	mean = 1,036 yr (658 to 1,131 yr)

Climate Data (in "climato2.dat")

100,000 yr climate cycle (symmetric)

no repeating cycles/not symmetric/varying relative maximums/minimums with varying durations during 1,000,000 yrs

Flow of Water into WP

determined from "ebsflo.dat" and multiplicative constant factors for Fmult, Fow, and flowfactor

determined from "ebsflo.dat" and multiplicative time dependent factors for Fmult and Fow; also using time varying factors for the drip shield and the weld; flowfactor is still constant (note: also applying a time varying sawet factor that is specified in "wpflow.dat")

Retardation Factors - SAV

(minimum; average; maximum)
Pu (500; 24,000; 300,000)
Am (8E+04; 8E+08; 7E+10)

(minimum; average; maximum)
Pu (500; 13,0 00; 62,000)
Am (1.7E+05; 5E+8; 8E+09)
Colloid Rd Factor (1; 500; 5,000)

Volcanism - Conditional Peak Expected Dose

	(with ASHREMOB)	Previous Model
100 yr: 230,000 mrem/yr	100 yr: 2,340 mrem/yr (all ~100x less)	5,920 mrem/yr
500 yr: 110,000 mrem/yr	500 yr: 1,230 mrem/yr	2,840 mrem/yr
1,000 yr: 60,000 mrem/yr	1,000 yr: 790 mrem/yr	1,760 mrem/yr
5,000 yr: 25,000 mrem/yr	5,000 yr: 360 mrem/yr	737 mrem/yr

(note: new ASHREMOB model that assumes inhalation pathway dominates [RARI Report]

Number of WPs in Repository/Subareas

```
===================================
   exec: Welcome to TPA Version 4.1j
  Job started: Thu Jul 14 07:22:03 2005
===================================
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
  #     [m^2]      [MTU]
  1   723591.3   11479.9     1455
  2   784763.0   12371.5     1568
  3   390372.0    6114.8      775
  4   207581.3    3361.1      426
  5   378972.8    5996.4      760
  6   424872.5    6714.4      851
  7   163938.3    2548.5      323
  8   393468.9    6674.9      846
  9   660785.5    7708.5      977
 10   589497.1    7069.4      896

Total Area [acre]          =  1165.76297799608
Total Buried Waste [MTU]   =  70039.530000
Repository AML [MTU/acre]  =  60.0804205674
```

```
======================================
   exec: Welcome to TPA Version 5.0.1betaD
  Job started: Wed Jul 06 16:03:12 2005
======================================
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
  #     [m^2]      [MTU]
  1   224091.0    4150.1      526
  2   448476.0    8379.2     1062
  3  2621741.5   41959.0     5318
  4   152357.0    2706.3      343
  5   318122.0    5491.4      696
  6   439350.0    7345.6      931

Total Area [acre]          =  1038.828144304423
Total Buried Waste [MTU]   =  70031.6400000
Repository AML [MTU/acre]  =  67.4140765091
Watts per MTU [W/MTU]      =  967.5799977250
Watts per linear meter of drift [W/m] = 1449.992
```

There are 8,877 WPs in both 4.1j and 5.0.1betaD.

% of WPs in a Subarea

Subarea	%
1	16
2	18
3	9
4	5
5	9
6	10
7	4
8	10
9	11
10	10

Subarea	%
1	6
2	12
3	60
4	4
5	8
6	10

DCFs - Ingestion of Drinking Water

These DCFs decrease by factors of 2 to 5. Average decrease is estimated to be about 50%.

WP Temperature

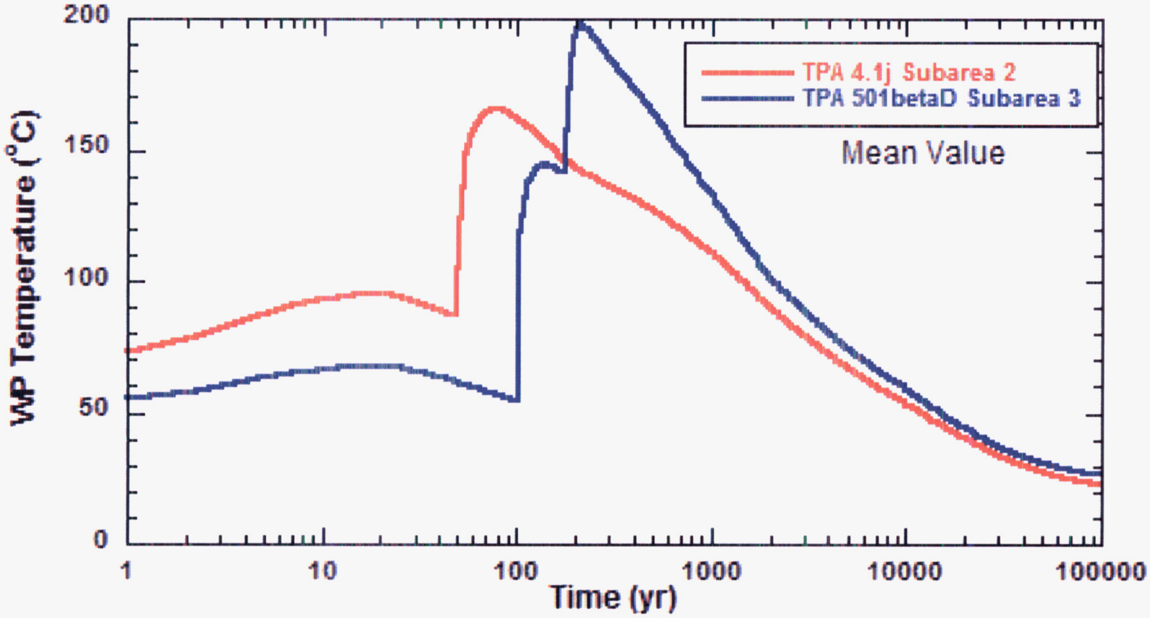
Mean Values
Subarea 2 (largest)
Time of Closure = 50 yr
Peak Temperature = 165 deg C
Time of Peak = 81 yr

Mean Values
Subarea 3 (largest)
Time of Closure = 100 yr
Peak Temperature = 199 deg C
Time of Peak = 208 yr

At times past ~1000 yr to 100,000 yr, both WP temperatures are approximately equal.

At times < 100 yrs, lower WP temperatures in TPA 501betaD (ventilation effects).

In TPA 501betaD, there are rockfall effects on WP temperature.



TPA 4.1j Subarea 2
TPA 501betaD Subarea 3
Mean Value
WP Temperature (°C)
Time (yr)
0
50
100
150
200
1
10
100
1000
10000
100000

Results from TPA 501betaE

Peak Expected Dose in mrem/yr (Time of the Peak)
364 realizations with Simulation Time = 10,000 yr

Subarea	WPs (%total)	Basecase (w/ glass)	WPs (% total)	Basecase (w/o glass)
1	526 (4%)	4.1 (5,676yr)	526 (6%)	3.7 (5,971 yr)
2	1,062 (9%)	9.0 (7,376 yr)	1,062 (12%)	8.4 (8,101 yr)
3	6,148 (50%)	125 (10,000 yr)	5,318 (60%)	99 (10,000 yr)
4	343 (3%)	1.2 (5,696 yr)	343 (4%)	0.87 (5,970 yr)
5	696 (6%)	7.7 (8,101 yr)	696 (8%)	7.6 (7,730 yr)
6	931 (8%)	16.7 (5,063 yr)	931 (10%)	18.2 (5,307 yr)
7	723 (6%)	4.3 (9,107 yr)		
8	1,747 (14%)	194 (10,000 yr)		
Totals	**12,176**	**349 mrem/yr (10,000 yr)**	**8,876**	**124 mrem/yr (10,000 yr)**

(Subareas 3 and 8 have the shortest average and minimum GWTT in UZ and SZ)

Also, note the following.

	Peak Expected Dose in mrem/yr (Time of the Peak)
364 Realizations:	349 mrem/yr (10,000 yr)
1,024 Realizations	278 mrem/yr (10,000 yr)
Simulation Time 10,000 yrs:	278 mrem/yr (10,000 yr) for 1,024 realizations
Simulation Time 100,000 yrs:	365 mrem/yr (10,900 yr) for 1,024 realizations

GWTT UZ and SZ Minimum, Average, and Maximum Values (Basecase/364 Realizations)

	sa1uz	sa2uz	sa3uz	sa4uz	sa5uz	sa6uz	sa7uz	sa8uz	aveuz
min	2.01E+01	2.00E+01	1.50E+01	2.41E+02	4.05E+01	4.43E+01	5.85E+01	1.50E+01	9.24E+01
average	2.73E+02	1.64E+02	7.49E+01	7.43E+02	1.68E+02	3.28E+02	5.58E+02	3.83E+01	2.93E+02
max	1.48E+03	5.87E+02	4.14E+03	3.38E+03	5.44E+02	3.19E+03	3.10E+03	3.44E+03	2.35E+03

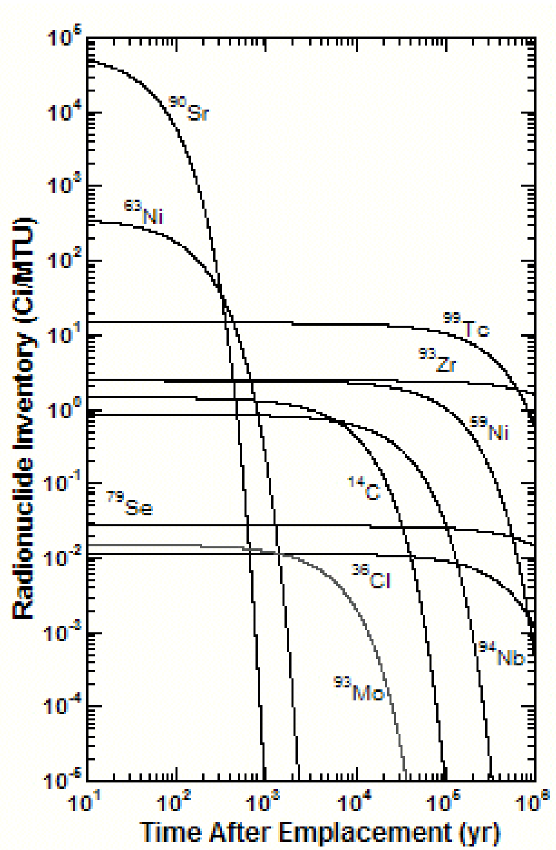
	sa1sz	sa2sz	sa3sz	sa4sz	sa5sz	sa6sz	sa7sz	sa8sz	avesz
min	1.24E+02	1.45E+02	1.40E+02	1.23E+02	1.21E+02	1.19E+02	1.20E+02	1.13E+02	1.26E+02
average	7.23E+02	8.19E+02	7.84E+02	7.13E+02	6.97E+02	6.87E+02	6.92E+02	6.83E+02	7.25E+02
max	2.31E+03	2.55E+03	2.45E+03	2.28E+03	2.24E+03	2.21E+03	2.22E+03	2.29E+03	2.32E+03

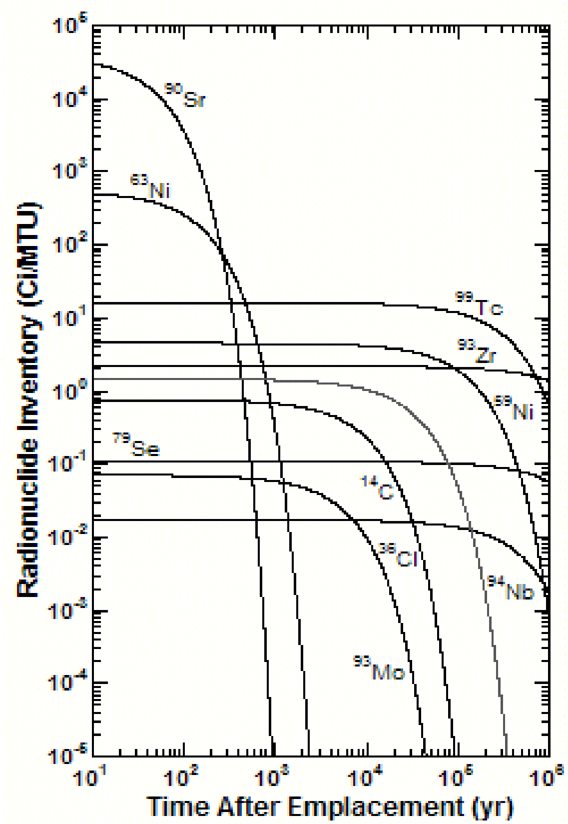
	sa1uzsz	sa2uzsz	sa3uzsz	sa4uzsz	sa5uzsz	sa6uzsz	sa7uzsz	sa8uzsz	aveuzsz
min	2.42E+02	2.16E+02	1.64E+02	5.58E+02	2.03E+02	2.79E+02	2.83E+02	1.46E+02	3.12E+02
average	9.95E+02	9.83E+02	8.59E+02	1.46E+03	8.65E+02	1.01E+03	1.25E+03	7.21E+02	1.02E+03
max	2.58E+03	2.70E+03	4.68E+03	4.03E+03	2.40E+03	3.62E+03	3.53E+03	3.86E+03	2.82E+03

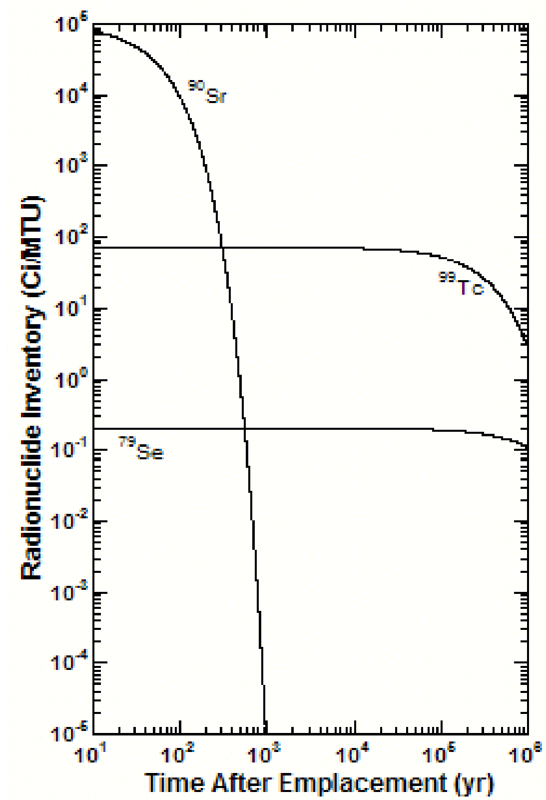
July 30, 2005 - prepared plots of inventories using inventories from the TPA code - Versions 4.1jpd for spent fuel and 5.0.1betaD for spent fuel and glass. These plots are equivalent to four plots in Chapter 3 of the TPA code User's Guide. To generate these plots the *invent.f* file was modified with the following lines were added to the *invent.f* code.

```
cc rwr 07/28/05 use to get Ci/MTU for the 43 radionuclides
      rzero = -0.001d0
      do jjj = 1,1001
        if (rzero .lt. 1.0d0 ) then
          rzero = rzero + 0.001d0
        elseif (rzero .lt. 10.0d0 ) then
          rzero = rzero + 0.01d0
        elseif (rzero .lt. 100.0d0 ) then
          rzero = rzero + 0.1d0
        elseif (rzero .lt. 1000.0d0 ) then
          rzero = rzero + 1.0d0
        elseif (rzero .lt. 10000.0d0 ) then
          rzero = rzero + 10.0d0
        elseif (rzero .lt. 100000.0d0 ) then
          rzero = rzero + 100.0d0
        elseif (rzero .lt. 1000000.0d0 ) then
          rzero = rzero + 1000.0d0
        elseif (rzero .lt. 10000000.0d0 ) then
          print *,'finished all times through 1e6yr'
          STOP
        endif
        call decay43mol( rzero, ammtu)
        print *,jjj,rzero,(ammtu(ijk)*activityperiso(ijk),ijk=1,43)
      enddo
cc rwr end of changes
```

The TPA Version 5.0.1betaD code, with the modified *invent.f* file, was compiled and executed and the screenprint captured to generate the plots below.

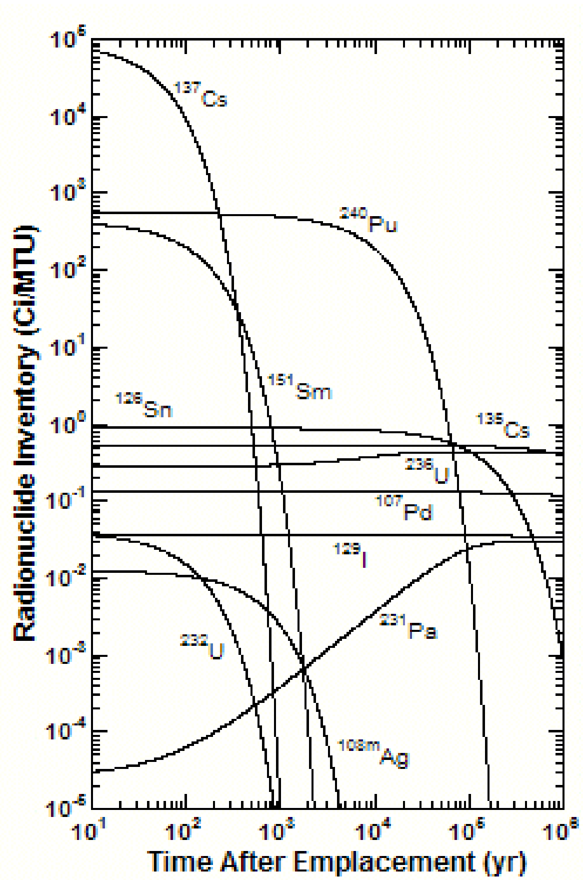


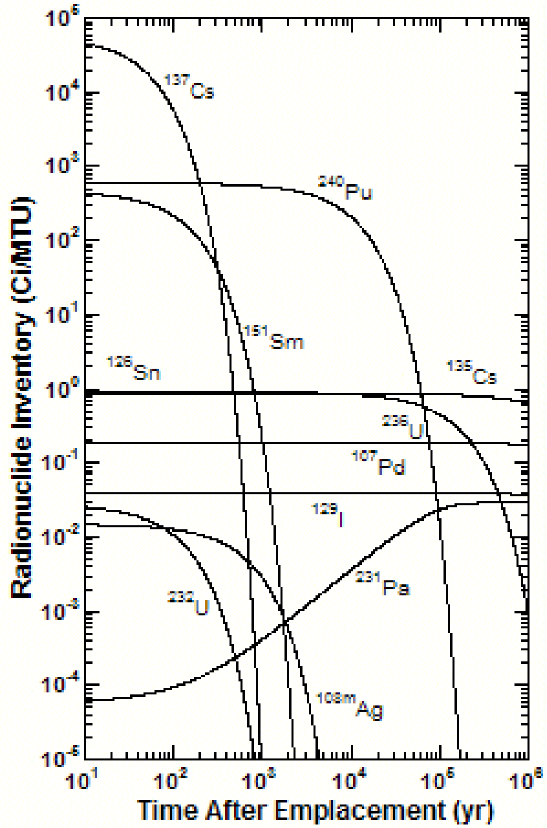


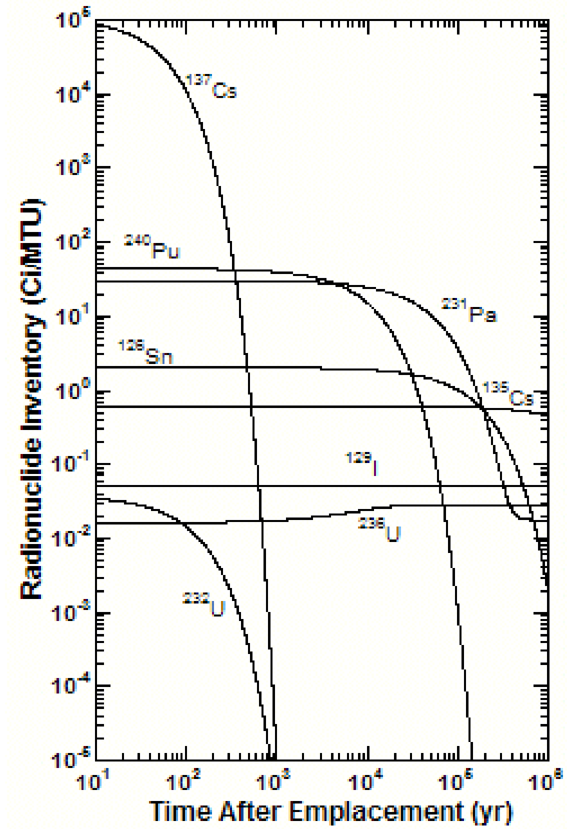


TPA 4.1jpd **TPA501betaD_SF** **TPA501betaD_glass**

(upper left plot in Figure 3-9 of TPA User's Guide)







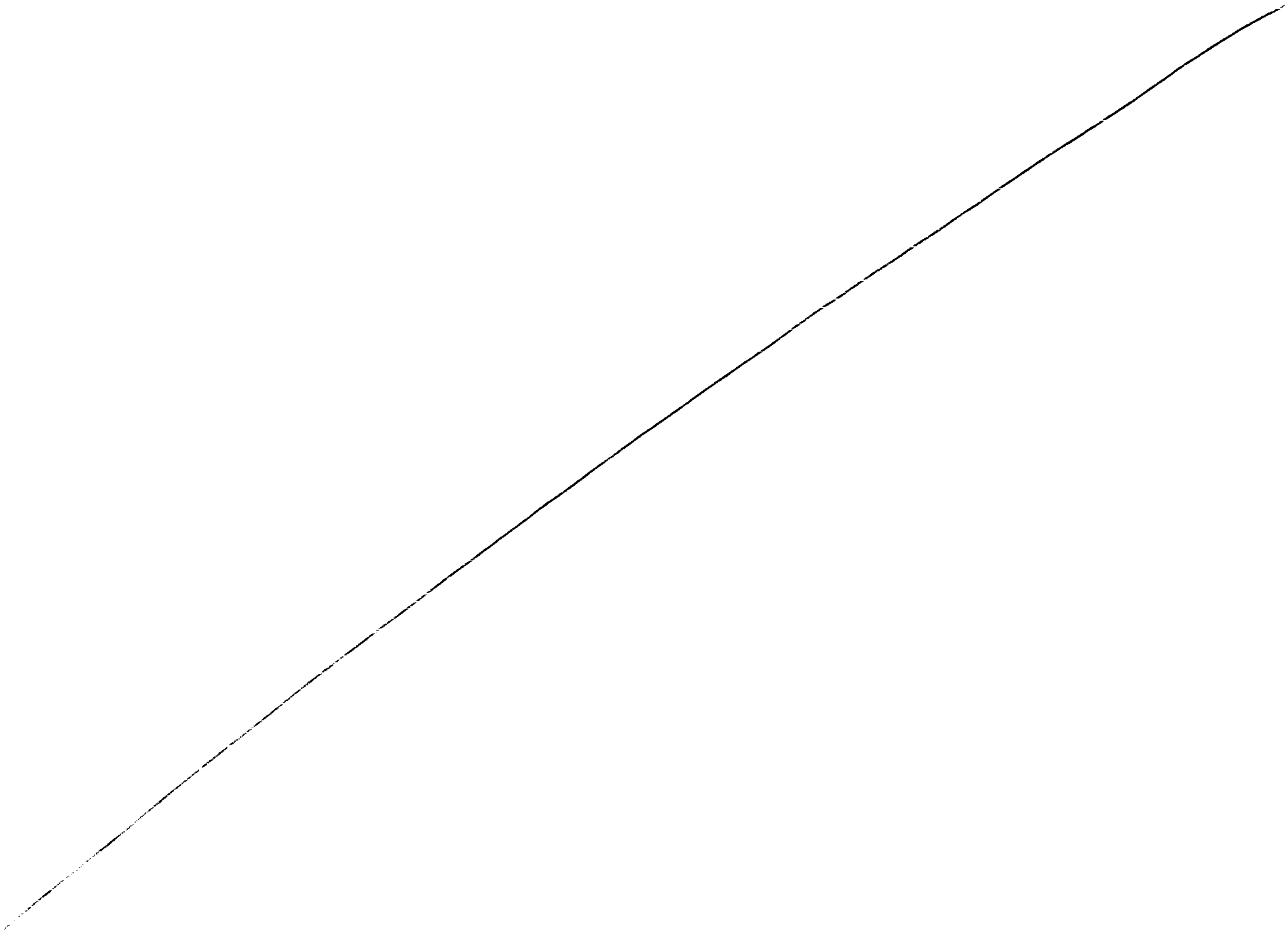
TPA 4.1jpd

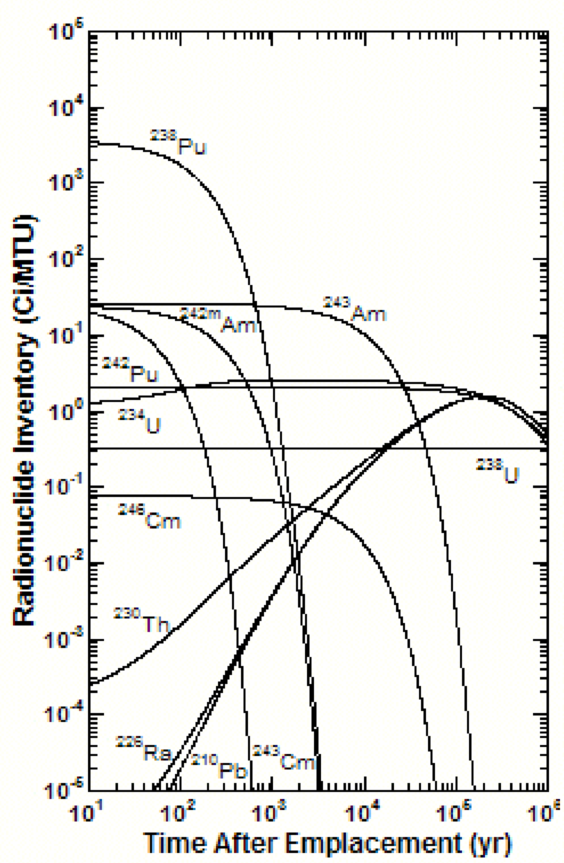
T
P
A
5
0
1

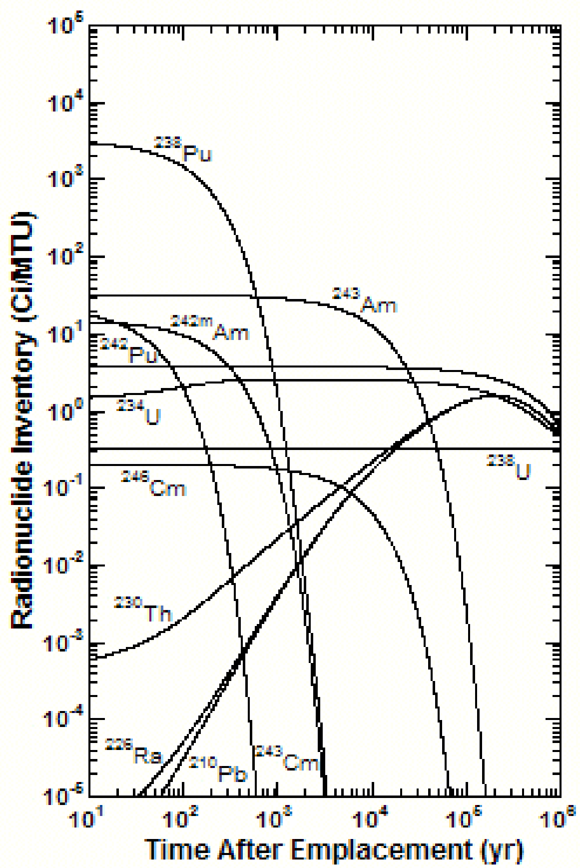
b

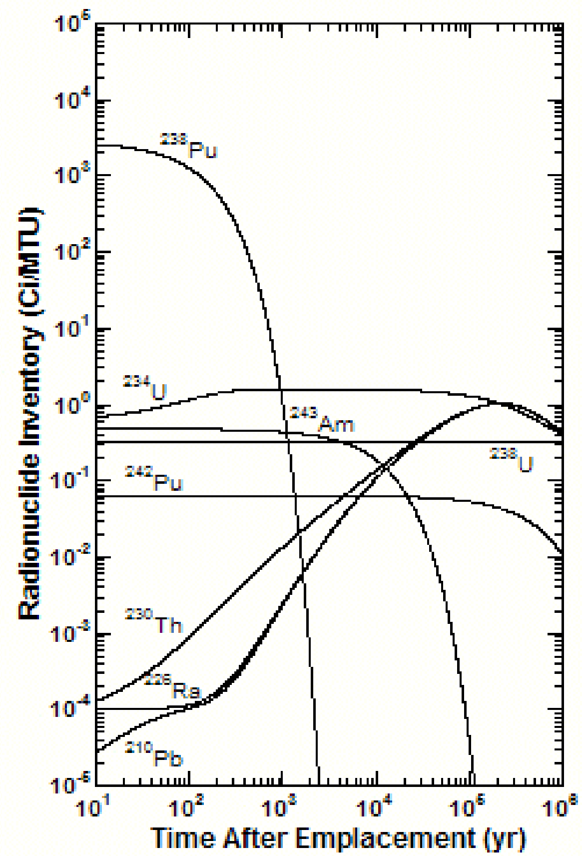
etaD_SFTPA501betaD_glass

(upper right plot in Figure 3-9 of TPA User's Guide)





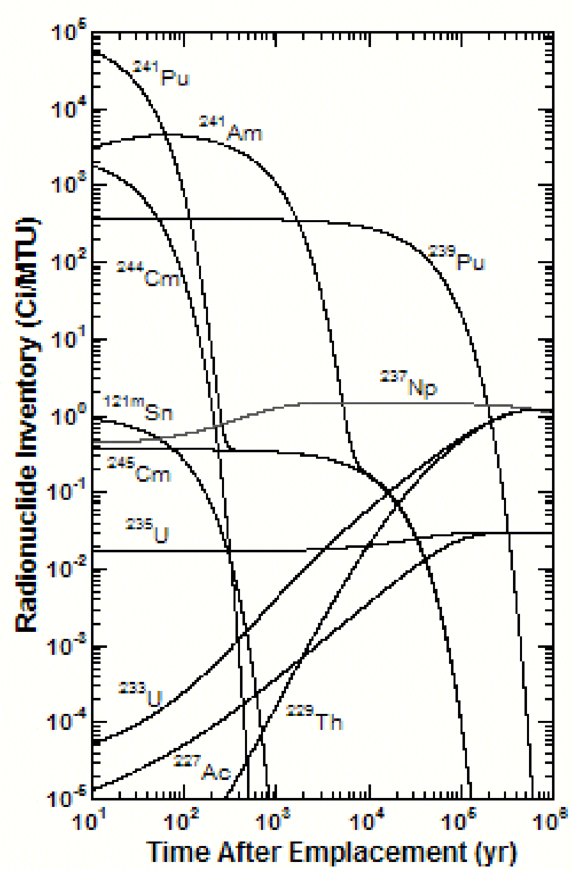


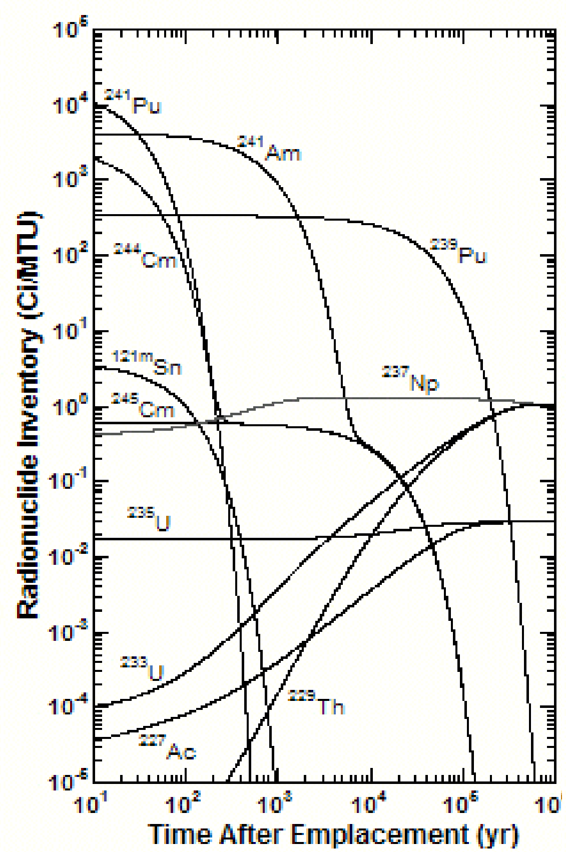


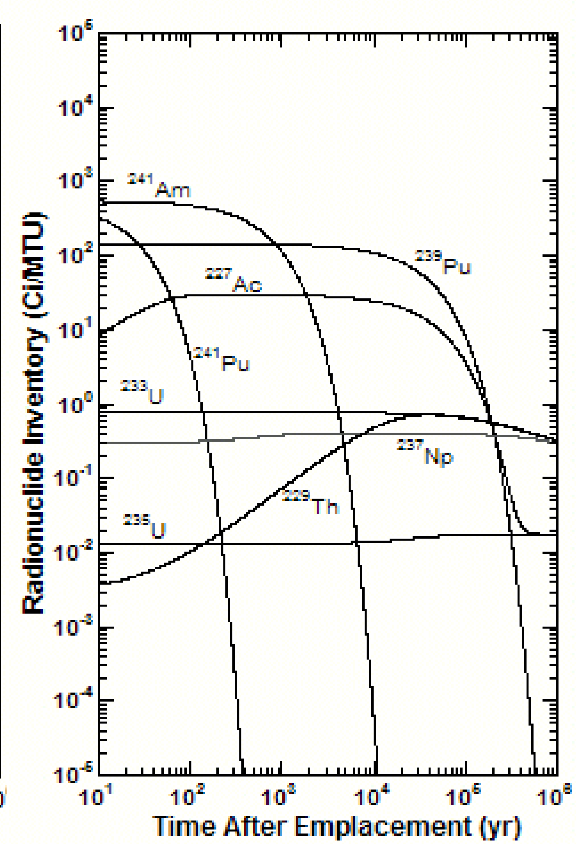
TPA 4.1jpd
(lower left plot in Figure 3-9 of TPA User's Guide)

TPA501betaD_SF **TPA501betaD_glass**

TPA 4.1jpd **TPA501betaD_SF** **TPA501betaD_glass**







(lower right plot in Figure 3-9 of TPA User's Guide)

August 3, 2005 - various TPA code simulations have been performed to examine an number of effects such as removing irreversible colloids, no WP corrosion failure, no weld failure, no seismic activity, no drip shield failure by rockfall, and adding glass. The following information summarizes the changes made to the TPA code to perform these simulations.

fc_ashremob_volcano
(to perform a simulation using ASHREMOB with a volcanic events fixed at 100 yr)

```
Comparing files tpa.inp and ..\..\..\TPA.INP
***** tpa.inp
VolcanismDisruptiveScenarioFlag(yes=1,no=0)
1
*0
**
***** ..\..\..\TPA.INP
VolcanismDisruptiveScenarioFlag(yes=1,no=0)
0
**
*****

***** tpa.inp
DirectReleaseOnlyFlag(yes=1,no=0)
1
*0
**
***** ..\..\..\TPA.INP
DirectReleaseOnlyFlag(yes=1,no=0)
0
**
*****

***** tpa.inp
**
*finiteexponential
*TimeOfNextVolcanicEventinRegionOfInterest[yr]
*100.0, 10000.0, 1.0e-7
uniform
TimeOfNextVolcanicEventinRegionOfInterest[yr]
99.99, 100.01
**
***** ..\..\..\TPA.INP
**
finiteexponential
TimeOfNextVolcanicEventinRegionOfInterest[yr]
100.0, 10000.0, 1.0e-7
**
*****
```

fc_no_ashremob_volcano_previous_model_instead
(same as above except use the previous TPA code model for ash remobilization)

```
Comparing files tpa.inp and ..\..\..\..\TPA.INP
```

```
***** tpa.inp
VolcanismDisruptiveScenarioFlag(yes=1,no=0)
1
*0
**
***** ..\..\..\..\TPA.INP
VolcanismDisruptiveScenarioFlag(yes=1,no=0)
0
**
*****

***** tpa.inp
DirectReleaseOnlyFlag(yes=1,no=0)
1
*0
**
***** ..\..\..\..\TPA.INP
DirectReleaseOnlyFlag(yes=1,no=0)
0
**
*****

***** tpa.inp
**
*finiteexponential
*TimeOfNextVolcanicEventinRegionOfInterest[yr]
*100.0, 10000.0, 1.0e-7
uniform
TimeOfNextVolcanicEventinRegionOfInterest[yr]
99.99, 100.01
**
***** ..\..\..\..\TPA.INP
**
finiteexponential
TimeOfNextVolcanicEventinRegionOfInterest[yr]
100.0, 10000.0, 1.0e-7
**
*****

***** tpa.inp
AshEvolutionMode[0=no_ashremob,1=ashremob]
0
*1
**
***** ..\..\..\..\TPA.INP
AshEvolutionMode[0=no_ashremob,1=ashremob]
1
**
*****
```

fc_initial_only_no_ds_mech_fail

(for 10,000 yr, this is equivalent to TPA 4.1jpd since there is only initial WP failures and only drip shield failure by corrosion in 10,000 yr)

Comparing files tpa.inp and ..\TPA.INP
***** tpa.inp
WPWeldThickness[m]
1.0e99
*2.03e-2
**
***** ..\TPA.INP
WPWeldThickness[m]
2.03e-2
**
*****

***** tpa.inp
OuterWPThickness[m]
1.0e99
*0.02
**
***** ..\TPA.INP
OuterWPThickness[m]
0.02
**
*****

***** tpa.inp
WastePackageOuterBarrierUltimateTensileStrength[MPa]
1.0e99
*679.134
**
***** ..\TPA.INP
WastePackageOuterBarrierUltimateTensileStrength[MPa]
679.134
**
*****

***** tpa.inp
DripShieldBucklingLoadSubarea_1[kg/m]
2.5e98, 1.50e99, 2.08134, 8.92986
*25000.0, 150000.0, 2.08134, 8.92986
**
***** ..\TPA.INP
DripShieldBucklingLoadSubarea_1[kg/m]
25000.0, 150000.0, 2.08134, 8.92986
**
*****

***** tpa.inp
DripShieldBucklingLoadSubarea_2[kg/m]
2.5e98, 1.50e99, 2.08134, 8.92986
*25000.0, 150000.0, 2.08134, 8.92986
**
***** ..\TPA.INP
DripShieldBucklingLoadSubarea_2[kg/m]
25000.0, 150000.0, 2.08134, 8.92986
**

```
*****

***** tpa.inp
DripShieldBucklingLoadSubarea_3[kg/m]
2.5e98,  1.50e99,  2.08134,  8.92986
*25000.0,  150000.0,  2.08134,  8.92986
**
***** ..\TPA.INP
DripShieldBucklingLoadSubarea_3[kg/m]
25000.0,  150000.0,  2.08134,  8.92986
**
*****

***** tpa.inp
DripShieldBucklingLoadSubarea_4[kg/m]
2.5e98,  1.50e99,  2.08134,  8.92986
*25000.0,  150000.0,  2.08134,  8.92986
**
***** ..\TPA.INP
DripShieldBucklingLoadSubarea_4[kg/m]
25000.0,  150000.0,  2.08134,  8.92986
**
*****

***** tpa.inp
DripShieldBucklingLoadSubarea_5[kg/m]
2.5e98,  1.50e99,  2.08134,  8.92986
*25000.0,  150000.0,  2.08134,  8.92986
**
***** ..\TPA.INP
DripShieldBucklingLoadSubarea_5[kg/m]
25000.0,  150000.0,  2.08134,  8.92986
**
*****

***** tpa.inp
DripShieldBucklingLoadSubarea_6[kg/m]
2.5e98,  1.50e99,  2.08134,  8.92986
*25000.0,  150000.0,  2.08134,  8.92986
**
***** ..\TPA.INP
DripShieldBucklingLoadSubarea_6[kg/m]
25000.0,  150000.0,  2.08134,  8.92986
**
*****

***** tpa.inp
DripShieldBucklingLoadSubarea_7[kg/m]
2.5e98,  1.50e99,  2.08134,  8.92986
*25000.0,  150000.0,  2.08134,  8.92986
**
***** ..\TPA.INP
DripShieldBucklingLoadSubarea_7[kg/m]
25000.0,  150000.0,  2.08134,  8.92986
```

```
**
*****

***** tpa.inp
IrreversibleColloidModel[0=no,1=yes]
0
*1
**
***** ..\TPA.INP
IrreversibleColloidModel[0=no,1=yes]
1
**
*****
```

fc_no_irrev
(remove the irreversible colloids from calculations)

```
Comparing files tpa.inp and ..\TPA.INP
***** tpa.inp
IrreversibleColloidModel[0=no,1=yes]
0
*1
**
***** ..\TPA.INP
IrreversibleColloidModel[0=no,1=yes]
1
**
*****
```

fc_no_corr
(no failures of the WP by corrosion)

```
Comparing files tpa.inp and ..\TPA.INP
***** tpa.inp
OuterWPThickness[m]
1.0e99
*0.02
**
***** ..\TPA.INP
OuterWPThickness[m]
0.02
**
*****
```

fc_no_seis
(no seismic activity that fails the WP)

```
Comparing files tpa.inp and ..\..\TPA.INP
***** tpa.inp
WastePackageOuterBarrierUltimateTensileStrength[MPa]
1.0e99
*679.134
**
```

```
***** ..\..\TPA.INP
WastePackageOuterBarrierUltimateTensileStrength[MPa]
679.134
**
*****
```

fc_no_weld
(no weld failures)

```
Comparing files tpa.inp and ..\..\TPA.INP
***** tpa.inp
WPWeldThickness[m]
1.0e99
*2.03e-2
**
***** ..\..\TPA.INP
WPWeldThickness[m]
2.03e-2
**
*****
```

fc_only_initial
(no releases from WP failures by corrosion or rockfall and no irreverisibles - this is similar to TPA 41jpd (see above))

```
Comparing files tpa.inp and ..\TPA.INP
***** tpa.inp
WPWeldThickness[m]
1.0e99
*2.03e-2
**
***** ..\TPA.INP
WPWeldThickness[m]
2.03e-2
**
*****

***** tpa.inp
OuterWPThickness[m]
1.0e99
*0.02
**
***** ..\TPA.INP
OuterWPThickness[m]
0.02
**
*****

***** tpa.inp
WastePackageOuterBarrierUltimateTensileStrength[MPa]
1.0e99
*679.134
**
***** ..\TPA.INP
```

```
WastePackageOuterBarrierUltimateTensileStrength[MPa]
679.134
**
*****

***** tpa.inp
IrreversibleColloidModel[0=no,1=yes]
0
*1
**
***** ..\TPA.INP
IrreversibleColloidModel[0=no,1=yes]
1
**
*****
```

fc_no_corr_weld_that_is_no_WP_corrosion_failures
(no WP failure by corrosion - either from WP general/local corrosion or weld failure)

```
Comparing files tpa.inp and ..\..\TPA.INP
***** tpa.inp
WPWeldThickness[m]
1.0e99
*2.03e-2
**
***** ..\..\TPA.INP
WPWeldThickness[m]
2.03e-2
**
*****

***** tpa.inp
OuterWPThickness[m]
1.0e99
*0.02
**
***** ..\..\TPA.INP
OuterWPThickness[m]
0.02
**
*****
```

fc_no_glass
(run the TPA code with only spent fuel and no glass - note that there are 6 subareas needed, instead of 8, and that a betaD version of *burnup.dat* needs to be used instead of the betaE or later version since this file has been adjusted to include the effects of glass on the heat load. Both the betaD and betaE versions of the *burnup.dat* file are also provided below.

```
Comparing files tpa.inp and ..\..\TPA.INP
***** tpa.inp
**
*subarea
```

*8
subarea
6
Subarea 1 (Top Left)
***** ..\..\TPA.INP
**
subarea
8
Subarea 1 (Top Left)
*****

***** tpa.inp
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.
**
***** ..\..\TPA.INP
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.
**
*****

***** tpa.inp
NumberOfRealizations
364
*1
**
***** ..\..\TPA.INP
NumberOfRealizations
1
**
*****

```
***** tpa.inp
FractionOfRepositoryWasteInGlassForm[]
0.0
*0.0126
**
***** ..\..\TPA.INP
FractionOfRepositoryWasteInGlassForm[]
0.0126
**
*****
```

The betaD version of *burnup.dat* is below.

```
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
** OPR: Multiplied by 0.8208 to get 1.45 kW/m at 25 yr, assuming
WastePackagePayload[MTU]=7.89, WPLength[m]=5.165, WP spacing = 0.1 m
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       6316.022254     11665.96807
2       3639.407755     6358.703626
3       2515.738559     4126.139554
5       1647.336798     2427.913428
10      1161.425795     1548.020529
15      1012.040993     1309.169005
20      912.7247234     1163.888181
25      825.5060095     1044.081376
30      760.4671369     955.4060953
50      550.3434595     681.3424396
100     297.4563307     361.3142295
200     164.1591229     195.7597541
300     126.6487633     150.0414383
500     91.51871102     107.6883846
1000    52.40779999     60.49263679
2000    27.42278148     30.55001277
5000    17.38445112     18.97679461
10000   12.4268456      13.63341516
20000   7.149129803     7.924781658
50000   2.545287201     2.870322264
100000  1.007116219     1.156501021
200000  0.636526999     0.747498566
500000  0.524488398     0.618305336
1000000         0.375513994     0.441341802
```

The betaE version of *burnup.dat* is below.

```
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
** OPR: Multiplied by 0.8208 to get 1.45 kW/m at 25 yr, assuming
WastePackagePayload[MTU]=7.89, WPLength[m]=5.165, WP spacing = 0.1 m
** RWJ (7-13-05): Multiplied by 1.37217 to get 1.45 kW/m at 25 yr, assuming
WastePackagePayload[MTU]=5.75, WPLength[m]=5.165, WP spacing = 0.1 m
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       8666.656256    16007.69141
2       4993.886139    8725.222354
3       3452.020979    5661.764912
5       2260.426134    3331.509968
10      1593.673633    2124.147329
15      1388.692289    1796.402434
20      1252.413484    1597.052445
25      1132.734581    1432.657142
30      1043.490191    1310.979582
50      755.1647848    934.9176553
100     408.1606533    495.7845463
200     225.2542237    268.6156618
300     173.7836335    205.8823604
500     125.5792297    147.7667707
1000    71.91241091    83.00618142
2000    37.62871806    41.91981102
5000    23.85442229    26.03938826
10000   17.05174473    18.70736328
20000   9.809821442    10.87414765
50000   3.492566739    3.938570101
100000  1.381934662    1.586916006
200000  0.873423252    1.025695107
500000  0.719687245    0.848420033
1000000         0.515269037    0.60559598
```

August 22 - began modifications associated with a *tpa.inp* file parameter for "TimeOfEndOfVentilation[yr]" and something like the following parameter name "FactorForHeatLossesAfterVentilationAndBeforeClosure[]". See the emails below.

From: opensado@cnwra.swri.edu
To: rwrice@aol.com
Cc:
Bcc:
Subject: Re: Ventilation period, TimeOfRepositoryClosure[yr]
Date: Tue, 09 Aug 2005 16:49:40 -0500

You got it right. Just in case, I would insert another heat loss parameter in case we want to adjust to a number greater than zero. Such parameter would be user defined and controled from tpa.inp.

----- Original Message -----

From: rwrice@aol.com

Date: Tuesday, August 9, 2005 4:33 pm

Subject: Re: Ventilation period, TimeOfRepositoryClosure[yr]

>
> Osvaldo,
>
> The heat loss parameter due to ventilation is 0.83 (constant) and
> is applied
> prior to the time of repository closure (previously the time of
> backfill).
> A parameter for the "EndOfVentilation" could be added to the
> tpa.inp file
> and at all times prior, this heat loss factor could be applied.
> After this time, but prior
> to the "TimeOfRepositoryClosure", there could be no heat loss
> factor applied.
> Then, after "TimeOfRepositoryClosure" (which is the time that
> maintenancestop) the effects of natural backfill on temperature
> could accounted for.
>
> At least this is my understanding of what we just discussed and
> how it could
> be addressed in a straightforward way in the TPA code.
>
> Am I understanding this correctly? What do you think?
>
> Thanks,
>
> Rob
>

> -----Original Message-----
> From: Osvaldo Pensado <opensado@cnwra.swri.edu>
> To: ofoegbu@swri.edu; opensado@swri.edu; rwrice@aol.com; 'George
> Adams' <gadams@cnwra.swri.edu>; 'Sitakanta Mohanty'
> <smohanty@cnwra.swri.edu>; 'James Winterle'
> <jwinterle@cnwra.swri.edu>; 'Ronald Janetzke'
> <rjanetzke@cnwra.swri.edu>Cc: 'Chandrika Manepally'
> <cmanepally@cnwra.swri.edu>Sent: Tue, 09 Aug 2005 14:03:31 -0500
> Subject: RE: Ventilation period, TimeOfRepositoryClosure[yr]
>
>
> There is no EndOfVentilationTime[yr] parameter in the TPA
> 5.0.1betaF version.
>
> The end of the ventilation is controlled by the
> TimeOfRepositoryClosure[yr]. There appears to be no time to
> introduce an EndOfVentilationTime[yr] parameter into the TPA code.
> Given that constraint, what should be the value of
> TimeOfRepositoryClosure[yr]?
> -----Original Message-----
> From: Goodluck Ofoegbu [ofoegbu@swri.edu]
> Sent: Tuesday, August 09, 2005 1:46 PM
> To: opensado@swri.edu; rwrice@aol.com; 'George Adams'; 'Goodluck I
> Ofoegbu'; 'Sitakanta Mohanty'; 'James Winterle'; 'Ronald Janetzke'
> Cc: 'Chandrika Manepally'
> Subject: RE: Ventilation period, TimeOfRepositoryClosure[yr]
>
>
> TimeOfRepositoryClosure[yr] = 100.0
> EndOfVentilationTime[yr] = 50.0
>
> This is the current DOE design as we know it. If your analysis
> departs from the design, then be prepared to justify the
> departure. I think we have discussed this before.
>
> Goodluck Ofoegbu
>
>
> -----Original Message-----
> From: Osvaldo Pensado [opensado@swri.edu]
> Sent: Tuesday, August 09, 2005 10:04 AM
> To: rwrice@aol.com; George Adams; Goodluck I Ofoegbu; Sitakanta
> Mohanty; James Winterle; Ronald Janetzke
> Cc: Chandrika Manepally
> Subject: Ventilation period, TimeOfRepositoryClosure[yr]
>
> I want to initiate a needed discussion to decide on the parameter
> TimeOfRepositoryClosure[yr], motivated by some discussions with
> Rob Rice.
>
> The current TPA setting for the "time of closure" is 100 years.
> This causes the system to be ventilated for 100 years; however,
> according to DOE design documents, active ventilation prevails for
> 50 years only.

>
> I understand that there are some discussions about closure at 100
> years, preceded by a 50 year passive ventilation period. This
> "real" system produces temperatures between our 50 year and 100
> year "time of closure" cases in the TPA code, because in the TPA
> code active ventilation acts throughout until closure.
>
> Do we want
>
> constant
> TimeOfRepositoryClosure[yr]
> 100.0
>
> in our base case?
>
> I am afraid that by doing so, we underestimate temperatures.
> Should we change the value to 50.0?
>
> Please comment against or in favor.
>
> ================================
> Osvaldo Pensado, Ph.D.
> Senior Research Scientist, SwRI
> 6220 Culebra Road. San Antonio TX 78238
> (210) 522 6084
> Fax: (210) 522 6081
> ================================
>
>

Performed a "grep" on the occurrences of "TimeOfRepository" for the TPA Version 501betaF code and found the following.

```
exec.f:     name = 'TimeOfRepositoryClosure[yr]'
nfenv.f:       name = 'TimeOfRepositoryClosure[yr]'
seismo2.f:       ch_tpa_name = 'TimeOfRepositoryClosure[yr]'
seismo2.f:       ch_tpa_name = 'TimeOfRepositoryClosure[yr]'
seismo2.f:       ch_tpa_name = 'TimeOfRepositoryClosure[yr]'
seismo2.f:    &  'Closure time[yr] {TimeOfRepositoryClosure[yr]}')
tpa.inp:**TimeOfRepositoryClosure[yr]
tpa.inp:TimeOfRepositoryClosure[yr]
```

Modified the TPA Version 501betaF code to allow for a time that ventilation ends and heat losses in the time period between the end of ventilation and repository closure. The files *tpa.inp*, *condxyzt.f*, *nfenv.f*, *driftcmn.i* and *tpanames.dbs* were modified. It is noted that *exec.f* and *seismo2.f* which were identified in the "grep" above did not need to be modified because the time of repository closure in these files were used to determine the time rockfall accumulates. A list of the four file comparisons (using "fc" in the command prompt window) follows.

tpa.inp

```
Comparing files tpa.inp and TPA.INP.ORIGINAL
***** tpa.inp
0.83
** rwr 8/22/05 added time of ventilation ending
** and a passive heat loss factor
** (Note: passive heat loss occurs after
**  ventilation ends, but prior to repository
**  closure)
constant
TimeVentilationEnds[yr]
50.0
constant
FactorForPassiveHeatlosses[]
0.0
**
***** TPA.INP.ORIGINAL
0.83
**
*****
```

condxyzt.f

```
Comparing files condxyzt.f and CONDXYZT.F.ORIGINAL
***** condxyzt.f
c     &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, bftimein,
c     &  hloss_factin, npoints,tempbump )
cc rwr 8/22/05 add passive heat losses
cc       subroutine cond3dxyzt(  aLin, aBin, aHin,
cc     &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, closetimein,
cc     &  hloss_factin, npoints, tempbump )
      subroutine cond3dxyzt(  aLin, aBin, aHin,
     &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, closetimein,
     &  ventendtimein, hloss_factin_vent, hloss_factin_pass, npoints,
     &  tempbump )

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** CONDXYZT.F.ORIGINAL
c     &  rhoin, cpin, condin, amlin, xin, yin, zin, timin, bftimein,
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
*****

***** condxyzt.f
c                  in units of [yr]

cc rwr 8/22/05 add passive heat losses
cc c           closetimein = double precision, ventilation end time.
cc c           hloss_factin =
c           closetimein = double precision, repository closure time.
c           ventendtimein = double precision, ventilation end time.
c           hloss_factin_vent =
c           hloss_factin_pass =
```

```
c         npoints =
c
***** CONDXYZT.F.ORIGINAL
c                in units of [yr]
c         closetimein = double precision, ventilation end time.
c         hloss_factin =
c         npoints =
c
*****

***** condxyzt.f
c          [m^2/s]

cc rwr 8/22/05 add passive heat losses
cc c     closetime = double precision, ventilation end time.
c     closetime = double precision, repository closure time.
c     ventendtime = double precision, ventilation end time.

c     aml =
***** CONDXYZT.F.ORIGINAL
c          [m^2/s]
c     closetime = double precision, ventilation end time.
c     aml =
*****

***** condxyzt.f
c     cpin = specific heat of geophysical rock in units of [J/(kg-C)]

cc rwr 8/22/05 add passive heat losses
cc c     hloss_fact =
cc c     hloss_factin =
c     hloss_fact_vent =
c     hloss_factin_vent =
c     hloss_fact_pass =
c     hloss_factin_pass =

c     npoints =
c     qpermtu =
***** CONDXYZT.F.ORIGINAL
c     cpin = specific heat of geophysical rock in units of [J/(kg-C)]
c     hloss_fact =
c     hloss_factin =
c     npoints =
c     qpermtu =
*****

***** condxyzt.f
c     tempbump1 =
c     tempbump2 =

cc rwr 8/22/05 add passive heat losses
c     tempbump3 =
```

```
c    tempgl =
***** CONDXYZT.F.ORIGINAL
c    tempbump1 =
c    tempbump2 =
c    tempgl =
*****

***** condxyzt.f
c     double precision bftime

      double precision closetime

cc rwr 8/22/05 add passive heat losses
      double precision ventendtime
      double precision ventendtimein

c    GADAMS PA-SCR-553 2-4-2005: End of change

***** CONDXYZT.F.ORIGINAL
c     double precision bftime
      double precision closetime
c    GADAMS PA-SCR-553 2-4-2005: End of change

*****

***** condxyzt.f
      double precision cp

cc rwr 8/22/05 add passive heat losses
cc      double precision hloss_fact
      double precision hloss_fact_vent
      double precision hloss_fact_pass
      double precision hloss_factin_vent
      double precision hloss_factin_pass


      double precision rho
***** CONDXYZT.F.ORIGINAL
      double precision cp
      double precision hloss_fact
      double precision rho
*****

***** condxyzt.f
      double precision tempbump2

cc rwr 8/22/05 add passive heat losses
      double precision tempbump3

      double precision tend
***** CONDXYZT.F.ORIGINAL
      double precision tempbump2
      double precision tend
*****
```

```
***** condxyzt.f
c     & hloss_fact

cc rwr 8/22/05 add passive heat losses
cc       common / tempgl1 / aL, aB, aH, x, y, z,
cc      & aml, rho, cp, cond, tend, alpha, closetime,
cc      & hloss_fact
      common / tempgl1 / aL, aB, aH, x, y, z,
     & aml, rho, cp, cond, tend, alpha, closetime, ventendtime,
     & hloss_fact_vent, hloss_fact_pass

c     GADAMS PA-SCR-553 2-4-2005: End of change

***** CONDXYZT.F.ORIGINAL
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

*****

***** condxyzt.f
      closetime = closetimein

cc rwr 8/22/05 add passive heat losses
      ventendtime = ventendtimein

c     GADAMS PA-SCR-553 2-4-2005: End of change

cc rwr 8/22/05 add passive heat losses
cc       hloss_fact = hloss_factin
      hloss_fact_vent = hloss_factin_vent
      hloss_fact_pass = hloss_factin_pass

***** CONDXYZT.F.ORIGINAL
      closetime = closetimein
c     GADAMS PA-SCR-553 2-4-2005: End of change

      hloss_fact = hloss_factin

*****

***** condxyzt.f
c      if (tend.le.bftime) then

cc rwr 8/22/05 add passive heat losses
cc        if (tend.le.closetime) then
cc c     GADAMS PA-SCR-553 2-4-2005: End of change
cc
cc          call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
cc          tempbump = tempbump1
cc        else
cc
```

```
cc c      GADAMS PA-SCR-553 2-4-2005: Replaced bftime with closetime
cc c       call xgauleg(tempgl, 0.0d0, bftime, npoints, tempbump1)
cc        call xgauleg(tempgl, 0.0d0, closetime, npoints, tempbump1)
cc c       call xgauleg(tempgl, bftime, tend, npoints, tempbump2)
cc        call xgauleg(tempgl, closetime, tend, npoints, tempbump2)
cc c      GADAMS PA-SCR-553 2-4-2005: End of change
cc
cc        tempbump = tempbump1 + tempbump2
cc      endif
      if (tend.lt.ventendtime) then
         call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
***** CONDXYZT.F.ORIGINAL
c      if (tend.le.bftime) then
      if (tend.le.closetime) then
c     GADAMS PA-SCR-553 2-4-2005: End of change

         call xgauleg(tempgl, 0.0d0, tend, npoints, tempbump1)
*****

***** condxyzt.f
         tempbump = tempbump1
      elseif (tend.ge.ventendtime .and. tend.lt.closetime) then
        call xgauleg(tempgl, 0.0d0, ventendtime, npoints, tempbump1)
        call xgauleg(tempgl, ventendtime, tend, npoints, tempbump2)
        tempbump = tempbump1 + tempbump2
      else
        call xgauleg(tempgl, 0.0d0, ventendtime, npoints, tempbump1)
        call xgauleg(tempgl, ventendtime, closetime, npoints, tempbump2)
        call xgauleg(tempgl, closetime, tend, npoints, tempbump3)
        tempbump = tempbump1 + tempbump2 + tempbump3

      endif
***** CONDXYZT.F.ORIGINAL
         tempbump = tempbump1
      else

c       GADAMS PA-SCR-553 2-4-2005: Replaced bftime with closetime
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

        tempbump = tempbump1 + tempbump2
      endif
*****

***** condxyzt.f
c     aml = areal mass loading of plate in units of [MTU/acre]

cc rwr 8/22/05 add passive heat losses
cc c     closetime = time of repository closure when ventilation ends
c     closetime = time of repository closure
c     ventendtime = time when ventilation ends
```

```
c     cond = thermal conductivity of geophysical rock in units of
c           [W/(m-C)]
***** CONDXYZT.F.ORIGINAL
c     aml = areal mass loading of plate in units of [MTU/acre]
c     closetime = time of repository closure when ventilation ends
c     cond = thermal conductivity of geophysical rock in units of
c           [W/(m-C)]
*****

***** condxyzt.f
c     cp = specific heat of geophysical rock in units of [J/(kg-C)]
c     dmyexp =

cc rwr 8/22/05 add passive heat losses
cc c     hloss_fact =
c     hloss_fact_vent =
c     hloss_fact_pass =

c     qpp =
***** CONDXYZT.F.ORIGINAL
c     cp = specific heat of geophysical rock in units of [J/(kg-C)]
c     dmyexp =
c     hloss_fact =
c     qpp =
*****

***** condxyzt.f
c      double precision bftime
      double precision closetime

cc rwr 8/22/05 add passive heat losses
      double precision ventendtime

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** CONDXYZT.F.ORIGINAL
c      double precision bftime
      double precision closetime
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** condxyzt.f
      double precision cp

cc rwr 8/22/05 add passive heat losses
cc       double precision hloss_fact
      double precision hloss_fact_vent
      double precision hloss_fact_pass

      double precision qpp
***** CONDXYZT.F.ORIGINAL
      double precision cp
      double precision hloss_fact
      double precision qpp
```

```
*****

***** condxyzt.f
c     & hloss_fact

cc rwr 8/22/05 add passive heat losses
cc       common / tempgl1 / aL, aB, aH, x, y, z,
cc      & aml, rho, cp, cond, tend, alpha, closetime,
cc      & hloss_fact
      common / tempgl1 / aL, aB, aH, x, y, z,
     & aml, rho, cp, cond, tend, alpha, closetime, ventendtime,
     & hloss_fact_vent, hloss_fact_pass

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** CONDXYZT.F.ORIGINAL
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
*****

***** condxyzt.f
c      if (t.lt.bftime) then

cc rwr 8/22/05 add passive heat losses
cc        if (t.lt.closetime) then
cc c     GADAMS PA-SCR-553 2-4-2005: End of change
cc
cc          qpp = qpermtu( t ) * (1.d0 - hloss_fact) * aml / 4047.0d0
cc        else
cc          qpp = qpermtu( t ) *  aml / 4047.0d0
cc        endif
      if (t.lt.ventendtime) then
        qpp = qpermtu( t ) * (1.d0 - hloss_fact_vent) * aml / 4047.0d0
      elseif (t.ge.ventendtime .and. t.lt.closetime) then
        qpp = qpermtu( t ) * (1.d0 - hloss_fact_pass) * aml / 4047.0d0
      else
        qpp = qpermtu( t ) *  aml / 4047.0d0
      endif
***** CONDXYZT.F.ORIGINAL
c      if (t.lt.bftime) then
      if (t.lt.closetime) then
c     GADAMS PA-SCR-553 2-4-2005: End of change

         qpp = qpermtu( t ) * (1.d0 - hloss_fact) * aml / 4047.0d0
      else
         qpp = qpermtu( t ) *  aml / 4047.0d0
      endif
*****

***** condxyzt.f
     &    dmyexp( - (z-2.0 * aH)**2/ ( 4.0d0 * alpha * (tend-t) ) )  )
      include 'tempgl.t2'
```

```
***** CONDXYZT.F.ORIGINAL
     &    dmyexp( - (z-2.0 * aH)**2/ ( 4.0d0 * alpha * (tend-t) ) )  )

      include 'tempgl.t2'
*****
```

nfenv.f

```
Comparing files nfenv.f and NFENV.F.ORIGINAL
***** nfenv.f
      double precision rh_weight2

cc rwr 8/22/05 add passive heat loss
cc       double precision rh_closure
      double precision rh_ventends

c     GADAMS SCR520 11-4-2004: End of change
***** NFENV.F.ORIGINAL
      double precision rh_weight2
      double precision rh_closure
c     GADAMS SCR520 11-4-2004: End of change
*****

***** nfenv.f
      save i_timeofclosure

cc rwr 8/22/05 add passive heat losses
      double precision timeventends
      integer i_timeventends
      save i_timeventends


c     GADAMS PA-SCR-553 2-4-2005: End of change
***** NFENV.F.ORIGINAL
      save i_timeofclosure
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** nfenv.f
c      common / nfenv17 / iconde_n, icondbf, icondds, ihloss_fact

cc rwr 8/22/05 add passive heat losses
cc       common / nfenv17 / iconde_n, icondbf1, icondbf2, icondds,
cc      &                   ihloss_fact
      common / nfenv17 / iconde_n, icondbf1, icondbf2, icondds,
     &                   ihloss_fact_vent, ihloss_fact_pass

c     GADAMS SCR562 4-18-2005: End of change
***** NFENV.F.ORIGINAL
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
*****
```

```
***** nfenv.f
c       GADAMS PA-SCR-553 2-4-2005: End of change

cc rwr 8/22/05 add passive heat losses
        call clearchar(60, name)
        name = 'TimeVentilationEnds[yr]'
        i_timeventends = ispquery(name)


        call clearchar(60, name)
***** NFENV.F.ORIGINAL
c       GADAMS PA-SCR-553 2-4-2005: End of change

        call clearchar(60, name)
*****

***** nfenv.f

cc rwr 8/22/05 add passive heat losses
cc        call clearchar( 60, name )
cc        name = 'FactorForVentilationHeatlosses[]'
cc        ihloss_fact = ispquery( name )
        call clearchar( 60, name )
***** NFENV.F.ORIGINAL

        call clearchar( 60, name )
*****

***** nfenv.f
        name = 'FactorForVentilationHeatlosses[]'
        ihloss_fact_vent = ispquery( name )
        call clearchar( 60, name )
        name = 'FactorForPassiveHeatlosses[]'
        ihloss_fact_pass = ispquery( name )

***** NFENV.F.ORIGINAL
        name = 'FactorForVentilationHeatlosses[]'
        ihloss_fact = ispquery( name )

*****

***** nfenv.f
      timeofclosure = valuesp(i_timeofclosure)

cc rwr 8/22/05 add passive heat losses
      timeventends = valuesp(i_timeventends)
      if (timeventends .gt. timeofclosure) then
        print *, '***>>> Error in nfenv <<<***'
        print *, ' problem with:'
        print *, '    Ventilation ends after repository closure'
        print *, ' timeventends = ', timeventends
        print *, ' timeofclosure = ', timeofclosure
        print *, ' timeventends should be .le. timeofclosure'
        STOP
```

```
      endif

      rho       = valuesp( irho )
***** NFENV.F.ORIGINAL
      timeofclosure = valuesp(i_timeofclosure)

      rho       = valuesp( irho )
*****

***** nfenv.f
      aB = driftdia/2.0d0

cc rwr 8/22/05 add passive heat losses
cc      hloss_fact = valuesp( ihloss_fact )
      hloss_fact_vent = valuesp( ihloss_fact_vent )
      hloss_fact_pass = valuesp( ihloss_fact_pass )

      npoints = ivaluesp ( inpoints )
***** NFENV.F.ORIGINAL
      aB = driftdia/2.0d0
      hloss_fact = valuesp( ihloss_fact )
      npoints = ivaluesp ( inpoints )
*****

***** nfenv.f
c     &         npoints, tbump )

cc rwr 8/22/05 add passive heat losses
cc          call cond3dxyzt(  aL, aB, aH,
cc     &         rho, cp, cond, amld,
cc     &         x, y, z, tend, timeofclosure, hloss_fact,
cc     &         npoints, tbump )
          call cond3dxyzt(  aL, aB, aH,
***** NFENV.F.ORIGINAL
c     &         npoints, tbump )
          call cond3dxyzt(  aL, aB, aH,
*****

***** nfenv.f
     &         rho, cp, cond, amld,
     &         x, y, z, tend, timeofclosure, timeventends,
     &         hloss_fact_vent, hloss_fact_pass,
     &         npoints, tbump )
***** NFENV.F.ORIGINAL
     &         rho, cp, cond, amld,
     &         x, y, z, tend, timeofclosure, hloss_fact,
     &         npoints, tbump )
*****

***** nfenv.f
        D_WPPayload = wppayload

cc rwr 8/22/05 add passive heat loss
cc        D_HLossFact = hloss_fact
```

```
         D_HLossFact_vent = hloss_fact_vent
         D_HLossFact_pass = hloss_fact_pass

        D_FracInv = frac_inv
***** NFENV.F.ORIGINAL
        D_WPPayload = wppayload
        D_HLossFact = hloss_fact
        D_FracInv = frac_inv
*****

***** nfenv.f
c          rh_transition_point = timeofbackfill

cc rwr 8/22/05 add passive heat loss
cc           rh_closure = 0.0d0
         rh_ventends = 0.0d0

c        GADAMS SCR520 11-3-2004: End of change
***** NFENV.F.ORIGINAL
c          rh_transition_point = timeofbackfill
         rh_closure = 0.0d0
c        GADAMS SCR520 11-3-2004: End of change
*****

***** nfenv.f
c     &         temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)

cc rwr 8/22/05 add passive heat losses
cc              call calcTempsLinear(tim(it), timeofclosure,
cc      &         tempwp(it), tempdsiA(it), tempdsiB(it),
cc      &         tempdsoA(it), tempdsoB(it),
cc      &         tempbfoA(it), tempbfoB(it),
cc      &         temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
            call calcTempsLinear(tim(it), timeofclosure,
     &         timeventends,
     &         tempwp(it), tempdsiA(it), tempdsiB(it),
***** NFENV.F.ORIGINAL
c     &         temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
            call calcTempsLinear(tim(it), timeofclosure,
     &         tempwp(it), tempdsiA(it), tempdsiB(it),
*****

***** nfenv.f
     &         temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)

c           GADAMS PA-SCR-553 2-4-2005: End of change
***** NFENV.F.ORIGINAL
     &         temprep(it), qwp, qwp_i, qwp_dA, qwp_dB)
c           GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** nfenv.f
c     &         tempwp(it), qwp, qwp_dA, qwp_i)
```

```
cc rwr 8/22/05 add passive heat losses
cc          call calcTempsIterative(tim(it), timeofclosure,
cc     &        temprep(it), tempbfoA(it),
cc     &        tempdsoA(it), tempdsiA(it),
cc     &        tempwp(it), qwp, qwp_dA, qwp_i)
          call calcTempsIterative(tim(it), timeofclosure,
     &        timeventends,
     &        temprep(it), tempbfoA(it),
***** NFENV.F.ORIGINAL
c    &        tempwp(it), qwp, qwp_dA, qwp_i)
          call calcTempsIterative(tim(it), timeofclosure,
     &        temprep(it), tempbfoA(it),
*****

***** nfenv.f
     &        tempwp(it), qwp, qwp_dA, qwp_i)

c          GADAMS PA-SCR-553 2-4-2005: End of change
***** NFENV.F.ORIGINAL
     &        tempwp(it), qwp, qwp_dA, qwp_i)
c          GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** nfenv.f
c         if(tim(it) .lt. timeofbackfill) then

cc rwr 8/22/05 add passive heat loss
cc         if(tim(it) .lt. timeofclosure) then
         if(tim(it) .lt. timeventends) then
          rh_drift_wall = rh_ventilated_air
***** NFENV.F.ORIGINAL
c         if(tim(it) .lt. timeofbackfill) then
         if(tim(it) .lt. timeofclosure) then
          rh_drift_wall = rh_ventilated_air
*****

***** nfenv.f
     &        pvap( tempwp(it) )

cc rwr 8/22/05 add passive heat loss
cc          rh_closure = relhumwp(it)
          rh_ventends = relhumwp(it)

         elseif(
***** NFENV.F.ORIGINAL
     &        pvap( tempwp(it) )
          rh_closure = relhumwp(it)
         elseif(
*****

***** nfenv.f
c    &      (tim(it) .le. (timeofbackfill + rh_transition_time))

cc rwr 8/22/05 add passive heat loss
```

```
cc     &      (tim(it) .le. (timeofclosure + rh_transition_time))
   &      (tim(it) .le. (timeventends + rh_transition_time))
   &      .and.
***** NFENV.F.ORIGINAL
c    &      (tim(it) .le. (timeofbackfill + rh_transition_time))
   &      (tim(it) .le. (timeofclosure + rh_transition_time))
   &      .and.
*****

***** nfenv.f
c    &        (tim(it) - timeofbackfill)
cc rwr 8/22/05 add passive heat loss
cc     &        (tim(it) - timeofclosure)
   &        (tim(it) - timeventends)

cc rwr 8/22/05 add passive heat loss
cc c          If there is a relative humidity at closure...
cc
cc            if(rh_closure .gt. 0.0d0) then
c          If there is a relative humidity at the end of ventilation...

          if(rh_ventends .gt. 0.0d0) then

c            Calculate weighting factors for the relative humidity
c             rh_weight2 = (tim(it) - timeofbackfill) /

cc rwr 8/22/05 add passive heat loss
cc              rh_weight2 = (tim(it) - timeofclosure) /
            rh_weight2 = (tim(it) - timeventends) /
   &         rh_transition_time
***** NFENV.F.ORIGINAL
c    &        (tim(it) - timeofbackfill)
   &        (tim(it) - timeofclosure)

c          If there is a relative humidity at closure...
          if(rh_closure .gt. 0.0d0) then
c            Calculate weighting factors for the relative humidity
c             rh_weight2 = (tim(it) - timeofbackfill) /
            rh_weight2 = (tim(it) - timeofclosure) /
   &         rh_transition_time
*****

***** nfenv.f
c            Weight the relative humidity

cc rwr 8/22/05 add passive heat loss
cc              relhumwp(it) = rh_closure * rh_weight1 +
            relhumwp(it) = rh_ventends * rh_weight1 +
   &         (rh_drift_wall *
***** NFENV.F.ORIGINAL
c            Weight the relative humidity
            relhumwp(it) = rh_closure * rh_weight1 +
   &         (rh_drift_wall *
*****
```

```
***** nfenv.f
c     &  qwp, qwpInvert, qwpRWA, qwpRWB)

cc rwr 8/22/05 add passive heat losses
cc       subroutine calcTempsLinear(time, timeClosure,
cc      &  tempWP, tempDSIA, tempDSIB, tempDSOA, tempDSOB, tempBFOA,
cc      &  tempBFOB, tempRep,
cc      &  qwp, qwpInvert, qwpRWA, qwpRWB)
      subroutine calcTempsLinear(time, timeClosure, timenovent,
     &  tempWP, tempDSIA, tempDSIB, tempDSOA, tempDSOB, tempBFOA,
***** NFENV.F.ORIGINAL
c     &  qwp, qwpInvert, qwpRWA, qwpRWB)
      subroutine calcTempsLinear(time, timeClosure,
     &  tempWP, tempDSIA, tempDSIB, tempDSOA, tempDSOB, tempBFOA,
*****

***** nfenv.f
     &  qwp, qwpInvert, qwpRWA, qwpRWB)

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** NFENV.F.ORIGINAL
     &  qwp, qwpInvert, qwpRWA, qwpRWB)
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** nfenv.f
c           double precision, timeClosure

cc rwr 8/22/05 add passive heat losses
c           double precision, timenovent

c           double precision, tempRep
***** NFENV.F.ORIGINAL
c           double precision, timeClosure
c           double precision, tempRep
*****

***** nfenv.f
      double precision timeClosure

cc rwr 8/22/05 add passive heat losses
      double precision timenovent

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** NFENV.F.ORIGINAL
      double precision timeClosure
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** nfenv.f
c        if(time .lt. timeBF) then

        if(time .lt. timeClosure) then
```

```
c      GADAMS PA-SCR-553 2-4-2005: End of change

***** NFENV.F.ORIGINAL
c       if(time .lt. timeBF) then
       if(time .lt. timeClosure) then
c      GADAMS PA-SCR-553 2-4-2005: End of change

*****

***** nfenv.f
c        Calculate the heat flux during the ventilation period

cc rwr 8/22/05 add passive heat losses
cc          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
        if(time .lt. timenovent) then
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact_vent)
        else
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact_pass)
        endif

c        Conduction through the floor and invert
***** NFENV.F.ORIGINAL
c        Calculate the heat flux during the ventilation period
        qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)

c        Conduction through the floor and invert
*****

***** nfenv.f
c        Calculate the heat flux during the ventilation period
cc rwr 8/22/05 add passive heat losses
cc          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
        if(time .lt. timenovent) then
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact_vent)
        else
          qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact_pass)
        endif

c        Conduction through the floor and invert
***** NFENV.F.ORIGINAL
c        Calculate the heat flux during the ventilation period
        qwp = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)

c        Conduction through the floor and invert
*****

***** nfenv.f
c     &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)

cc rwr 8/22/05 add passive heat losses
cc       subroutine calcTempsIterative(time, timeClosure, tempRW, tempBF,
cc      &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
      subroutine calcTempsIterative(time, timeClosure, timenovent,
     &   tempRW, tempBF,
```

```
    &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
***** NFENV.F.ORIGINAL
c     &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
      subroutine calcTempsIterative(time, timeClosure, tempRW, tempBF,
    &  tempDSO, tempDSI, tempWP, qwpTotal, qwpAbove, qwpInvert)
*****

***** nfenv.f
c           double precision, timeClosure

cc rwr 8/22/05 add passive heat losses
c           double precision, timenovent

c           double precision, tempRW
***** NFENV.F.ORIGINAL
c           double precision, timeClosure
c           double precision, tempRW
*****

***** nfenv.f
      double precision timeClosure

cc rwr 8/22/05 add passive heat losses
      double precision timenovent

c     GADAMS PA-SCR-553 2-4-2005: End of change
***** NFENV.F.ORIGINAL
      double precision timeClosure
c     GADAMS PA-SCR-553 2-4-2005: End of change
*****

***** nfenv.f
c     GADAMS PA-SCR-553 2-4-2005: End of change

cc rwr 8/22/05 add passive heat losses
cc         qwpTotal = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
        if(time .lt. timenovent) then
          qwpTotal =
     &     qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact_vent)
        else
          qwpTotal =
     &     qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact_pass)
        endif

        B_Early = .true.
***** NFENV.F.ORIGINAL
c     GADAMS PA-SCR-553 2-4-2005: End of change

        qwpTotal = qpermtu(time) * D_WPPayload * (1.d0-D_HLossFact)
        B_Early = .true.
*****
```

driftcmn.i

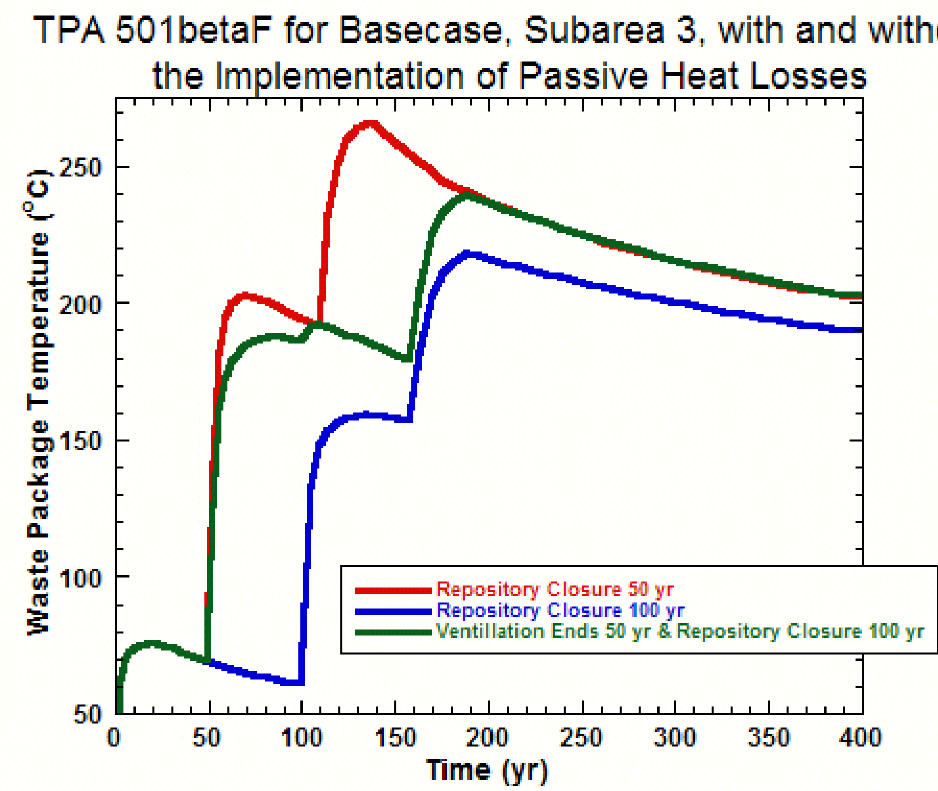
Comparing files driftcmn.i and DRIFTCMN.I.ORIGINAL

```
***** driftcmn.i
      double precision D_WPPayload

cc rwr 8/22/05 add passive heat losses
cc      double precision D_HLossFact
      double precision D_HLossFact_vent
      double precision D_HLossFact_pass

      double precision D_FracInv
***** DRIFTCMN.I.ORIGINAL
      double precision D_WPPayload
      double precision D_HLossFact
      double precision D_FracInv
*****

***** driftcmn.i
      double precision D_EmissBF

cc rwr 8/22/05 add passive heat losses
cc       common /nfenv_thermal1/ D_SBolt, D_ViewFactor, D_WPPayload,
cc     &  D_HLossFact, D_FracInv, D_FracWedge,
cc     &  D_WPSpace, D_WPDia, D_DSDiaI, D_DSThick, D_DriftDiaFloor,
cc     &  D_CondFloor, D_CondRW, D_CondConv, D_CondBF, D_EmissWP,
cc     &  D_EmissRW, D_EmissDS, D_EmissBF
      common /nfenv_thermal1/ D_SBolt, D_ViewFactor, D_WPPayload,
     &  D_HLossFact_vent, D_HLossFact_pass, D_FracInv, D_FracWedge,
     &  D_WPSpace, D_WPDia, D_DSDiaI, D_DSThick, D_DriftDiaFloor,
***** DRIFTCMN.I.ORIGINAL
      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,
*****
```

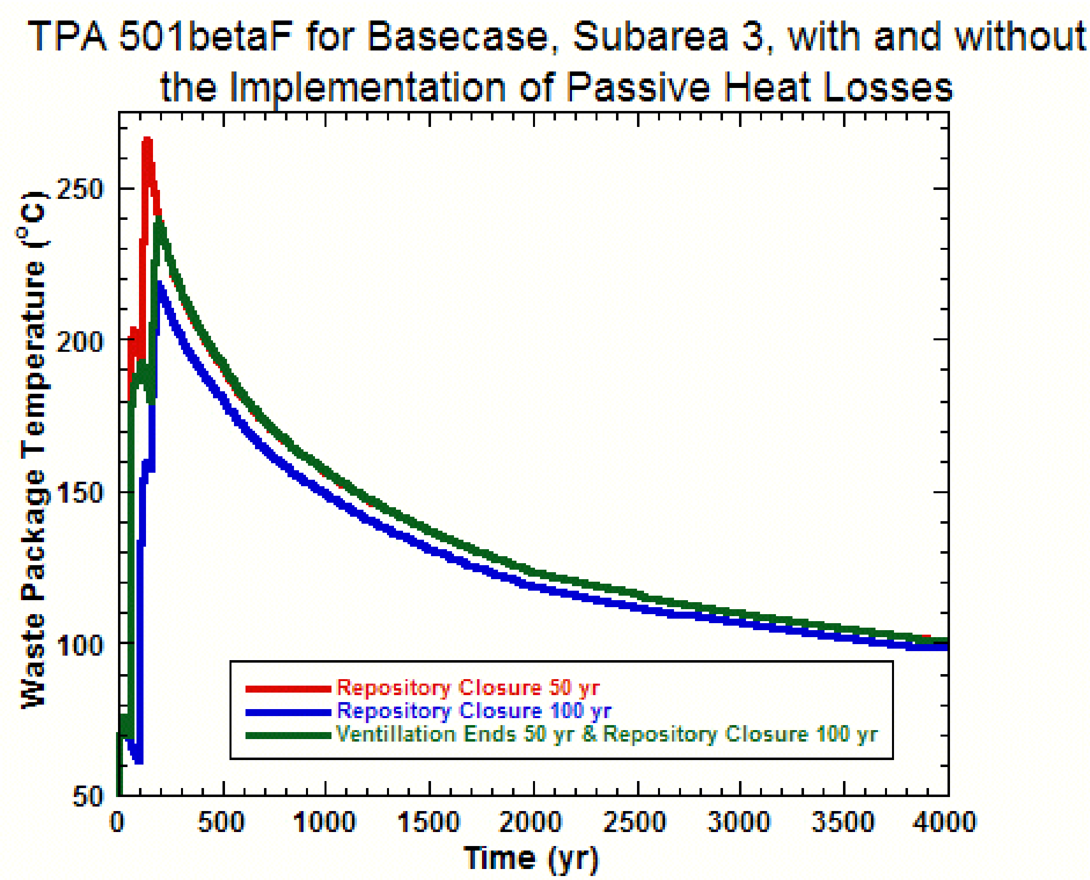
tpanames.dbs

```
Comparing files tpanames.dbs and TPANAMES.DBS.ORIGINAL
***** tpanames.dbs
FactorForVentilationHeatlosses[]                    VentFctr
FactorForPassiveHeatlosses[]                        PassFctr
NumberOfWeightsForGaussLegendreIntegration[]            GLIntWts
***** TPANAMES.DBS.ORIGINAL
FactorForVentilationHeatlosses[]                    VentFctr
NumberOfWeightsForGaussLegendreIntegration[]            GLIntWts
*****

***** tpanames.dbs
TimeOfRepositoryClosure[yr]                         TimClosr
TimeVentilationEnds[yr]                           TimVent
ThermalConductivityOfBackfillModelOne[W/(m-C)]          ThCndBM1
***** TPANAMES.DBS.ORIGINAL
TimeOfRepositoryClosure[yr]                         TimClosr
ThermalConductivityOfBackfillModelOne[W/(m-C)]          ThCndBM1
*****
```

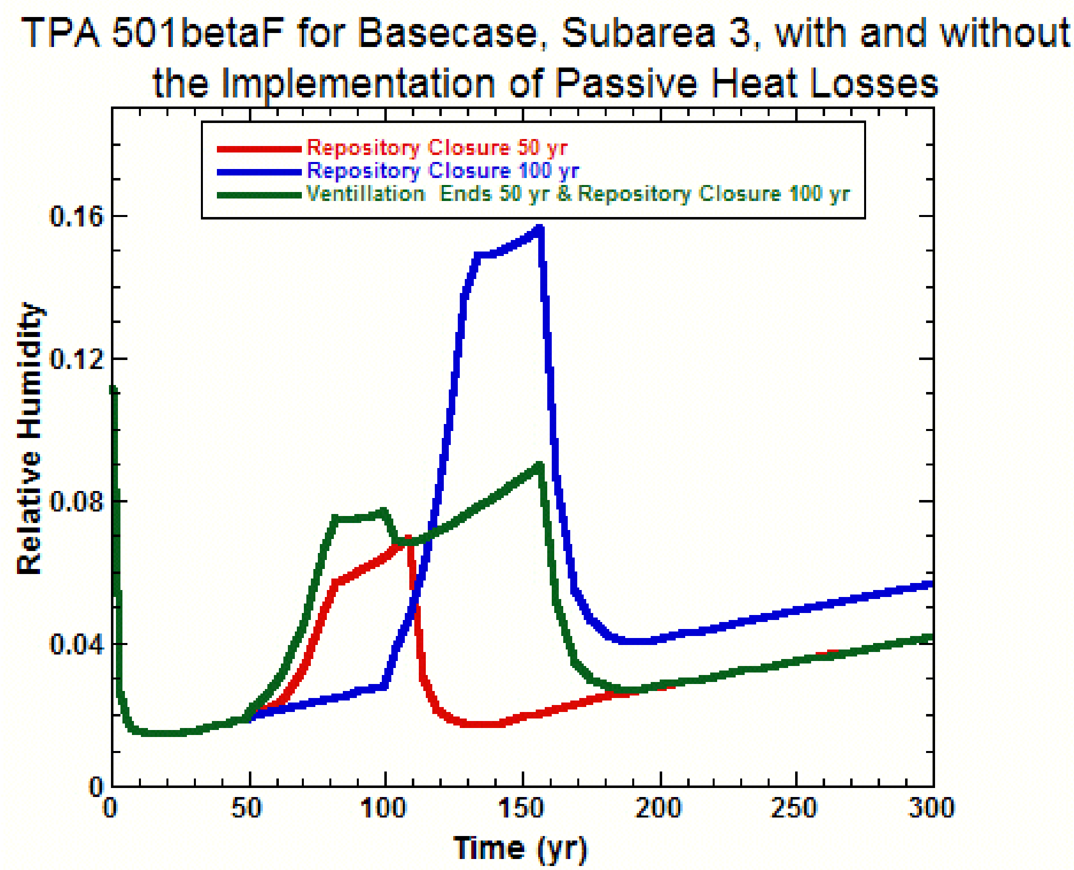
The following plots illustrates the 3 situations in which repository closure is at 50 and 100 years with ventilation heat losses occurring until repository closure (i.e., this represents TPA Version 501betaF results for repository closure at 50 and 100 years). The third case represents ventilation ending at 50 years (with ventilation heat losses) and then no ventilation (with no passive heat losses) until repository closure at 100 years.

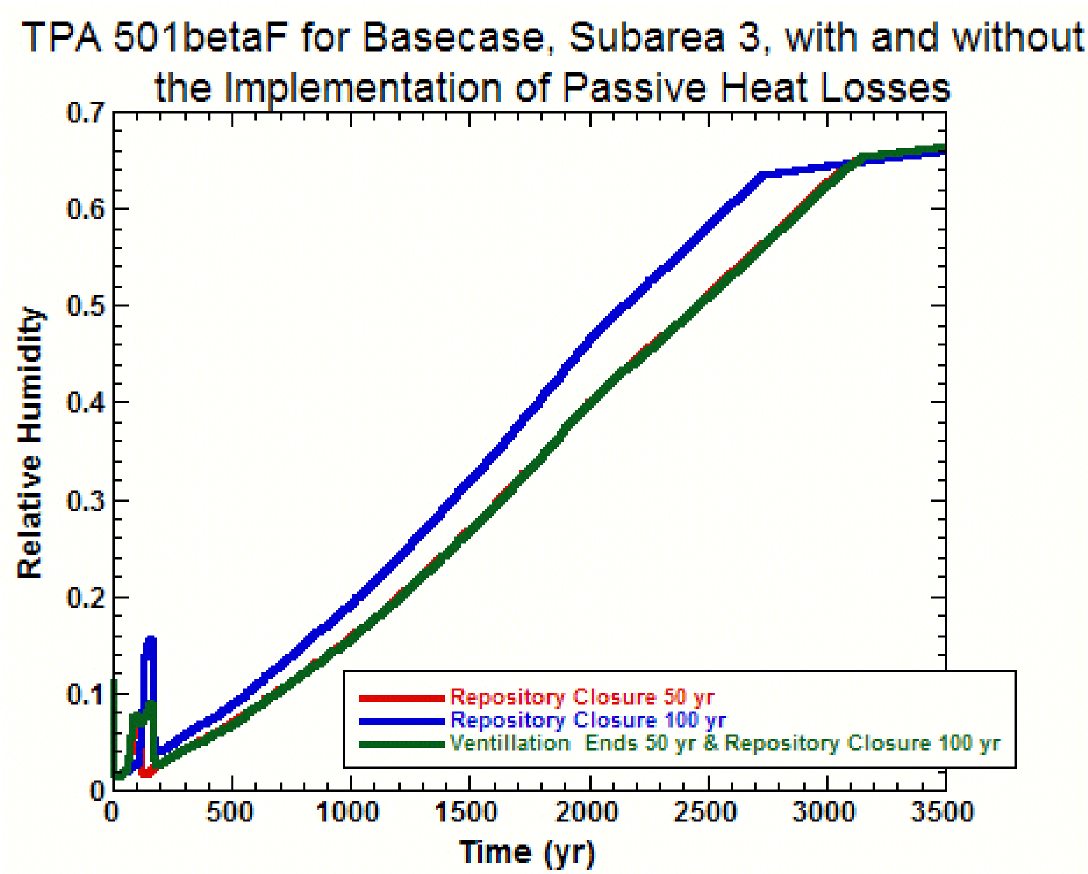


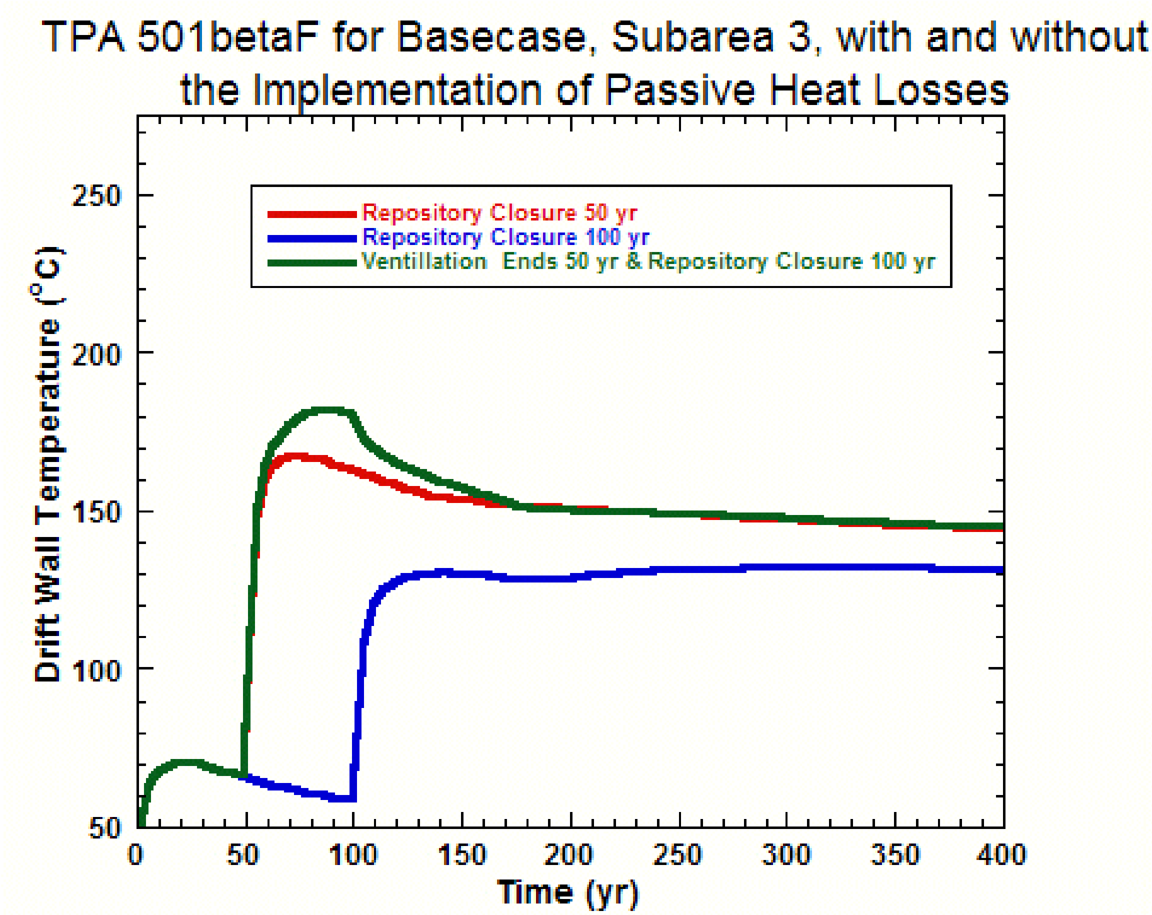
TPA 501betaF for Basecase, Subarea 3, with and without the Implementation of Passive Heat Losses
Waste Package Temperature (°C)
Time (yr)
50
100
150
200
250
0
50
100
150
200
250
300
350
400
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr

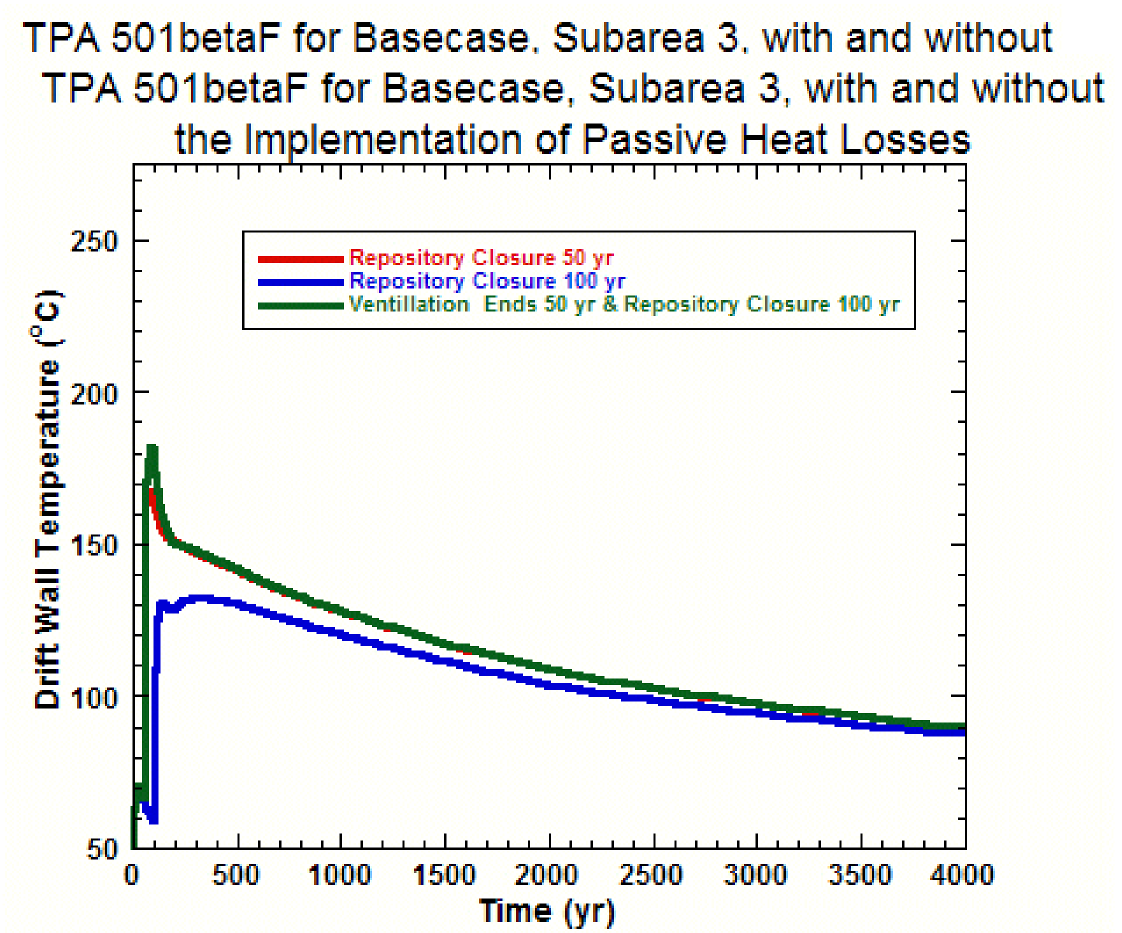


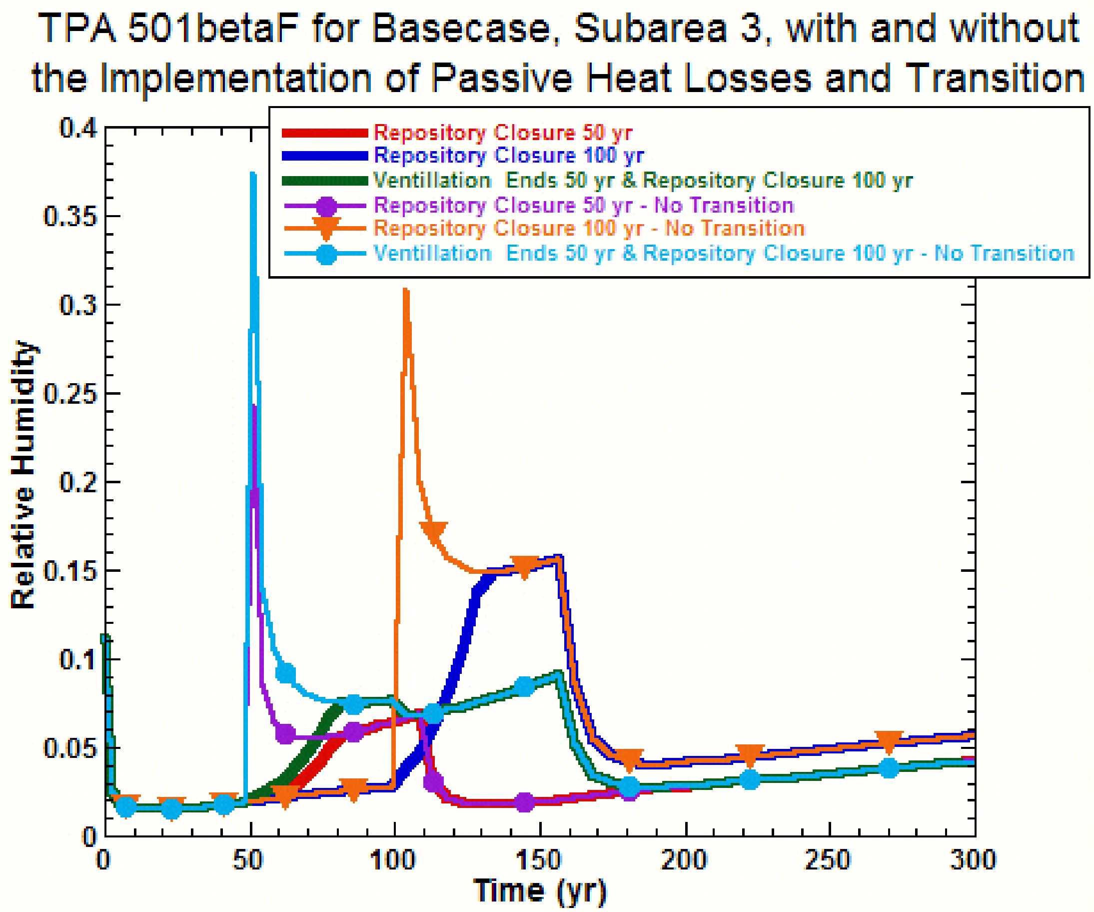
TPA 501betaF for Basecase, Subarea 3, with and without the Implementation of Passive Heat Losses
Waste Package Temperature (°C)
Time (yr)
50
100
150
200
250
0
500
1000
1500
2000
2500
3000
3500
4000
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr


TPA 501betaF for Basecase, Subarea 3, with and without the Implementation of Passive Heat Losses
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Relative Humidity
0
0.04
0.08
0.12
0.16
0
50
100
150
200
250
300
Time (yr)

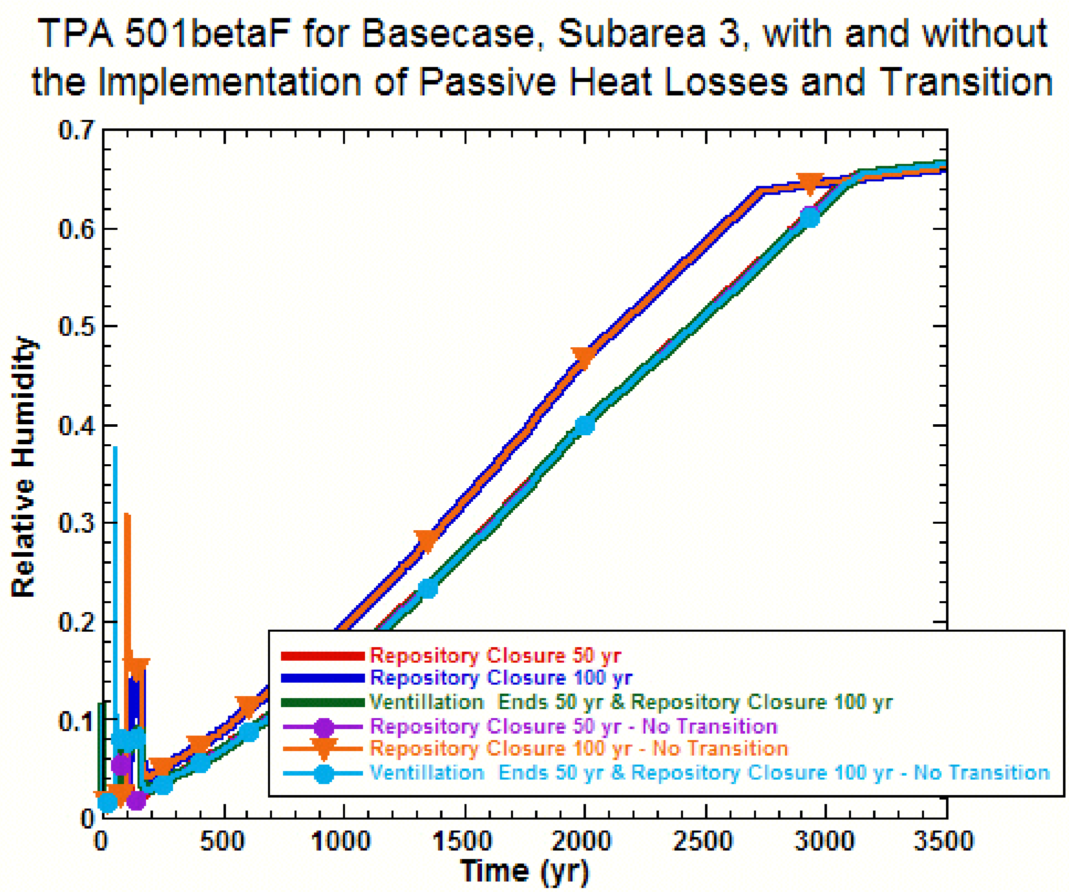

TPA 501betaF for Basecase, Subarea 3, with and without the Implementation of Passive Heat Losses
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Relative Humidity
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000
2500
3000
3500
Time (yr)


TPA 501betaF for Basecase, Subarea 3, with and without
the Implementation of Passive Heat Losses
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Drift Wall Temperature (°C)
Time (yr)
250
200
150
100
50
0
50
100
150
200
250
300
350
400

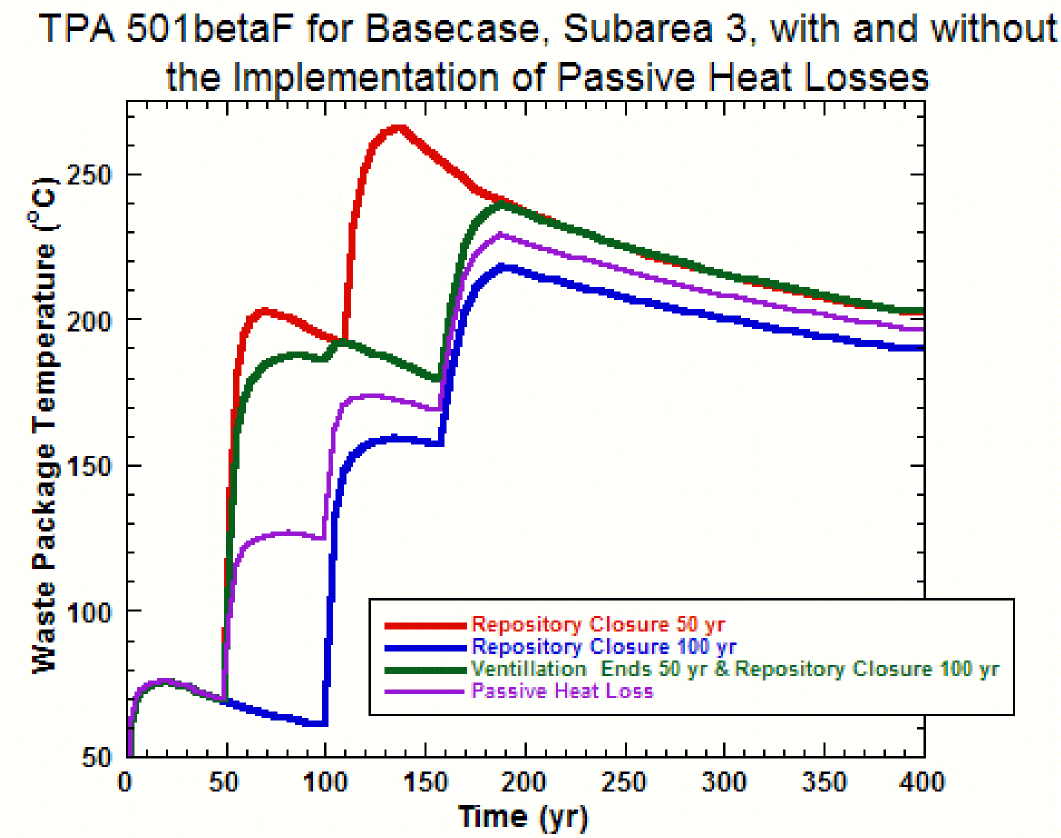

TPA 501betaF for Basecase, Subarea 3, with and without
TPA 501betaF for Basecase, Subarea 3, with and without
the Implementation of Passive Heat Losses
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Drift Wall Temperature (°C)
Time (yr)
250
200
150
100
50
0
500
1000
1500
2000
2500
3000
3500
4000

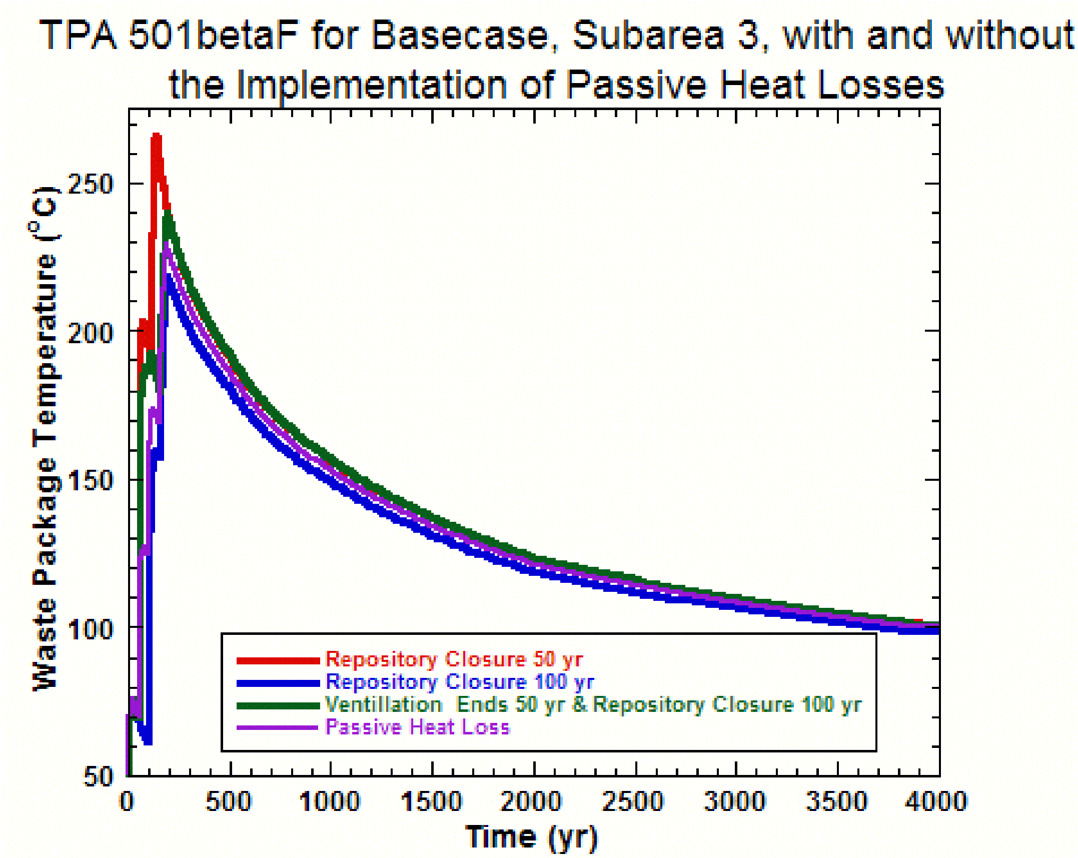


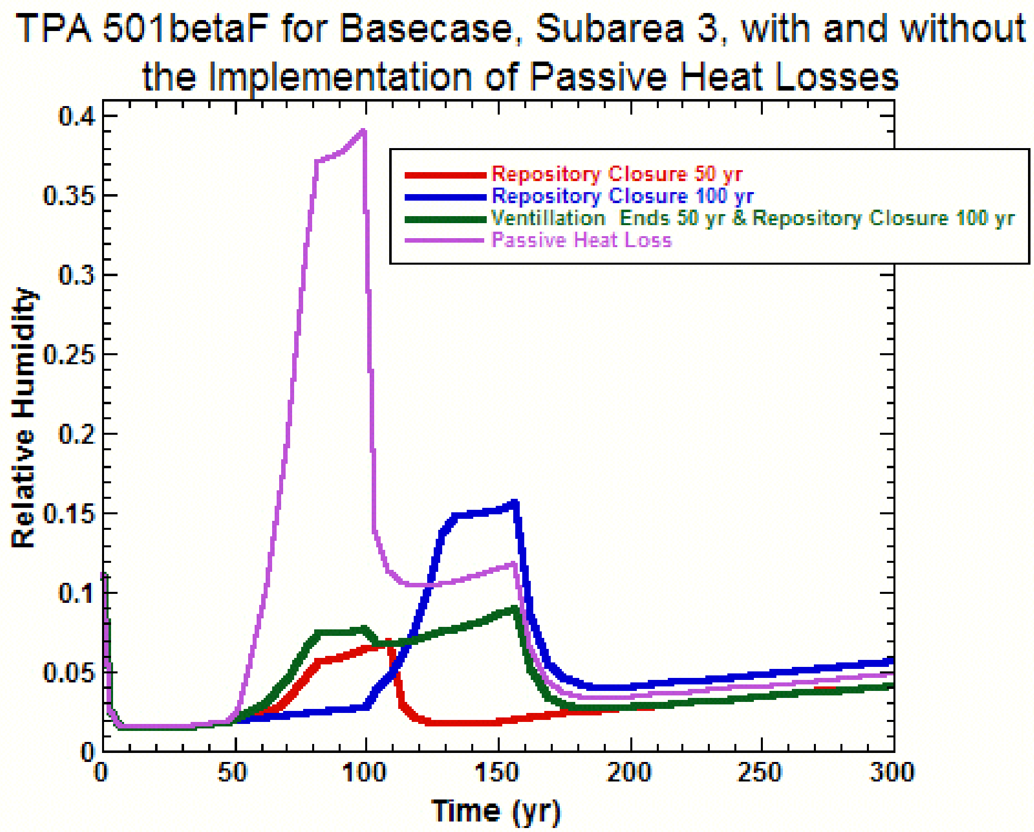
TPA 501betaF for Basecase, Subarea 3, with and without the Implementation of Passive Heat Losses and Transition
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Repository Closure 50 yr - No Transition
Repository Closure 100 yr - No Transition
Ventillation Ends 50 yr & Repository Closure 100 yr - No Transition
Relative Humidity
Time (yr)

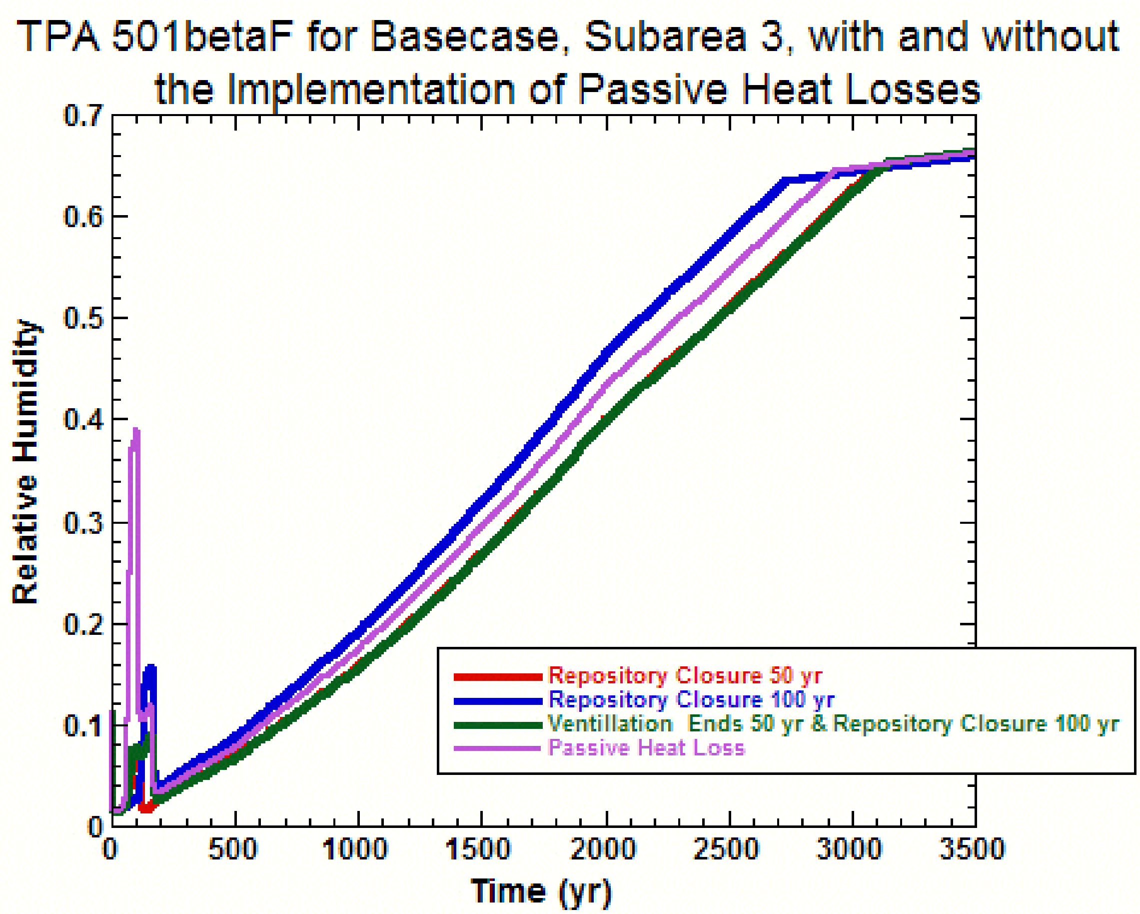


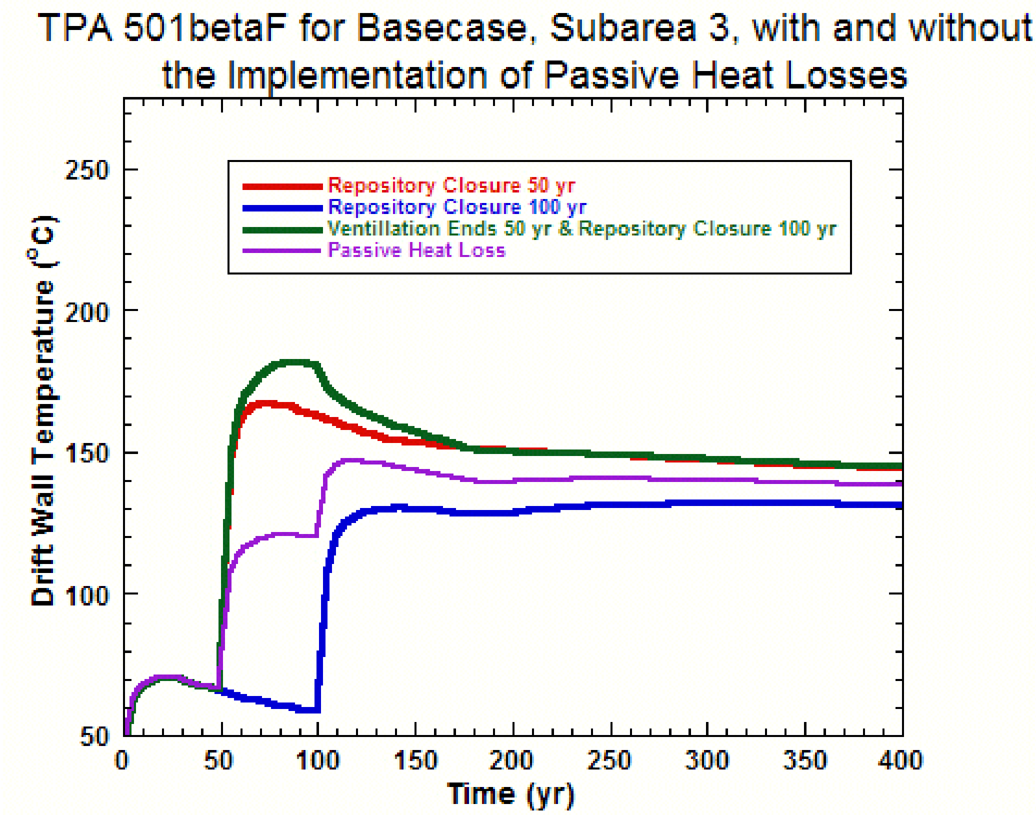
TPA 501betaF for Basecase, Subarea 3, with and without the Implementation of Passive Heat Losses and Transition
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Repository Closure 50 yr - No Transition
Repository Closure 100 yr - No Transition
Ventillation Ends 50 yr & Repository Closure 100 yr - No Transition
Relative Humidity
Time (yr)

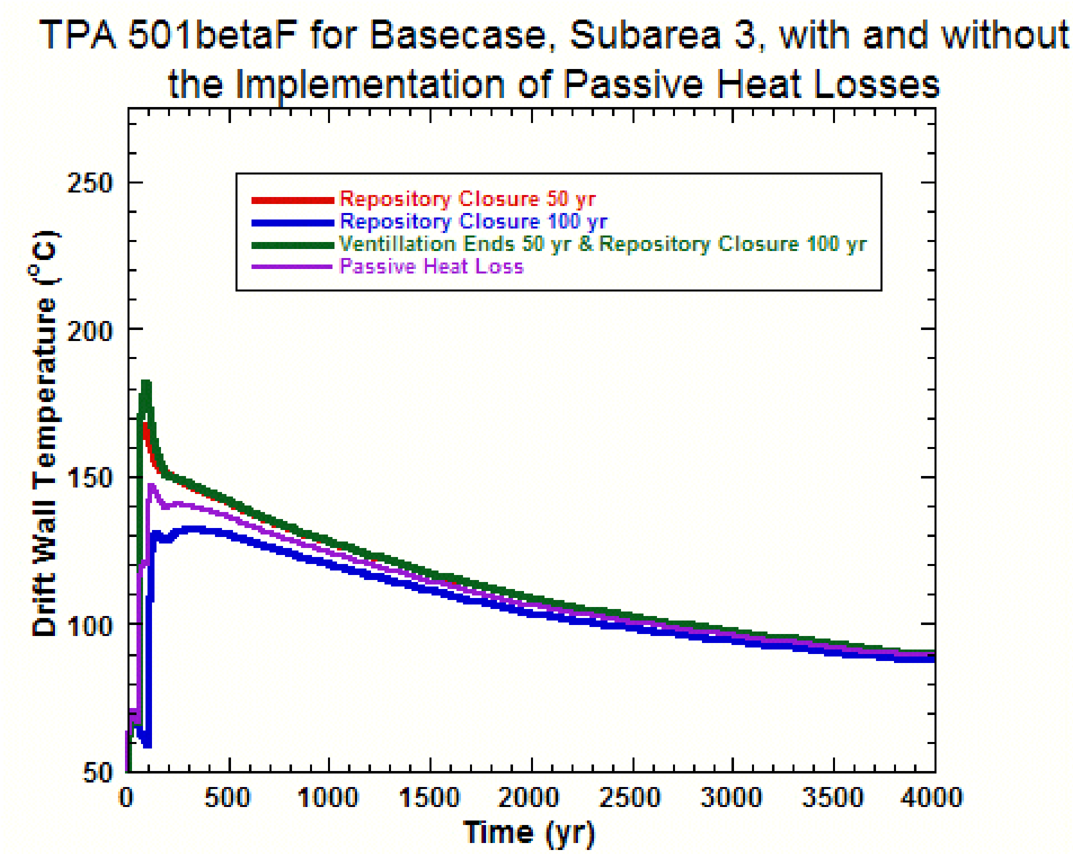

TPA 501betaF for Basecase, Subarea 3, with and without
the Implementation of Passive Heat Losses
Waste Package Temperature (°C)
Time (yr)
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Passive Heat Loss
50
100
150
200
250
0
50
100
150
200
250
300
350
400


TPA 501betaF for Basecase, Subarea 3, with and without
the Implementation of Passive Heat Losses
Waste Package Temperature (°C)
Time (yr)
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Passive Heat Loss
50
100
150
200
250
0
500
1000
1500
2000
2500
3000
3500
4000


TPA 501betaF for Basecase, Subarea 3, with and without the Implementation of Passive Heat Losses
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Passive Heat Loss
Relative Humidity
Time (yr)


TPA 501betaF for Basecase, Subarea 3, with and without the Implementation of Passive Heat Losses
Repository Closure 50 yr
Repository Closure 100 yr
Ventillation Ends 50 yr & Repository Closure 100 yr
Passive Heat Loss
Relative Humidity
Time (yr)





August 30, 2005 - Sent the following email to R. Janetzke to identify the TPA code changes for "Passive" heat losses and an end to the ventilation period. Also note that this email discusses changes to the TPA code for “Penetration” of corrosion. The changes in TPA code files made to accomplish allowing for “Penetration” of corrosion is presented after the text of the email below.

From: Rwrice
To: rjanetzke@cnwra.swri.edu
Cc: opensado@cnwra.swri.edu, jwinterle@swri.org, Rwrice
Bcc:
Subject: TPA code changes for End of Ventilation and Fraction Corrosion Penetration
Date: Tue, 30 Aug 2005 16:32:18 -0400

Ron,

I have made modifications to the TPA 501betaF code to address two situations. For purposes of my modifications, I labeled these two situations as "Passive" and "Penetration".

1) "Passive" - Allow for specification of the time for end of ventilation and for passive heat losses from that time to the time of repository closure (currently, the TPA code permits specification of a time of repository closure and heat losses during ventilation only).

2) "Penetration" - Allow for specification of three fractions of penetration by corrosion of the weld, WP, and drip shield thicknesses. Once this fraction of the thickness is penetrated by corrosion, then failure occurs.

These modifications were recommended by Osvaldo, who gave me explanations of the reasons for the changes and ideas of how to implement the changes in the TPA code. For "Passive", Osvaldo received and examined plots of results and expressed to me that the results seemed reasonable.

You can find the modified files, original files, and a comparison between the modified files and the original files in "passive\modified_files" and "penetration\modified_files" subdirectories located on the Scratch drive in SMohanty\Rob.

I tested these changes and found that they were correctly implemented in the TPA code. I recompiled the TPA code and performed the test runs on my laptop computer.

Please contact me if you have any questions.

Thanks,

Rob

(I'd email these files to you, but AOL creates a ZIP file whenever there is more than one file attached and your email can not receive ZIP files as attachments.)

Modifications made to the TPA code to allow for “Penetration” of corrosion failure associated with the thicknesses of the weld, waste package, and drip shield. Changes were made to the files *tpa.inp*, *tpanames.dbs*, *dsfail.f*, and *ebsfail.f*.

tpa.inp

```
Comparing files tpa.inp and TPA.INP.ORIGINAL
***** tpa.inp
**
** rwr 8/23/05 add fraction thickness penetration for corrosion failure
**         (note that there is a parameter for weld, waste package,
**          and drip shield)
**
constant
WPWeldFractionThicknessPenetratedForFailureByCorrosion[]
1.0
**
constant
WPFractionThicknessPenetratedForFailureByCorrosion[]
1.0
**
constant
DripShieldFractionThicknessPenetratedForFailureByCorrosion[]
1.0
**

***** TPA.INP.ORIGINAL

*****
```

tpanames.dbs

```
Comparing files tpanames.dbs and TPANAMES.DBS.ORIGINAL
***** tpanames.dbs
WPWeldThickness[m]                                  WPWThick
WPWeldFractionThicknessPenetratedForFailureByCorrosion[]    WeldPene
WPFractionThicknessPenetratedForFailureByCorrosion[]        WPPene
DripShieldFractionThicknessPenetratedForFailureByCorrosion[]DSPene
StandardExchangeCurrentDensityforOxygenReduction[C/(m^2 yr)]SECDOR
EquilibriumPotentialOxygenReduction[VSHE]                EPOR
***** TPANAMES.DBS.ORIGINAL
WPWeldThickness[m]                                  WPWThick
StandardExchangeCurrentDensityforOxygenReduction[C/(m^2 yr)]SECDOR
EquilibriumPotentialOxygenReduction[VSHE]                EPOR
*****
```

dsfail.f

```
Comparing files dsfail.f and DSFAIL.F.ORIGINAL
***** dsfail.f
c     drip_shield_thickness =

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
c     dspenetration =

c     drip_shield_slope =
***** DSFAIL.F.ORIGINAL
c     drip_shield_thickness =
c     drip_shield_slope =
```

```
*****

***** dsfail.f
      INTEGER index_thickness

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      integer i_dspenetration

***** DSFAIL.F.ORIGINAL
      INTEGER index_thickness

*****

***** dsfail.f
      DOUBLE PRECISION drip_shield_thickness

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
       double precision dspenetration

c      DOUBLE PRECISION drip_shield_slope
***** DSFAIL.F.ORIGINAL
      DOUBLE PRECISION drip_shield_thickness
c      DOUBLE PRECISION drip_shield_slope
*****

***** dsfail.f
c     &  index_min_fluoride, index_max_fluoride, index_FluorideEnh

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
cc       COMMON /dsfail2/ index_corrosion, index_thickness
      COMMON /dsfail2/ index_corrosion, index_thickness, i_dspenetration

c     GADAMS SCR562 4-4-2005: End of change
c
***** DSFAIL.F.ORIGINAL
c     &  index_min_fluoride, index_max_fluoride, index_FluorideEnh
      COMMON /dsfail2/ index_corrosion, index_thickness
c     GADAMS SCR562 4-4-2005: End of change
c
*****

***** dsfail.f
      drip_shield_thickness = valuesp(index_thickness)

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      dspenetration = valuesp(i_dspenetration)

c     GADAMS SCR562 4-4-2005: Removed slope, minF, maxF, and
***** DSFAIL.F.ORIGINAL
      drip_shield_thickness = valuesp(index_thickness)

c     GADAMS SCR562 4-4-2005: Removed slope, minF, maxF, and
*****
```

```
***** dsfail.f
c   Retrieve the drip shield thickness

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      drip_shield_thickness = drip_shield_thickness * dspenetration

      WRITE(line7(1:18), FMT = '(F15.3, 3x)') drip_shield_thickness
***** DSFAIL.F.ORIGINAL
c   Retrieve the drip shield thickness
      WRITE(line7(1:18), FMT = '(F15.3, 3x)') drip_shield_thickness
*****

***** dsfail.f
c     index_thickness =

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
c     i_dspenetration =

c     ispquery =
***** DSFAIL.F.ORIGINAL
c     index_thickness =
c     ispquery =
*****

***** dsfail.f
      INTEGER index_thickness

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      integer i_dspenetration

c     GADAMS SCR562 4-4-2005: Removed slope, minF, maxF, and
***** DSFAIL.F.ORIGINAL
      INTEGER index_thickness

c     GADAMS SCR562 4-4-2005: Removed slope, minF, maxF, and
*****

***** dsfail.f
c     &  index_min_fluoride, index_max_fluoride, index_FluorideEnh


cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
cc       COMMON /dsfail2/ index_corrosion, index_thickness
      COMMON /dsfail2/ index_corrosion, index_thickness, i_dspenetration

c     GADAMS SCR562 4-4-2005: End of change
c
***** DSFAIL.F.ORIGINAL
c     &  index_min_fluoride, index_max_fluoride, index_FluorideEnh
      COMMON /dsfail2/ index_corrosion, index_thickness
c     GADAMS SCR562 4-4-2005: End of change
c
*****
```

```
***** dsfail.f
      index_thickness = ispquery(sample_name)

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      CALL clearchar(60, sample_name)
      sample_name =
     &    'DripShieldFractionThicknessPenetratedForFailureByCorrosion[]'
      i_dspenetration = ispquery(sample_name)

c     GADAMS SCR562 4-4-2005: Removed slope, minF, maxF, and
***** DSFAIL.F.ORIGINAL
      index_thickness = ispquery(sample_name)

c     GADAMS SCR562 4-4-2005: Removed slope, minF, maxF, and
*****
```

ebsfail.f.

```
Comparing files ebsfail.f and EBSFAIL.F.ORIGINAL
***** ebsfail.f
c     i_terpslope     =
c     i_thickness     =

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
c     i_weldpenetration =
c     i_wppenetration   =

c     iaa_1_1         =
***** EBSFAIL.F.ORIGINAL
c     i_terpslope     =
c     i_thickness     =
c     iaa_1_1         =
*****

***** ebsfail.f
c     thickness       =

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
c     weldpenetration =
c     wppenetration   =

c     thist           =
c     timr            =
***** EBSFAIL.F.ORIGINAL
c     thickness       =
c     thist           =
c     timr            =
*****

***** ebsfail.f
      integer i_thickness

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      integer i_weldpenetration
```

```
      integer i_wppenetration

      integer iaa_1_1
***** EBSFAIL.F.ORIGINAL
      integer i_thickness
      integer iaa_1_1
*****

***** ebsfail.f
      double precision thickness

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      double precision weldpenetration
      double precision wppenetration

      double precision timr
***** EBSFAIL.F.ORIGINAL
      double precision thickness
      double precision timr
*****

***** ebsfail.f
      common /ebsfail19/ itend

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
cc      common / ebsfail20/ i_thickness, i_ErpInt,
cc     &  i_TErpInt, i_ErpSlope, i_TErpSlope
      common / ebsfail20/ i_thickness,
     &  i_weldpenetration, i_wppenetration,i_ErpInt,
     &  i_TErpInt, i_ErpSlope, i_TErpSlope
***** EBSFAIL.F.ORIGINAL
      common /ebsfail19/ itend

      common / ebsfail20/ i_thickness, i_ErpInt,
     &  i_TErpInt, i_ErpSlope, i_TErpSlope
*****

***** ebsfail.f
        i_thickness = ispquery(name)

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
        CALL clearchar(60, name)
        name =
     &        'WPWeldFractionThicknessPenetratedForFailureByCorrosion[]'
        i_weldpenetration = ispquery(name)

        CALL clearchar(60, name)
        name = 'WPFractionThicknessPenetratedForFailureByCorrosion[]'
        i_wppenetration = ispquery(name)

c  ZW SCR478 05-07-04 deleted:
***** EBSFAIL.F.ORIGINAL
        i_thickness = ispquery(name)
```

```
c  ZW SCR478 05-07-04 deleted:
*****

***** ebsfail.f

c ZW SCR478 05-07-04 new to end:
***** EBSFAIL.F.ORIGINAL


c ZW SCR478 05-07-04 new to end:
*****

***** ebsfail.f

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
cc           (note that these lines are repeated from above - they are
cc            commented out here)
cc      call clearchar( 60, name )
cc      name = 'OuterWPThickness[m]'
cc      cthick1 = valuesp( icthick1 )
cc
cc      call clearchar( 60, name )
cc      name = 'InnerWPThickness[m]'
cc      cthick2 = valuesp( icthick2 )
      cthick1 = valuesp( icthick1 )
      cthick2 = valuesp( icthick2 )



***** EBSFAIL.F.ORIGINAL

      call clearchar( 60, name )
        name = 'OuterWPThickness[m]'
        cthick1 = valuesp( icthick1 )

      call clearchar( 60, name )
        name = 'InnerWPThickness[m]'
        cthick2 = valuesp( icthick2 )

*****

***** ebsfail.f
      thickness = valuesp(i_thickness)

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      weldpenetration = valuesp(i_weldpenetration)
      wppenetration = valuesp(i_wppenetration)

c     std_iO2o = valuesp(i_iO2o)    ZW SCR478 05-07-04
***** EBSFAIL.F.ORIGINAL
      thickness = valuesp(i_thickness)
c     std_iO2o = valuesp(i_iO2o)    ZW SCR478 05-07-04
*****
```

```
***** ebsfail.f

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      cthick1 = cthick1 * wppenetration

      read(iebsfailtmp,100)aline
***** EBSFAIL.F.ORIGINAL

      read(iebsfailtmp,100)aline
*****

***** ebsfail.f
c     Alloy thickness of the weld

cc rwr 8/23/05 add fraction thickness penetration for corrosion failure
      thickness = thickness * weldpenetration

      READ(iebsfailtmp, 100) aline
***** EBSFAIL.F.ORIGINAL
c     Alloy thickness of the weld
      READ(iebsfailtmp, 100) aline
*****
```

Also, observed that the NEFTRAN output (not infrequently) may compute release rates at times greater than the maximum simulation time. For example, it was observed that the NEFTRAN SZ release rates for a 10,000 yr maximum simulation were computed for 11,000 yrs. The TPA code in reading the NEFTRAN output in *uzft.f* (subroutine aftnefmks) does not read NEFTRAN output at times greater than the maximum simulation time. Instead, the last time less than to equal to the maximum simulation time are read and the subroutine maplist will set all release rates equal for all TPA code times from at that last time read-in through the maximum simulation time. Release rates computed by NEFTRAN at times greater than the maximum simulation time may occur in a number of cases, including when NEFTRAN SZ is executed for tuff and alluvium separately. To test the effects of this approach/assumption of not reading in release rates at times greater than the maximum simulation time on TPA code results, the *uzft.f* file was modified and the TPA Version 501betaF code recompiled to read all NEFTRAN output (i.e., any release rates at times greater than the maximum simulation time will be used in maplist to determine release rates at TPA code times). The following changes were made in the *uzft.f* file.

```
Comparing files uzft.f and UZFT.F.ORIGINAL
***** uzft.f

cc rwr debug          if(timnew(i) .le.   tim(ntim)) then
cc (i.e., checking if limiting NEFTRAN output to
cc  times .le. tim(ntim) affects results)
            icounttimnew = icounttimnew +1
***** UZFT.F.ORIGINAL

          if(timnew(i) .le.   tim(ntim)) then
            icounttimnew = icounttimnew +1
*****
```

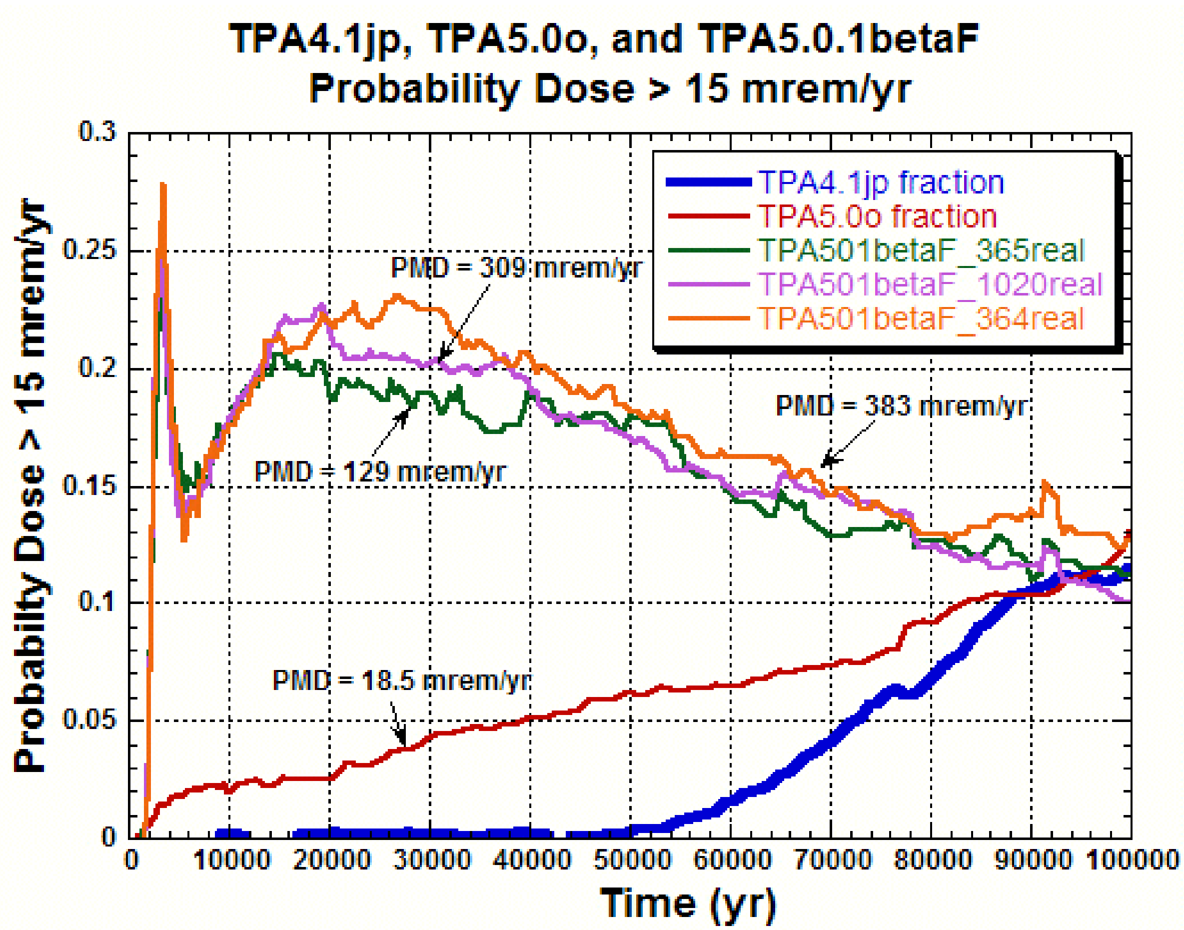
```
***** uzft.f

cc rwr debug          end if

***** UZFT.F.ORIGINAL

          end if

*****
```

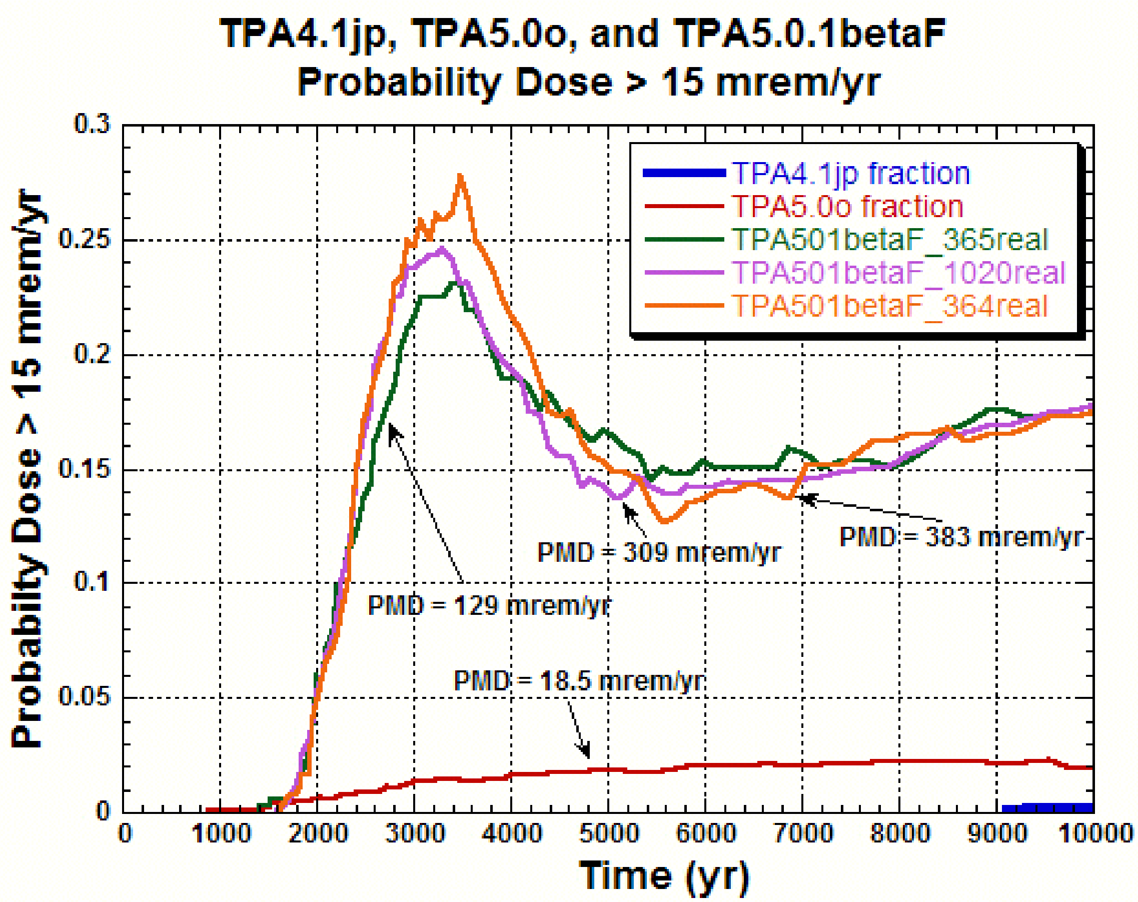
A TPA code run on the "tpa" machine was executed for 364 realizations. These results will be compared with basecase TPA Version 501betaF code results for 364 realizations. RESULTS - The peak expected dose decreased from 383 mrem/yr to 354 mrem/yr (about an 8% decrease) by using the recompiled code relative to the basecase.

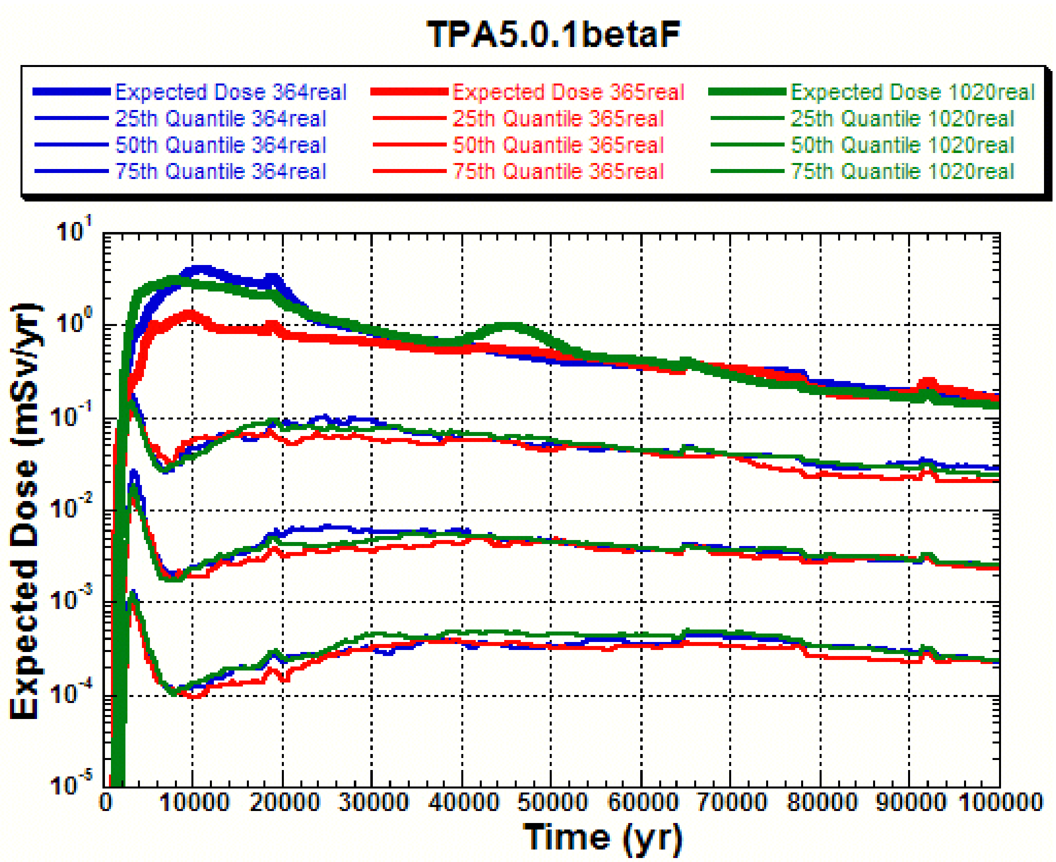
Additionally, the TPA code was modified to allow for simulations with greater than 1,024 realizations. The *snllhs.f* file in Version 501betaF is dimensioned in its include file for 4,000 realizations. The TPA code files *exec.f* and *execd.i* were the only files that needed to be modified to enable capabilities for greater than 1,024 realizations. The variables in these files were increased from 1,024 to 4,000. The TPA code was executed on the "tpa" machine using a number of realizations ranging to 4,000 realizations to compare output and convergence in the results (i.e., convergence of results for peak mean dose with increasing number of realizations). These results will be reported once these simulations successfully completed their execution.

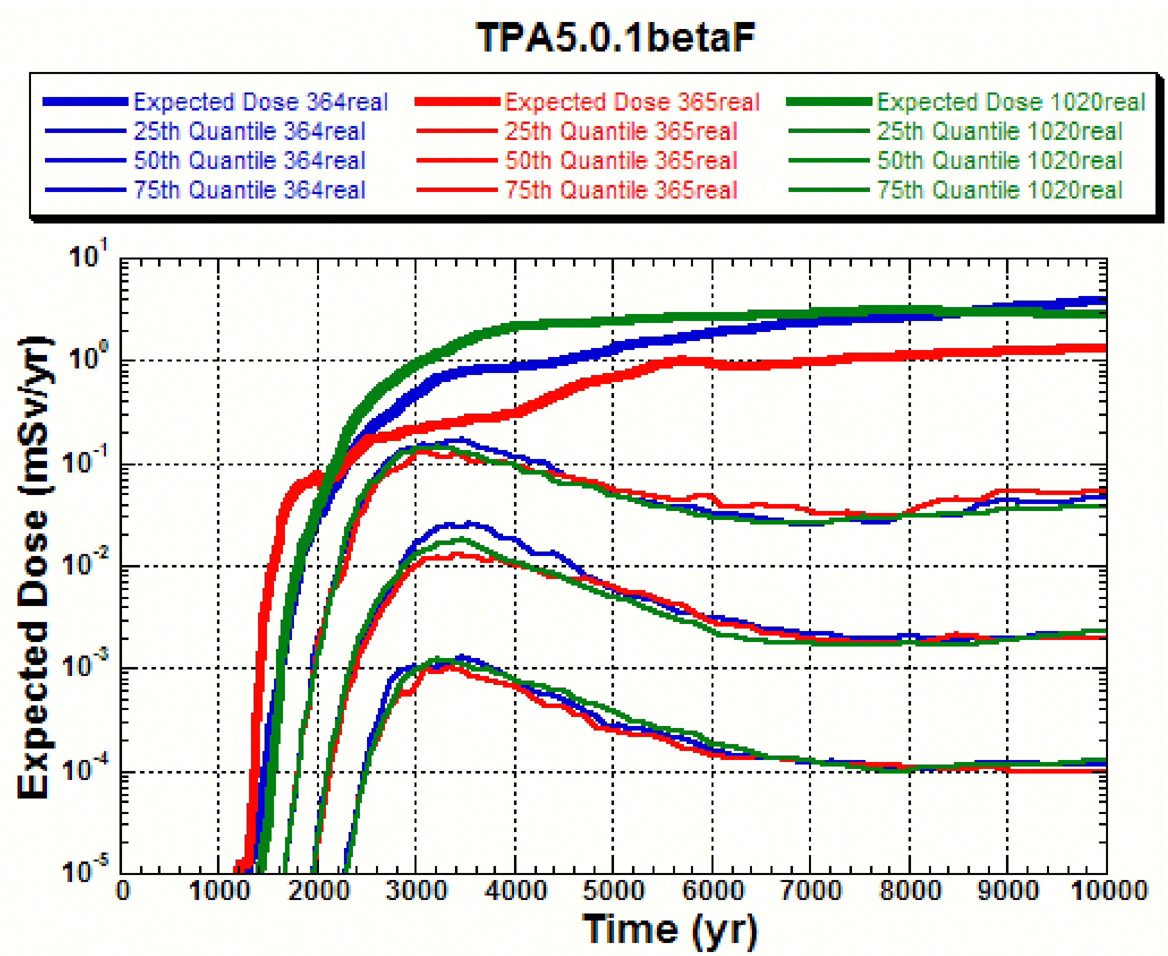
At the request of a query from J. Winterle, modified the *uzft.f* file by resetting the "gwttmin" to zero instead of 20 years. (This is value used to determine whether a leg will be included in the NEFTRAN input file *nefii.inp*. Thus, legs may not be used and in fact no legs may pass this test in which case NEFTRAN is skipped. NEFTRAN is skipped about 1/7 cases so this skipping raises the question of what are the implications of ignoring the UZ barrier on TPA code results.) The modified code was recompiled and executed for 364 realizations. TPA code execution was stopped in realization 23 in subarea 8 because the "BF" array dimensions were exceeded. Another TPA code simulation will be conducted using gwttmin = 5.0yr.

September 14, 2005 - Plotted TPA Version 501betaF code results to investigate the reasons for the behavior associated with a seeming lack of convergence in the peak expected dose with increasing number of realizations. From the plots below, it appears that a small number of realizations (<1%) are driving situations in which the peak expected dose varies considerably (i.e., from about 100 to 500 even though the number of realizations in the simulation differs by only 1 or 2 realizations). See the various plots below.


TPA4.1jp, TPA5.0o, and TPA5.0.1betaF
Probability Dose > 15 mrem/yr
Probabilty Dose > 15 mrem/yr
Time (yr)
TPA4.1jp fraction
TPA5.0o fraction
TPA501betaF_365real
TPA501betaF_1020real
TPA501betaF_364real
PMD = 309 mrem/yr
PMD = 129 mrem/yr
PMD = 383 mrem/yr
PMD = 18.5 mrem/yr
0
0.05
0.1
0.15
0.2
0.25
0.3
0
10000
20000
30000
40000
50000
60000
70000
80000
90000
100000


TPA4.1jp, TPA5.0o, and TPA5.0.1betaF
Probability Dose > 15 mrem/yr
TPA4.1jp fraction
TPA5.0o fraction
TPA501betaF_365real
TPA501betaF_1020real
TPA501betaF_364real
PMD = 309 mrem/yr
PMD = 383 mrem/yr
PMD = 129 mrem/yr
PMD = 18.5 mrem/yr
Probabilty Dose > 15 mrem/yr
Time (yr)


TPA5.0.1betaF
Expected Dose 364real
25th Quantile 364real
50th Quantile 364real
75th Quantile 364real
Expected Dose 365real
25th Quantile 365real
50th Quantile 365real
75th Quantile 365real
Expected Dose 1020real
25th Quantile 1020real
50th Quantile 1020real
75th Quantile 1020real
Expected Dose (mSv/yr)
Time (yr)


TPA5.0.1betaF
Expected Dose 364real
25th Quantile 364real
50th Quantile 364real
75th Quantile 364real
Expected Dose 365real
25th Quantile 365real
50th Quantile 365real
75th Quantile 365real
Expected Dose 1020real
25th Quantile 1020real
50th Quantile 1020real
75th Quantile 1020real
Expected Dose (mSv/yr)
Time (yr)
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
0
1000
2000
3000
4000
5000
6000
7000
8000
9000
10000

September 15, 2005 - Prepared and sent the following email to R. Janetzke. This list of items was requested by R. Janetzke and is intended to be my list of items that may need to be addressed in TPA code development, testing, and validation. The text of the email is:

Ron,

In response to your request during our meeting yesterday (see below), I have prepared the following list of items that may need to be addressed during TPA code development, testing, and validation. I mentioned these items to you yesterday, following the meeting, but am supplying this list as documentation for your and my reference in the future.

1. The output from NEFTRAN oftentimes extends beyond the maximum TPA code simulation time. The UZFT module which reads the NEFTRAN output file ignores any times greater than the maximum TPA code simulation time. When mapping these values to TPA code times, the UXFT module flat-lines all release rates at time greater than the last time read-in until the maximum TPA code simulation time. I've seen TPA code peak mean release rates change from 40 to 28 rem/yr. This could be solved by reading in all NEFTRAN output and allowing the TPA code to maplist those values to TPA code times. I saw a difference in peak mean dose for 364 realizations using TPA501betaF of 383 mrem/yr compared to 350 mrem/yr with the basecase and with this recommended changed introduced.

2. Suggest permanently changing the Courant number in the tpa.inp file from 1.5 to 0.15 to avoid NEFTRAN array out-of-bounds situations for 100,000 yr simulations. This problem occurs quickly in 1,000,000 yr simulations and in about 1/4 instances for 100,000 yr simulations.

3. At the request of and in consultation with Osvaldo, modified TPA501betaF and tested those changes to allow for (a) a time when ventilation stops maybe at 50 yr (during which time there are heat losses due to ventilation) and (b) passive heat losses maybe from 50 - 100 yr. At 100 yr, maintenance stops and natural drift degradation occurs. Ron thought we could also add the ability to specify a time for engineered backfill too. Osvaldo and Goodluck discussed the importance of ventilation stopping at 50yrs and natural drift degradation beginning at repository closure (100 yr). The modified TPA code is available on the scratch drive in the SMohanty/Rob/Passive subdirectory.

4. Similar to #3 above, Osvaldo recommended (following NRC/Center meeting) to modify the TPA code to allow the user to set a fraction of the thickness of the (a) drip shield; (b) weld; and (c) WP thickness (i.e., 3 different parameters) that is required to be penetrated for corrosion failure. That is, only partial, not complete, penetration of these entire thickness would result in failure by corrosion. Note that because these thicknesses are used in thermal calculations, these thicknesses needed to be changed during writing the values in the DSFAIL and FAILT input files and not in the tpa.inp file.

5. The fluoride.dat file only extends to 100,000 yrs, instead of to 1,000,000 yrs. If this file is not used, it is recommended that this file (and any others in this same situation of not being used) are removed from the delivered version of the TPA code.

6. In NFENV.F, there are parameters named "_DRY" (such as "PH_DRY") that are hard-coded. Note that the concentrations are set equal to zero and the pH equal to 7.0. If these parameters are used, suggest removing the hard-coded values from NFENV.F and moving them to tpa.inp.

7. In EBSREL.F, there is comment that the minimum invert permeability is 2e-18 m2; however, in the tpa.inp file the minimum is equal to 2.1e-19 m2. Also, this value is used in a

test to determine the average flow. Suggest making the EBSREL and tpa.inp minimum permeabilities consistent.

8. Suggest updating drythick.dat because the thermal loading of the repository and its payout has changed; thus the thickness and time-history of the dryout zone might be expected to be affected too. (Note that during an NRC/Center presentation, it was mentioned that this file needed to be updated.)

9. Suggest saving RELEASET input files for ebsrel.inp form both SF (spent fuel) and glass, instead of allowing them to overwritten. Also suggest ensuring that other files are renamed too (i.e., glass and SF; tuft and alluvium separation) - like what is done with the UZ and SZ NEFTRAN files.

10. The velocity files for SZ NEFTRAN when separating tuff and alluvium use lengths and velocity for LEG #1 that appear to be inconsistent with the approach used to set the LEG #1 lengths and velocity in the UZ and SZ without separation. Suggest examining the approach to determine whether this consistency is desired.

11. Examine the dependence of UZ NEFTRAN velocities in the nefii.vel file on the number of TPA code time steps specified in the tpa.inp file. This should be done mindful of the behavior of values in the climato2.dat file. It has been noted that difference TPA code time steps can result in nefii.vel values that are inconsistent due to mapping in the UZFT module.

12. The end of reflux is hard-coded in NFENV.F at 20,000 yr. Suggest examining whether this value should be hard-coded, if this value is correct (justify it), and it the REFLUX3 model is correct (i.e., remove this hard-coded value and check if the REFLUX3 output is as expected).

13. As was discussed with R. Codell, should implement a switch in RELEASET to use a different minimum volume that is dependent on the maximum TPA code simulation time (cutoff at 10,000 yr), since the release rates can be impacted by the value of the assumed minimum volume.

14. RELEASET output shows release rates at time prior filling the waste package. There doesn't appear to be a mechanism intentionally included in the TPA code that would explain these releases.

Please contact me if you have any questions regarding these items.

Thanks,

Rob

October 12, 2005 - Completed testing associated with SCR576. The SCR and Test Plan follow.

SOFTWARE CHANGE REPORT (SCR)

<table>
<tr><td>1. SCR No. (Software Developer Assigns):
PA-SCR-576</td><td>2. Software Title and Version:
TPA 5.0.0y</td><td>3. Project No:
20.06002.01.354</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td>5. Change Requested by:
R. Rice
5-12-05</td><td colspan="2">6. Change Authorized by (Software Developer):
R. Janetzke
Date: 5-12-05</td></tr>
<tr><td colspan="3">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.</td></tr>
<tr><td>8. Implemented by:
R. Janetzke</td><td colspan="2">Date:
5-16-05</td></tr>
<tr><td colspan="3">9. Description of Acceptance Tests: The file named “Test_Plan_SCR576.wpd” on the CD attached to this SCR contains a description of the Acceptance Tests for the change listed above in Box #4.</td></tr>
<tr><td>10. Tested by:
R. Rice</td><td colspan="2">Date: 10-12-05</td></tr>
</table>

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**

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.
October 25, 2005 - Completed testing for SCR578. The SCR and Test Plan follow.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-578	**2. Software Title and Version:** TPA 5.0.1beta	**3. Project No:** 20.06002.01.354
4. Affected Software Module(s), Description of Problem(s): *tpa.inp, releaset.f,, ebsfail.f, uzft.f, reader.f.* Sampling **CHnv** thicknesses with a PDF with a minimum of zero meters can result in very thin leg lengths for NEFMKS, thus causing run time inefficiencies in the code. The array element **rlmass(1,1,1)** is uninitialized in *releaset.f.* The *ebsfail.f* variables **outweldc** and **outwelds** are not calculated correctly. There are unused variables in *reader.f.*		
5. Change Requested by: R. Codell/ O. Pensado 5-26-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 5-27-05	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): See Attachment A.		
8. Implemented by: R. Janetzke	**Date:** 5-16-05	
9. Description of Acceptance Tests: See Attachment B.		
10. Tested by: R. Rice	**Date:** 10-25-05	

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP
SCR 578

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**
Modify to	EBSFAIL	OuterInhibitingCarbonateToCl		constant	0.2		O. Pensado
Modify to	NFENV	EnvironmentII_Wastepackage_DeltaECrit[VSHE]		constant	0.0		O. Pensado

Modify to	UZFT	LogCO2PartialPressure_AllUZ_SZLayers[atm]		usersuppliedpwisecdf	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		P. Bertetti

Modify to	UZFT	pH_AllUZ_SZLayers[StandardUnits]		usersuppliedpwisecdf	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		P. Bertetti
Modify to	EBSFAIL	OuterOverpackErpIntercept		triangular	1025.04,1180.76,1336.49		D. Dunn
Modify to	EBSFAIL	TempCoefOfOuterPackErpIntercept		constant	-9.35026		D. Dunn
Modify to	EBSFAIL	OuterOverpackErpSlope		constant	-752.034		D. Dunn
Modify to	EBSFAIL	TempCoefOfOuterPackErpSlope		constant	5.20131		D. Dunn

Modify to	EBSREL	RD_Invert_Cm	Retardation factor of Cm in invert	beta	2001, 20001, 9.039, 18.079		D. Pickett
Modify to	EBSREL	RD_Invert_U	Retardation factor of U in invert	beta	1, 21, 4.091, 4.091		D. Pickett
Modify to	EBSREL	RD_Invert_Am	Retardation factor of Am in invert	beta	2001, 20001, 9.039, 18.079		D. Pickett
Modify to	EBSREL	RD_Invert_Np	Retardation factor of Np in invert	beta	1, 21, 4.091, 4.091		D. Pickett
Modify to	EBSREL	RD_Invert_Th	Retardation factor of Th in invert	beta	2001, 20001, 9.039, 18.079		D. Pickett
Modify to	EBSREL	RD_Invert_Ni	Retardation factor of Ni in invert	beta	1, 1001, 3.061, 2.041		D. Pickett
Modify to	EBSREL	RD_Invert_Se	Retardation factor of Se in invert	beta	1, 21, 4.091, 4.091		D. Pickett

Modify to	EBSREL	RD_Invert_Nb	Retardation factor of Nb in invert	beta	2001, 20001, 9.039, 18.079		D. Pickett

Attachment A

This list contains the method of resolution for the following items:

1) Sampling **CHnv** thicknesses with a PDF with a minimum of zero meters can result in very thin leg lengths for NEFMKS, thus causing run time inefficiencies in the code.

The **CHnv** thickness is limited to values greater than 2, or if the values are between 0 and 2 they are set to 0.

2) The array element **rlmass(1,1,1)** is uninitialized in *releaset.f.*

The array element is initialized at the point were the rest of the array is initialized.

3) The *ebsfail.f* variables **outweldc** and **outwelds** are not calculated correctly.

Usage of variable **inhToCl1** in line 2080 was changed to variable **inhToClw**.

4) There are unused variables in *reader.f.*

Variable **totnwp** was removed.

5) Update the *tpa.inp* file for the parameters starting on page 2 of this SCR in the table “UPDATE REQUIREMENTS for TPA.INP - SCR578"

Attachment B

Test Plan for TPA SCR#578

Test Plan Name: *uzft.f*, RELEASET, *ebsfail.f*, and *reader.f* Modifications and *tpa.inp* Data Updates

Tested By: R. Rice **Date:** October 25, 2005

Host Machine: Toshiba Laptop **Host OS:** XP Professional

Baseline Version: 5.0.1beta **Test Version:** 5.0.1betaA

System Level (SL) Tests

SL-1. Name: Set Minimum CHnv Thickness - *uzft.f*

Path for run directory: c:\SCR578\tpa501beta\run\test1
c:\SCR578\tpa501betaA\run\test1

Path for archive of results: \SCR578\tpa501beta\run\test1 (archived on CD "SCR#578 Testing")
\SCR578\tpa501betaA\run\test1 (archived on CD "SCR#578 Testing")

Environment variables: Baseline case
TPA_DATA=c:\SCR578\tpa501beta
TPA_DATA=c:\SCR578\tpa501beta

and

Test Case
TPA_DATA=c:\SCR578\tpa501betaA
TPA_DATA=c:\SCR578\tpa501betaA

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only; activate APPEND file flag; set the CHnv thickness greater than and less than 2; and set CHnv porosity to 0.99); because there are no parameter additions or deletions in the *tpa.inp* file (only values and distributions), use the *tpa.inp* file from TPA Version 5.0.1beta code also for TPA Version 5.0.1betaA code

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 TPA code was modified to set CHnv thickness in the *uzft.f* source code to 0 whenever a sampled value is less than 2. The test verifies the TPA Version 5.0.1betaA code correctly sets this value when the CHnv thickness in the *tpa.inp* file is greater than and less than 2. Results from TPA Version 5.0.1beta are compared with TPA Version 5.0.1betaA code results to demonstrate that this change was implemented correctly.

- Objective: Verify that the TPA Version 5.0.1betaA code sets the CHnv thickness to 0 when the sampled value is less than 2 Otherwise (i.e., Chnv thickness greater than 2), the sampled value is written to the *nefiiuz.inp* file.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *nefiiuz.inp*, screenprint

- Step by step test procedure to be used:

1. In the “run\test1” subdirectories in both the TPA Versions 5.0.1beta and 5.0.1betaA main source code directories, create two subdirectories named “CHnv_thickness_greater_than_2” and “CHnv_thickness_less_than_2”.
2. In each of these subdirectories, modify the *tpa.inp* file according to the “Special input files or modifications to input files required” given above. Note that values for the

CHnv thickness are set in this step at close to 2 (i.e., limits are 1.999, 1.9995 and 1.9999 together with 2.000, 2.005, 2.010 for cases less than and greater than 2, respectively).

3. Execute the TPA Versions 5.0.1beta and 5.0.1betaA code in the subdirectories created in #1 and capture the screenprint.

- Pass/Fail criteria:

Criterion 1: The differences in the TPA Version 5.0.1beta code screenprint (*tpa.out*) of less than 5% because the CHnv thicknesses both equal 2.0 at two significant digits (i.e., even though the values are less than and greater than 2 using the limits in #2 above, they are rounded to 2 in the *nefiiuz.inp* file) and only the dispersion in the *nefiiuz.inp* file should be different because this value is calculated using the CHnv thicknesses.

Criterion 2: The differences in dispersion for the TPA Version 5.0.1beta code in the *nefiiuz.inp* file should be less than 5%.

Criterion 3: For the TPA Version 5.0.1betaA code, the UZ should be skipped (see screenprint file *tpa.out*) when the CHnv thicknesses is less than 2.

Criterion 4: For the TPA Version 5.0.1betaA code, when the CHnv thicknesses is greater than 2, the NEFTRAN input files *nefiiuz.inp* and results in the screenprint (*tpa.out*) should be the same (other than the time and date of the TPA code run) as observed in TPA Version 5.0.1beta when the CHnv thicknesses is greater than 2.

Test Results: The files in the \SCR578\tpa501beta\run\test1 and \SCR578\tpa501betaA\run\test1 subdirectories contain results for this test. The results in these subdirectories indicate that the Pass/Fail Criteria for all 4 criteria were met. (Note that the text for the file comparisons [“differences”] shown below are in the \SCR578\tpa501beta\run\test1 and SCR578\tpa501betaA\run\test1 subdirectories in files with names starting with “fc_”.)

<u>For Criterion 1,</u> the differences in the screenprint (*tpa.out*) are:

```
    Comparing files tpa.out and ..\CHNV_THICKNESS_GREATER_THAN_2\TPA.OUT
***** tpa.out
   exec: Welcome to TPA Version 5.0.1beta
```

```
     Job started: Wed Oct 19 15:24:31 2005
==========================================================================
***** ..\CHNV_THICKNESS_GREATER_THAN_2\TPA.OUT
      exec: Welcome to TPA Version 5.0.1beta
     Job started: Wed Oct 19 15:27:31 2005
==========================================================================
*****

***** tpa.out
            Highest release rates from UZ
        Tc99    1.3716E-02 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   4.2437E-03 [Ci/yr/SA] at  1.000E+04 yr
        Ni59    9.4799E-04 [Ci/yr/SA] at  1.000E+04 yr
        Se79    8.0047E-04 [Ci/yr/SA] at  1.000E+04 yr
        Cl36    4.8049E-04 [Ci/yr/SA] at  1.000E+04 yr
        Np237   3.4641E-04 [Ci/yr/SA] at  1.000E+04 yr
exec: calling szft
***** ..\CHNV_THICKNESS_GREATER_THAN_2\TPA.OUT
            Highest release rates from UZ
        Tc99    1.3572E-02 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   4.1866E-03 [Ci/yr/SA] at  1.000E+04 yr
        Ni59    9.3039E-04 [Ci/yr/SA] at  1.000E+04 yr
        Se79    7.9208E-04 [Ci/yr/SA] at  1.000E+04 yr
        Cl36    4.7545E-04 [Ci/yr/SA] at  1.000E+04 yr
        Np237   3.4168E-04 [Ci/yr/SA] at  1.000E+04 yr
exec: calling szft
*****

***** tpa.out
        I129    1.1600E-04 [Ci/yr/SA] at  7.376E+03 yr
        Np237   3.3429E-08 [Ci/yr/SA] at  8.293E+03 yr
        U233    3.3737E-11 [Ci/yr/SA] at  1.000E+04 yr
exec: calling dcagw
***** ..\CHNV_THICKNESS_GREATER_THAN_2\TPA.OUT
        I129    1.1600E-04 [Ci/yr/SA] at  7.376E+03 yr
        Np237   3.3428E-08 [Ci/yr/SA] at  8.293E+03 yr
        U233    3.3736E-11 [Ci/yr/SA] at  1.000E+04 yr
exec: calling dcagw
*****

***** tpa.out
        Cl36    3.2258E-04 [mrem/yr]  at  7.376E+03 yr
        Np237   4.3270E-06 [mrem/yr]  at  8.293E+03 yr
        U233    1.6372E-09 [mrem/yr]  at  1.000E+04 yr
***** ..\CHNV_THICKNESS_GREATER_THAN_2\TPA.OUT
        Cl36    3.2258E-04 [mrem/yr]  at  7.376E+03 yr
        Np237   4.3269E-06 [mrem/yr]  at  8.293E+03 yr
        U233    1.6372E-09 [mrem/yr]  at  1.000E+04 yr
*****
```

```
***** tpa.out
        Se79    5.4939E-04 [mrem/yr]
        Cl36    1.5288E-04 [mrem/yr]
        Np237   2.2304E-06 [mrem/yr]
***** ..\CHNV_THICKNESS_GREATER_THAN_2\TPA.OUT
        Se79    5.4939E-04 [mrem/yr]
        Cl36    1.5287E-04 [mrem/yr]
        Np237   2.2304E-06 [mrem/yr]
*****
```

Note above that the maximum % difference in the results is 1.4% for CS135 UZ release. Therefore, Criterion 1 is passed.

For Criterion 2, the differences in the dispersion values from the *nefiiuz.inp* file are:

```
Comparing files nefiiuz.inp and ..\CHNV_THICKNESS_GREATER_THAN_2\NEFIIUZ.INP
***** nefiiuz.inp
  1 0.6000E-01    0.0     0    0.990E+00   0.000E+00   0.000E+00   0.100E+01
  2 0.1199E+00    0.0     0    0.990E+00   0.000E+00   0.000E+00   0.383E-01
                       DECAY CHAIN ARRAY
***** ..\CHNV_THICKNESS_GREATER_THAN_2\NEFIIUZ.INP
  1 0.6000E-01    0.0     0    0.990E+00   0.000E+00   0.000E+00   0.100E+01
  2 0.1200E+00    0.0     0    0.990E+00   0.000E+00   0.000E+00   0.383E-01
                       DECAY CHAIN ARRAY
*****
```

Note above that the maximum difference in the dispersion values is 0.1199 compared to 0.1200. Therefore, Criterion 2 is passed.

For Criterion 3, the screenprint (*tpa.out*) below shows UZ NEFTRAN was skipped.

```
=======================================================================
      exec: Welcome to TPA Version 5.0.1betaA
     Job started: Wed Oct 19 15:09:59 2005
=======================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
  #     [m^2]      [MTU]
  1    224091.0    4150.1       526
  2    448476.0    8379.2      1062
  3   2621741.5   41959.0       5318
  4    152357.0    2706.3       343
  5    318122.0    5491.4       696
  6    439350.0    7345.6       931

Total Area [acre]        =  1038.828144304423
Total Buried Waste [MTU]  =  70031.64000000000
Repository AML [MTU/acre] =  67.41407650915320
Watts per MTU [W/MTU]     =  967.5799977250001
```

```
Watts per linear meter of drift [W/m] =  1449.991677502422

Specified Global Parameters:

             Compliance Period =  10000.0 (yr)
        Maximum Simulation Time =  10000.0 (yr)
         Number Of Realizations =      1
             Number Of Subareas =      6
             Volcanism scenario =      0 (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    220 megs of disk space.
(NOTE: more disk space could be needed)

----------------------------------------------------------------------
    subarea   1 of   6         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: time of Weld failure =      841.4  yr
     *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =      2 at time =      0.0 yr
 *** failed WPs:  2   out of  526  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
                Highest release rates from Sub Area 1
```

```
        Pu239   1.4707E-01 [Ci/yr/SA] at  1.000E+04 yr
        Jp239   1.2501E-01 [Ci/yr/SA] at  1.000E+04 yr
        Pu240   1.1700E-01 [Ci/yr/SA] at  1.000E+04 yr
        Jp240   9.9450E-02 [Ci/yr/SA] at  1.000E+04 yr
        Tc99    2.0103E-02 [Ci/yr/SA] at  1.000E+04 yr
        C14     8.3011E-03 [Ci/yr/SA] at  1.000E+04 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
        Pu239   1.4707E-01 [Ci/yr/SA] at  1.000E+04 yr
        Jp239   1.2501E-01 [Ci/yr/SA] at  1.000E+04 yr
        Pu240   1.1700E-01 [Ci/yr/SA] at  1.000E+04 yr
        Jp240   9.9450E-02 [Ci/yr/SA] at  1.000E+04 yr
        Tc99    2.0103E-02 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   8.0213E-03 [Ci/yr/SA] at  1.000E+04 yr
exec: calling szft
             Highest release rates from SZ
        Tc99    4.3880E-03 [Ci/yr/SA] at  7.376E+03 yr
        Se79    2.6927E-04 [Ci/yr/SA] at  8.101E+03 yr
        Cl36    1.8660E-04 [Ci/yr/SA] at  7.205E+03 yr
        I129    1.1627E-04 [Ci/yr/SA] at  7.205E+03 yr
        Np237   3.3428E-08 [Ci/yr/SA] at  8.101E+03 yr
        U233    3.5642E-11 [Ci/yr/SA] at  1.000E+04 yr
exec: calling dcagw
             Highest annual dose GW pathway
        I129    1.4548E-02 [mrem/yr]  at  7.205E+03 yr
        Tc99    3.1089E-03 [mrem/yr]  at  7.376E+03 yr
        Se79    8.0374E-04 [mrem/yr]  at  8.101E+03 yr
        Cl36    3.2356E-04 [mrem/yr]  at  7.205E+03 yr
        Np237   4.3268E-06 [mrem/yr]  at  8.101E+03 yr
        U233    1.7297E-09 [mrem/yr]  at  1.000E+04 yr
       At end of TPI, annual dose GW pathway
        I129    6.8670E-03 [mrem/yr]
        Tc99    1.6528E-03 [mrem/yr]
        Se79    5.4047E-04 [mrem/yr]
        Cl36    1.5024E-04 [mrem/yr]
        Np237   2.3090E-06 [mrem/yr]
        U233    1.7297E-09 [mrem/yr]
          sum  9.2128E-03 [mrem/yr]
exec: end realizations

exec: Peak Mean Dose is 1.84030E-05 rem/yr at    7376.3 yr, based on     1 realizations.

exec:  Run Successfully Completed
```

Note above that the NEFTRAN UZ is now skipped since the CHnv thickness is less than 2. Therefore, Criterion 3 is passed.

For Criterion 4, the differences in the *nefiiuz.inp* and screenprint (*tpa.out*) from TPA Versions 5.0.1beta and 5.0.1betaA code with CHnv thickness greater than 2 are shown below.

```
Comparing files nefiiuz.inp and
C:\SCR578\TPA501BETA\RUN\TEST1\CHNV_THICKNESS_GREATER_THAN_2\NEFIIUZ.I
NP
FC: no differences encountered


Comparing files tpa.out and
C:\SCR578\TPA501BETA\RUN\TEST1\CHNV_THICKNESS_GREATER_THAN_2\TPA.OUT
***** tpa.out
=============================================================================
       exec: Welcome to TPA Version 5.0.1betaA
     Job started: Wed Oct 19 15:06:07 2005
=============================================================================
*****
C:\SCR578\TPA501BETA\RUN\TEST1\CHNV_THICKNESS_GREATER_THAN_2\TPA.OUT
=============================================================================
       exec: Welcome to TPA Version 5.0.1beta
     Job started: Wed Oct 19 15:27:31 2005
=============================================================================
*****
```

There are no differences (other than the time and date of the TPA code run) in the above "file comparison" between *nefiiuz.inp* and the screenprint (*tpa.out*). Therefore, Criterion 4 is passed.

- Overall test status: PASS

SL-2. Name: Initial All Elements in Array “rlmass(1,1,1)” - RELEASET

Path for run directory: c:\SCR578\tpa501beta\run\test2
c:\SCR578\tpa501betaA\run\test2

Path for archive of results: \SCR578\tpa501beta\run\test2 (archived on CD “SCR#578 Testing”)
\SCR578\tpa501betaA\run\test2 (archived on CD “SCR#578 Testing”)

Environment variables: Baseline case
TPA_DATA=c:\SCR578\tpa501beta
TPA_DATA=c:\SCR578\tpa501beta

and

Test Case
TPA_DATA=c:\SCR578\tpa501betaA
TPA_DATA=c:\SCR578\tpa501betaA

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only and activate APPEND file flag); because there are no parameter additions or deletions in the *tpa.inp* file (only values and distributions), use the *tpa.inp* file from TPA Version 5.0.1beta code also for TPA Version 5.0.1betaA code

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 RELEASET code was modified to initialize all elements in the array “rlmass(1,1,1)”. This initialization should not change results since the TPA code only calculates release rates at the first time step greater than zero (i.e., there is no release at time equals zero).

- Objective: Verify that the EBS release rates from the TPA Version 5.0.1beta and 5.0.1betaA code results are not changed from this initialization.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *ebsrel.rlt*, *ebsnef.dat*, and *releaset.f*

- Step by step test procedure to be used:

1. In the "run" subdirectories in both the TPA Versions 5.0.1beta and 5.0.1betaA main source code directories, execute the TPA code using the *tpa.inp* file described above.
2. Create subdirectories in these "run" subdirectories called "test2\standalone_run". Copy the files needed to run RELEASET in standalone mode here. Also, create a subdirectory to archive these files called "original_files".
3. Modify the *ebsflo.dat* file by setting the flow rate at time equals zero at 100 (i.e., force flow and therefore releases at early as possible since flow/release does not necessarily occur at the first time step
4. Run RELEASET in standalone mode for the set-up described above in #3.

- Pass/Fail criteria:

Criterion 1: The differences between source code of RELEASET (*releaset.f*) in TPA Versions 5.0.1beta and 5.0.1beta code should show that the array "rlmass(1,1,1)" is initialized.

Criterion 2: There should be no differences between the EBSREL output files *ebsrel.rlt* (other than the time and date of the TPA code run) from the TPA Versions 5.0.1beta and 5.0.1beta code results in corresponding "run" subdirectories.

Criterion 3: There should be no differences between the RELEASET output file *ebsnef.dat* (other than the time and date of the TPA code run) from the TPA Versions 5.0.1beta and 5.0.1beta code results in corresponding "run" subdirectories.

Criterion 4: There should be no differences between the RELEASET output file *ebsnef.dat* (other than the time and date of the TPA code run) from the TPA Versions 5.0.1beta and 5.0.1beta code results in corresponding "run\test2\standalone_run" subdirectories.

Test Results: The files in the \SCR578\tpa501beta\run\test2 and \SCR578\tpa501betaA\run\test2 subdirectories contain results for this test. The results in these subdirectories indicate that the Pass/Fail Criteria for all 4 criteria were met. (Note that the text for the file comparisons ["differences"] shown below are in the \SCR578\tpa501beta\run\test2 and SCR578\tpa501betaA\run\test2 subdirectories in files with names starting with "fc_".)

<u>For Criterion 1,</u> the differences in the RELEASET source code (*releaset.f*) are:

```
Comparing files releaset.f and C:\SCR578\TPA501BETA\RUN\TEST2\RELEASET.F
***** releaset.f
C File Name:         releaset.f
C File Date:        05/31/05
C Release Version:    5.0
***** C:\SCR578\TPA501BETA\RUN\TEST2\RELEASET.F
C File Name:         releaset.f
C File Date:        05/13/05
C Release Version:    5.0
*****

***** releaset.f

cc rwj 5-27-05; SCR578; initialize all elements of xmass, rlmass and
c                    amwp arrays.
c       do 1100 itemp = 2, ntemp
        do 1100 itemp = 1, ntemp

***** C:\SCR578\TPA501BETA\RUN\TEST2\RELEASET.F

        do 1100 itemp = 2, ntemp
*****
```

Note above that the array element "rlmass(1,1,1)" is initialized in the TPA Version 5.0.1betaA code compared TPA Version 5.0.1beta code. Therefore, <u>Criterion 1 is passed</u>.

<u>For Criterion 2,</u> the differences in the EBSREL output *ebsrel.rlt* are:

```
Comparing files ebsrel.rlt and C:\SCR578\TPA501BETA\RUN\TEST2\EBSREL.RLT
***** ebsrel.rlt
```

Base case.
TPA 5.0.1betaA, Job started: Wed Oct 19 14:23:37 2005
EBSREL Results
***** C:\SCR578\TPA501BETA\RUN\TEST2\EBSREL.RLT
Base case.
TPA 5.0.1beta, Job started: Wed Oct 19 14:26:18 2005
EBSREL Results
*****

The only differences between the *ebsrel.rlt* files from the TPA Versions 5.0.1beta and 5.0.1betaA code are the time and date of the TPA code run. Therefore, Criteria 2 is passed.

For Criterion 3, the differences in the RELEASET output file *ebsnef,dat* from the TPA code run are:

Comparing files ebsnef.dat and C:\SCR578\TPA501BETA\RUN\EBSNEF.DAT
FC: no differences encountered

Since there are no differences between these files, Criterion 3 is passed.

For Criterion 4, the differences in the RELEASET output file *ebsnef,dat* from the standalone RELEASET run are:

Comparing files ebsnef.dat and
C:\SCR578\TPA501BETA\RUN\TEST2\STANDALONE_RUN\EBSNEF.DAT
FC: no differences encountered

Since there are no differences between these files, Criterion 4 is passed.

- Overall test status: PASS

SL-3. Name: Modify Equations to Calculate “outweldc” and “outwelds” - *ebsfail.f*

Path for run directory: c:\SCR578\tpa501beta\run\test3
c:\SCR578\tpa501betaA\run\test3

Path for archive of results: \SCR578\tpa501beta\run\test3 (archived on CD “SCR#578 Testing”)
\SCR578\tpa501betaA\run\test3 (archived on CD “SCR#578 Testing”)

Environment variables: <u>Baseline case</u>
TPA_DATA=c:\SCR578\tpa501beta
TPA_DATA=c:\SCR578\tpa501beta

and

<u>Test Case</u>
TPA_DATA=c:\SCR578\tpa501betaA
TPA_DATA=c:\SCR578\tpa501betaA

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only and activate APPEND file flag); because there are no parameter additions or deletions in the *tpa.inp* file (only values and distributions), use the *tpa.inp* file from TPA Version 5.0.1beta code also for TPA Version 5.0.1betaA code

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 equations used to compute for “outweldc” and “outwelds” were modified. These parameters are used to compute values of variables written to the *ebstrhc.inp* file which is read by FAILT and used to determine corrosion of the waste package weld.

- Objective: Verify that the equations used to compute “outweldc” and “outwelds” are implemented as intended and that values in the FAILT input file *ebstrhc.inp* are computed as intended.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *ebstrhc.inp* and *ebsfail.f*

- Step by step test procedure to be used:

1. In the “run” subdirectories of both the TPA Versions 5.0.1beta and 5.0.1betaA main source code directories, execute the TPA code using the *tpa.inp* file described above.
2. Create subdirectories in these “run" subdirectories called “test3”.
3. Copy the files to examine for this test (*ebstrhc.inp* and *ebsfail.f*) into the step #2 subdirectories.
4. Compare the files in step #3 using the “fc” DOS command.
5. Extract the *ebsfail.f* source code that calculated the values written to the *ebstrhc.inp* file
6. Perform hand calculation using the information from #5 and values from the *tpa.inp* file to verify the values in the last two columns of the *ebstrhc.inp* file are calculated and written as intended.

- Pass/Fail criteria:

Criterion 1: The differences between *ebsfail.f* source code in TPA Versions 5.0.1beta and 5.0.1beta code in a modified equation to compute “outweldc” and “outwelds”.

Criterion 2: The differences between values in the last column of the *ebstrhc.inp* file in TPA Versions 5.0.1beta and 5.0.1beta code.

Criterion 3: Hand calculations using the equations from the *ebsfailf* file should yield values that are consistent with those values written in the last column of te *ebstrhc.inp* file.

Test Results: The files in the \SCR578\tpa501beta\run\test3 and \SCR578\tpa501betaA\run\test3 subdirectories contain results for this test. The results in these subdirectories indicate that the Pass/Fail Criteria for all 3 criteria were met. (Note that the text for the file comparisons ["differences"] shown below are in the \SCR578\tpa501beta\run\test3 and SCR578\tpa501betaA\run\test3 subdirectories in files with names starting with "fc_".)

For Criterion 1, the differences in the *ebsfail.f* source code are:

```
Comparing files ebsfail.f and C:\SCR578\TPA501BETA\RUN\TEST3\EBSFAIL.F
***** ebsfail.f
c File Name:         ebsfail.f
c File Date:       05/31/05
c Release Version:    5.0
***** C:\SCR578\TPA501BETA\RUN\TEST3\EBSFAIL.F
c File Name:         ebsfail.f
c File Date:       05/16/05
c Release Version:    5.0
*****

***** ebsfail.f
     wnws=inhToCl1 / inhsToCl1
cc rwj 5-27-05; SCR578
c     outweldc = inhToCl1 / inhcToClw
c     outwelds = inhToCl1 / inhsToClw
     outweldc = inhToClw / inhcToClw
     outwelds = inhToClw / inhsToClw

c SCR519:  add weld inhibiting concentrations
***** C:\SCR578\TPA501BETA\RUN\TEST3\EBSFAIL.F
     wnws=inhToCl1 / inhsToCl1
     outweldc = inhToCl1 / inhcToClw
     outwelds = inhToCl1 / inhsToClw
c SCR519:  add weld inhibiting concentrations
*****
```

Note above that the equations used to computed "outweldc" and "outwelds" have been modified. Therefore, Criterion 1 is passed.

For Criterion 2, the first six lines of the differences in the *ebstrhc.inp* files are:

```
Comparing files ebstrhc.inp and C:\SCR578\TPA501BETA\RUN\TEST3\EBSTRHC.INP
***** ebstrhc.inp
  750.2841   134.5828   98.3313    0.2937    7.0000    0.0000    0.0000
  770.1594   133.5036   97.9941    0.3031   10.6745    0.1687    0.1740
  790.5001   132.4383   97.6540    0.3128   10.6745    0.1687    0.1740
```

```
  811.3170   131.3859   97.3106   0.3227   10.6745   0.1687   0.1740
  832.6212   130.3461   96.9636   0.3324   10.6745   0.1687   0.1740
  854.4242   129.3072   96.6020   0.3384   10.6745   0.1687   0.1740
 ***** C:\SCR578\TPA501BETA\RUN\TEST3\EBSTRHC.INP
  750.2841   134.5828   98.3313   0.2937    7.0000   0.0000   0.0000
  770.1594   133.5036   97.9941   0.3031   10.6745   0.1687   0.1687
  790.5001   132.4383   97.6540   0.3128   10.6745   0.1687   0.1687
  811.3170   131.3859   97.3106   0.3227   10.6745   0.1687   0.1687
  832.6212   130.3461   96.9636   0.3324   10.6745   0.1687   0.1687
  854.4242   129.3072   96.6020   0.3384   10.6745   0.1687   0.1687
 *****
```

Note that the values in the last column (**bold**) are different. This column represents values for the weld, for which equations have been modified. Therefore, Criteria 3 is passed.

For Criterion 3, the equations in the *ebsfail.f* file used to compute values in the last column of the *ebstrhc.inp* file in Criteria 2 above are listed below.

```
      outweldc = inhToClw / inhcToClw
      outwelds = inhToClw / inhsToClw

c SCR519:  add weld inhibiting concentrations
c end change:  SCR519
c      tst=0.0

      do it = 1, ntemp

c ZW SCR478 05-25-04
c css 2-24-2005; SCR519:  calculate weld inhibitor vector
        inhEff= no3(it) + wnwc*co3(it) + wnws * so4(it)
        inhWeld = no3(it) + outweldc * co3(it) + outwelds * so4(it)
c end change: SCR519
```

Using the equation in **bold and underlined** above, hand calculations are performed.

"outweldc" = 0.3 / 0.2 = 1.5 (for Environment II from the *tpa.inp* file)
"outwelds" = 0.3 / 0.5 = 0.6 (for Environment II from the *tpa.inp* file)

"no3(it)" = 0.166 (from the sampled parameter for Environment II no3 in the *sp.tpa* file)
"so4(it)" = 1.31e-2 (from the sampled parameter for Environment II so4 in the *sp.tpa* file)
"co3(it)" = 2.26e-5 (from the sampled parameter for Environment II co3 in the *sp.tpa* file)

From these values and the highlighted equation, "inhWeld" = 0.1739. This value is compared to 1.740 in the last column of the TPA Version 5.0.1betaA code file named *ebstrhc.inp*. Because these values are consistent, Criterion 3 is passed.

- Overall test status: PASS

SL-4. Name: Removal of Variable"totnwp" - *reader.f*

Path for run directory: c:\SCR578\tpa501beta\run\test4
c:\SCR578\tpa501betaA\run\test4

Path for archive of results: \SCR578\tpa501beta\run\test4 (archived on CD "SCR#578 Testing")
\SCR578\tpa501betaA\run\test4 (archived on CD "SCR#578 Testing")

Environment variables: Baseline case
TPA_DATA=c:\SCR578\tpa501beta
TPA_DATA=c:\SCR578\tpa501beta

and

Test Case
TPA_DATA=c:\SCR578\tpa501betaA
TPA_DATA=c:\SCR578\tpa501betaA

(Note that there are no TPA code runs for this 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: None

Test description: The variable "totnwp" was removed from the *reader.f* file, which is the only file this variable was specified.

- Objective: Verify that the variable "totnwp" was removed from the *reader.f* file.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *reader.f* (source code)

- Step by step test procedure to be used:

1. Compare *reader.f* files from the TPA Versions 5.0.1beta and 5.0.1betaA source code directories.
2. Visually verify “totnwp”variable was removed from the *reader.f* file.
3. Perform a “grep” using the SUN UNIX OS with “totnwp” to verify this character string is not present in the TPA Version 5.0.1betaA.

- Pass/Fail criteria:

Criterion 1: The *reader.f* file comparison between the TPA Versions 5.0.1beta and 5.0.1betaA shows the variable “totnwp” is removed from this file.

Criterion 2: A “grep” on the TPA Version 5.0.1betaA using “totnwp” should show no occurrences of this character string.

Test Results:

The comparison file in the \SCR578\tpa501betaA\run\test4 subdirectory contains results for this test. (Note that the text for the file comparison [“difference”] shown below is in the \SCR578\tpa501betaA\run\test4 subdirectory in a file with a name starting with “fc_”.)

<u>For Criterion 1,</u> the differences in the *reader.f* source code are:

```
Comparing files reader.f and ..\TPA501BETA\READER.F
***** reader.f
c File Name:        reader.f
c File Date:      05/31/05
c Release Version:    5.0
***** ..\TPA501BETA\READER.F
c File Name:        reader.f
c File Date:      05/02/05
c Release Version:    5.0
*****

***** reader.f
   integer restart_flag

***** ..\TPA501BETA\READER.F
   integer restart_flag
cc rwj 4-22-05; SCR 564
   integer totnwp

*****

***** reader.f
    endif
```

```
***** ..\TPA501BETA\READER.F
      endif
cc rwj 4-22-05; scr564;
      totnwp = 0

*****

***** reader.f
     &          isa, area(isa), amtusa(isa), nwpsa(isa)
      end do
***** ..\TPA501BETA\READER.F
     &          isa, area(isa), amtusa(isa), nwpsa(isa)
cc rwj 4-22-05; scr564;
      totnwp = totnwp + nwpsa(isa)

      end do
*****
```

For Criterion 1, the differences show the variable "totnwp" was removed. Therefore, Criterion 1 is passed.

For Criterion 2, a "grep" on the source code for the TPA Version 5.0.1betaA code using "totnwp" returned no character strings. Therefore, Criterion 2 is passed.

- Overall test status: PASS

SL-5. Name: Update Data - *tpa.inp*

Path for run directory: c:\SCR578\tpa501beta\run\test5
c:\SCR578\tpa501betaA\run\test5

Path for archive of results: \SCR578\tpa501beta\run\test5 (archived on CD "SCR#578 Testing")
\SCR578\tpa501betaA\run\test5 (archived on CD "SCR#578 Testing")

Environment variables: Baseline case
TPA_DATA=c:\SCR578\tpa501beta
TPA_DATA=c:\SCR578\tpa501beta

and

Test Case
TPA_DATA=c:\SCR578\tpa501betaA
TPA_DATA=c:\SCR578\tpa501betaA

(Note that there are no TPA code runs for this 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: None

Test description: Data in the primary TPA code input file *tpa.inp* was updated using information in the table contained in this SCR.

- Objective: Using a file comparison, visually verify that the data in the table in this SCR was incorporated into the *tpa.inp* file of the TPA Version 5.01betaA code .

- Assumptions: None

- Constraints: None

- Output files to compare or examine: *tpa.inp*

- Step by step test procedure to be used:

1. Perform a file comparison between the *tpa.inp* files from TPA Versions 5.0.1beta and 5.0.1betaA code.
2. Visually verify the file comparison from step #1 is consistent with the information contained in the table in this SCR.

- Pass/Fail criteria:

Criterion 1: The *tpa.inp* file comparison between the TPA Versions 5.0.1beta and 5.0.1betaA should show the information in the table in this SCR is incorporated into the *tpa.inp* file for TPA Version 5.0.1betaA code.

Test Results:

The comparison file in the \SCR578\tpa501betaA\run\test5 subdirectory contains results for this test. (Note that the text for the file comparison ["difference"] shown below is in the \SCR578\tpa501betaA\run\test5 subdirectory in a file with a name starting with "fc_".)

<u>For Criterion 1,</u> the differences in the *tpa.inp* source code are:

```
Comparing files tpa.inp and ..\TPA501BETA\TPA.INP
***** tpa.inp
title
 Input file tpa.inp as supplied with TPA Version 5.0.1betaA Code.
 Base case.
***** ..\TPA501BETA\TPA.INP
title
 Input file tpa.inp as supplied with TPA Version 5.0.1beta Code.
 Base case.
*****

***** tpa.inp
**
** rwj scr578
**constant
**EnvironmentII_Wastepackage_DeltaECrit[VSHE]
**0.2
**
***** ..\TPA501BETA\TPA.INP
**
constant
EnvironmentII_Wastepackage_DeltaECrit[VSHE]
0.2
**
*****

***** tpa.inp
constant
```

EnvironmentII_Wastepackage_DeltaECrit[VSHE]
0.0
**
***** ..\TPA501BETA\TPA.INP
constant
EnvironmentIII_Fl[mol/L]
4.08e-4
**
*****

***** tpa.inp
constant
EnvironmentIII_Fl[mol/L]
4.08e-4
**
***** ..\TPA501BETA\TPA.INP
constant
EnvironmentIII_Cl[mol/L]
6.65e-3
**
*****

***** tpa.inp
constant
EnvironmentIII_Cl[mol/L]
6.65e-3
**
***** ..\TPA501BETA\TPA.INP
constant
EnvironmentIII_pH[]
8.37e0
**
*****

***** tpa.inp
constant
EnvironmentIII_pH[]
8.37e0
**
***** ..\TPA501BETA\TPA.INP
constant
EnvironmentIII_NO3[mol/L]
6.65e-3
**
*****

***** tpa.inp
constant
EnvironmentIII_NO3[mol/L]
6.65e-3

**
***** ..\TPA501BETA\TPA.INP
constant
EnvironmentIII_CO3[mol/L]
2.11e-3
**
*****

***** tpa.inp
constant
EnvironmentIII_CO3[mol/L]
2.11e-3
**
***** ..\TPA501BETA\TPA.INP
constant
EnvironmentIII_SO4[mol/L]
0.0
**
*****

***** tpa.inp
constant
EnvironmentIII_SO4[mol/L]
0.0
***** ..\TPA501BETA\TPA.INP
constant
EnvironmentIII_Wastepackage_DeltaECrit[VSHE]
0.0
*****

***** tpa.inp
**
constant
EnvironmentIII_Wastepackage_DeltaECrit[VSHE]
0.0
**
** relative humidity transition time is the time for relative
***** ..\TPA501BETA\TPA.INP
**
** relative humidity transition time is the time for relative
*****

***** tpa.inp
**
** rwj scr578
**constant
**OuterInhibitingCarbonateToCl
**0.1
**
***** ..\TPA501BETA\TPA.INP

```
**
constant
OuterInhibitingCarbonateToCl
0.1
**
*****

***** tpa.inp
constant
OuterInhibitingCarbonateToCl
0.2
**
***** ..\TPA501BETA\TPA.INP
constant
OuterInhibitingSulfateToCl
0.5
**
*****

***** tpa.inp
constant
OuterInhibitingSulfateToCl
0.5
**
***** ..\TPA501BETA\TPA.INP
constant
OuterDeltaEcritInh[mV]
800
**
*****

***** tpa.inp
constant
OuterDeltaEcritInh[mV]
800
**
constant
InnerInhibitingNitrateToCl
***** ..\TPA501BETA\TPA.INP
constant
InnerInhibitingNitrateToCl
*****

***** tpa.inp
**
** rwj 5-27-05; SCR578
**triangular
**OuterOverpackErpIntercept
**1541.2, 1591.2, 1641.2
**
```

triangular
***** ..\TPA501BETA\TPA.INP
**
triangular
*****

***** tpa.inp
OuterOverpackErpIntercept
1025.04, 1180.76, 1336.49
**
** rwj 5-27-05; SCR578
**constant
**TempCoefOfOuterPackErpIntercept
**-13.1
**
***** ..\TPA501BETA\TPA.INP
OuterOverpackErpIntercept
1541.2, 1591.2, 1641.2
**
*****

***** tpa.inp
TempCoefOfOuterPackErpIntercept
-9.35026
**
** rwj 5-27-05; SCR578
**constant
**OuterOverpackErpSlope
**-362.7
**
***** ..\TPA501BETA\TPA.INP
TempCoefOfOuterPackErpIntercept
-13.1
**
*****

***** tpa.inp
OuterOverpackErpSlope
-752.034
**
** rwj 5-27-05; SCR578
**constant
**TempCoefOfOuterPackErpSlope
**2.3
**
***** ..\TPA501BETA\TPA.INP
OuterOverpackErpSlope
-362.7
**
*****

```
***** tpa.inp
TempCoefOfOuterPackErpSlope
5.20131
**
***** ..\TPA501BETA\TPA.INP
TempCoefOfOuterPackErpSlope
2.3
**
*****

***** tpa.inp
**
** rwj 5-27-05 SCR578
**constant
**RD_Invert_Cm
**6.0e3
**
beta
RD_Invert_Cm
2001.0, 20001.0, 9.039, 18.079
**
***** ..\TPA501BETA\TPA.INP
**
constant
RD_Invert_Cm
6.0e3
**
**beta
**RD_Invert_Cm
**2001, 20001, 8001, 0.20
**
*****

***** tpa.inp
**
** rwj 5-27-05 SCR578
**constant
**RD_Invert_U
**6.01e2
***** ..\TPA501BETA\TPA.INP
**
constant
RD_Invert_U
6.01e2
**
**beta
**RD_Invert_U
**1, 21, 11, 0.30
**
constant
```

```
RD_Invert_Am
3.0e3
**
**beta
**RD_Invert_Am
**2001, 20001, 8001, 0.20
**
constant
RD_Invert_Np
1.2e3
**
**beta
**RD_Invert_Np
**1, 21, 7, 0.30
**
constant
RD_Invert_Th
3.0e3
**
**beta
**RD_Invert_Th
**2001, 20001, 8001, 0.20
**
**constant
**RD_Invert_Ra
**6.01e2
*****

***** tpa.inp
**
beta
RD_Invert_U
1.0, 21.0, 4.091, 4.091
**
** rwj 5-27-05 SCR578
**constant
**RD_Invert_Am
**3.0e3
**
beta
RD_Invert_Am
2001.0, 20001.0, 9.039, 18.079
**
** rwj 5-27-05 SCR578
**constant
**RD_Invert_Np
**1.2e3
**
beta
RD_Invert_Np
```

```
1.0, 21.0, 4.091, 4.091
**
** rwj 5-27-05 SCR578
**constant
**RD_Invert_Th
**3.0e3
**
beta
RD_Invert_Th
2001.0, 20001.0, 9.039, 18.079
**
***** ..\TPA501BETA\TPA.INP
**
uniform
RD_Invert_Ra
1001, 2001
**
*****

***** tpa.inp
**constant
**RD_Invert_Ra
**6.01e2
**
***** ..\TPA501BETA\TPA.INP
**constant
**RD_Invert_Pb
**3.01e2
**
*****

***** tpa.inp
uniform
RD_Invert_Ra
1001, 2001
**
***** ..\TPA501BETA\TPA.INP
uniform
RD_Invert_Pb
2001, 10001
**
*****

***** tpa.inp
**constant
**RD_Invert_Pb
**3.01e2
**
***** ..\TPA501BETA\TPA.INP
**constant
```

```
**RD_Invert_Cs
**1.21e2
**
*****

***** tpa.inp
uniform
RD_Invert_Pb
2001, 10001
**
***** ..\TPA501BETA\TPA.INP
uniform
RD_Invert_Cs
201, 2001
**
*****

***** tpa.inp
**constant
**RD_Invert_Cs
**1.21e2
**
uniform
RD_Invert_Cs
201, 2001
**
**constant
**RD_Invert_I
***** ..\TPA501BETA\TPA.INP
**constant
**RD_Invert_I
*****

***** tpa.inp
**
** rwj 5-27-05 SCR578
**constant
**RD_Invert_Ni
**6.1e1
****
beta
RD_Invert_Ni
1.0, 1001.0, 3.061, 2.041
**
***** ..\TPA501BETA\TPA.INP
**
constant
RD_Invert_Ni
6.1e1
**
```

```
**beta
**RD_Invert_Ni
**1, 1001, 601, 0.33
**
*****

***** tpa.inp
**
** rwj 5-27-05 SCR578
**constant
**RD_Invert_Se
**1.0
**
beta
RD_Invert_Se
1.0, 21.0, 4.091, 4.091
**
** rwj 5-27-05 SCR578
**constant
**RD_Invert_Nb
**6.01e2
**
beta
RD_Invert_Nb
2001.0, 20001.0, 9.039, 18.079
**
***** ..\TPA501BETA\TPA.INP
**
constant
RD_Invert_Se
1.0
**
**beta
**RD_Invert_Se
**1, 21, 3, 1.0
**
*****

***** tpa.inp
constant
GapFractionForCM246
0.0
**
***** ..\TPA501BETA\TPA.INP
constant
RD_Invert_Nb
6.01e2
**
**beta
**RD_Invert_Nb
```

```
**2001, 20001, 8001, 0.20
**
*****

***** tpa.inp
constant
GapFractionForU238
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForCM246
0.0
*****

***** tpa.inp
constant
GapFractionForCM245
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForU238
0.0
*****

***** tpa.inp
constant
GapFractionForAM241
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForCM245
0.0
*****

***** tpa.inp
constant
GapFractionForNP237
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForAM241
0.0
*****

***** tpa.inp
constant
GapFractionForAM243
0.0
***** ..\TPA501BETA\TPA.INP
constant
```

GapFractionForNP237
0.0
*****

***** tpa.inp
constant
GapFractionForPU239
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForAM243
0.0
*****

***** tpa.inp
constant
GapFractionForPU240
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForPU239
0.0
*****

***** tpa.inp
constant
GapFractionForU234
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForPU240
0.0
*****

***** tpa.inp
constant
GapFractionForTH230
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForU234
0.0
*****

***** tpa.inp
constant
GapFractionForRA226
0.0
***** ..\TPA501BETA\TPA.INP
constant

GapFractionForTH230
0.0
*****

***** tpa.inp
constant
GapFractionForPB210
0.0
***** ..\TPA501BETA\TPA.INP
constant
GapFractionForRA226
0.0
*****

***** tpa.inp
**
** cc rwr 2-4-05; SCR 530
***** ..\TPA501BETA\TPA.INP
**
constant
GapFractionForPB210
0.0
**
** cc rwr 2-4-05; SCR 530
*****

***** tpa.inp
**
constant
***** ..\TPA501BETA\TPA.INP
**
**constant
**SurfaceAreaOfGlass[m^2/kg]
**5.63e-2
**
constant
*****

***** tpa.inp
**
uniform
***** ..\TPA501BETA\TPA.INP
**
**uniform
**LogOfGlassDissolutionConstantHighRange[]
**6.4, 7.4
**
uniform
*****

```
***** tpa.inp
**
uniform
***** ..\TPA501BETA\TPA.INP
**
**uniform
**LogOfGlassDissolutionConstantLowRange[]
**8.0, 10.0
**
uniform
*****

***** tpa.inp
**
** rwj 5-27-05; SCR 578
**triangular
**LogCO2PartialPressure_AllUZ_SZLayers[atm]
**-4.0, -2.5, -1.0
**
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
**
**triangular
**pH_AllUZ_SZLayers[StandardUnits]
**6.7, 7.8, 9.2
**
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
**
***** ..\TPA501BETA\TPA.INP
**
triangular
LogCO2PartialPressure_AllUZ_SZLayers[atm]
-4.0, -2.5, -1.0
**
triangular
pH_AllUZ_SZLayers[StandardUnits]
6.7, 7.8, 9.2
**
*****
```

<u>For Criterion 1,</u> using the above file comparison, visual inspection reveals the information in the table in this SCR is contained in the *tpa.inp* file for the TPA Version 5.0.1betaA code. Therefore, <u>Criterion 1 is passed</u>.

- Overall test status: <u>PASS</u>

November 7, 2005 - Completed testing for SCR577. The SCR and Test Plan follow.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): PA-SCR-577	**2. Software Title and Version:** TPA 5.0.1betaA	**3. Project No:** 20.06002.01.354
4. Affected Software Module(s), Description of Problem(s): *failt.f, szft.f, tpa.inp, coefkdeq.dat, nuclides.dat* Curium Kd/Rd values are not similar to Americium values as suggested by D. Pickett. Nefiialluv.inp has incorrect format on the PC platform. FAILT continues to give lack of convergence error messages for cases when the environment is sampled and the overpack is thin.		
5. Change Requested by: R. Rice/ D. Turner/ R. Janetzke Date: 5-4-05	**6. Change Authorized by** (*Software Developer*): R. Janetzke Date: 6-3-05	
7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): 1) The americium values in *coefkdeq.dat* were copied and assigned to an additional section of the file for curium. Thus the curium Kds and Rds are now calculated. Associated changes were made in *tpa.inp* to remove curium parameters from the sampled data set. 2) *szft.f* was changed to write an integer 0 in *nefiialluv.inp* for the diffusion flag rather than floating point for the case when the separate runs for the SZ is selected . 3) See Attachment A for changes to *failt.f*		
8. Implemented by: R. Janetzke D. LeNeveu	**Date:** 6-6-05	
9. Description of Acceptance Tests: See Attachment B.		
10. Tested by: R. Rice	**Date:** 11-7-05	

CNWRA Form TOP-5 (05/2000)

SCR577 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	UZFT	MatrixKD_TSw_Cm[m3/kg]					DT
delete	UZFT	MatrixKD_CHnv_Cm[m3/kg]					
delete	UZFT	MatrixKD_CHnz_Cm[m3/kg]					
delete	UZFT	MatrixKD_PPw_Cm[m3/kg]					
delete	UZFT	MatrixKD_UCF_Cm[m3/kg]					

delete	UZFT	MatrixKD_BFw_Cm [m3/kg]					
delete	UZFT	MatrixKD_UFZ_Cm[m3/kg]					
delete	UZFT	FractureRD_TSw_C m					
delete	UZFT	FractureRD_CHnv_C m					
delete	UZFT	FractureRD_CHnz_C m					
delete	UZFT	FractureRD_PPw_C m					
delete	UZFT	FractureRD_UCF_C m					
delete	UZFT	FractureRD_BFw_C m					
delete	UZFT	FractureRD_UFZ_C m					
delete	SZFT	FractureRD_STFF_C m					
delete	SZFT	AlluviumMatrixRD_ SAV_cm					

delete	SZFT	ImmobileRD_STFF_ Cm					

Attachment A

The following is the output of the **diff** utility for the changes to *failt.f*:

```
3c3
< c File Date:          05/13/05
---
> c File Date:          06/13/05
1555,1556c1555,1557
<         DOUBLE PRECISION relercpass
<
---
> C*****code change by D.LeNeveu June 6, 2005; SCR577
>         DOUBLE PRECISION relercpass,piva,pivb,expfac
> C******end change
1744c1745,1747
<           yko2 = rkhy * exp(ghy * yyy1)
---
> cc DLN 6-6-05; SCR577
> c         yko2 = rkhy * exp(ghy * yyy1)
>
1772a1776,1788
> C*******Code change by D. LeNeveu move outside loop June 5 /2005; scr577
>        yko2 = rkhy * exp(ghy * yyy1)
>        if (yko2 .eq. 0.0) then
> c         Compute main contribution to cathodic current density constant
>           piva = (((10.0**(-ph))**npH * exp(-(gcath/(rgas*tk)))*
>      &       ire* xgas**nO*cbulko2)/cbulko2ref)
>          pivb= (max(scalthk, filmthk)/cbulko2)/
>      &            (4.0*cfarad*do2w*taus*spor)
>          expfac= (cfarad*zo2*beta)/(rgas*tk)
> c         Introduce diffusion control of partial cathodic current density
>          eec=Log((piva-cpass*pivb)/cpass)/expfac
>        else
> C*******End of code change
1774,1775c1790,1795
<         do 100 i = 1, 10
<           yko2 = rkhy * exp(ghy * yyy1)
---
> cc DLN 6-6-05; SCR577
> c       do 100 i = 1, 10
> c         yko2 = rkhy * exp(ghy * yyy1)
>         do 100 i = 1, 50
> C         yko2 = rkhy * exp(ghy * yyy1)
>
1778,1779c1798,1799
< c         Compute main contribution to cathodic current density
<           piv = (((10.0**(-ph))**npH * exp(-(gcath/(rgas*tk)) -
---
> c           Compute main contribution to cathodic current density
>             piv = (((10.0**(-ph))**npH * exp(-(gcath/(rgas*tk)) -
1782,1784c1802,1804
<           piv2=piv/cbulko2
< c         Introduce diffusion control of partial cathodic current density
<           curox = - piv/(1.0 + (max(scalthk, filmthk)*piv2)/
---
>             piv2=piv/cbulko2
> c           Introduce diffusion control of partial cathodic current density
>             curox = - piv/(1.0 + (max(scalthk, filmthk)*piv2)/
1787,1790c1807,1810
```

```
<           cathod = -(curox + curhy)
<           zc = cpass - cathod
< c         dzz is the derivative of the total current wrt potential, eec
< c         This derivative is always positive
---
>             cathod = -(curox + curhy)
>             zc = cpass - cathod
> c           dzz is the derivative of the total current wrt potential, eec
> c           This derivative is always positive
1792,1797c1812,1817
< 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           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
1799c1819
<           dzc = -xxx1 * curhy +
---
>             dzc = -xxx1 * curhy +
1805,1806c1825,1833
< c         if ( abs(zc).le.1.0e-8 ) go to 150
<           if ( abs(zc).le. abs(10.0d0*relercpass*eec*dzc) ) go to 150
---
> cc DLN  6-6-05; SCR577
> c           Since the Newton-Raphson loop is determining a value for ecc
> c           stop iterations when the change in ecc is insignificant
> c           with respect to machine precision
> c           This amounts the relative change in eec should be less than relercpass
> c           or abs(zc/dzc) <= abs(eec)*relercpass which can be converted to
> c           abs(zc) .le. abs(eec*10.d0*relercpass*eec*dzc) to avoid a divide by zero
case
> c           for dzc and to take into account the extra loss of precision in
evaluating eec repeatedly
>             if ( abs(zc).le. abs(10.0d0*relercpass*eec*dzc) ) go to 150
1811c1838
<         write (*, *) 'corrosion potential not converging in 10 '//
---
>           write (*, *) 'corrosion potential not converging in 50 '//
1814,1815c1841,1845
< c     Compare potentials with critical potentials
<   150   continue
---
> c         Compare potentials with critical potentials
>   150     continue
> C*******code change by D.LeNeveu June 6, 2005; SCR577
>         end if
> C*******end code change
```

Attachment B

Test Plan for TPA SCR#577

Test Plan Name: Cm Rds, *nefiizalluv.inp* Format, and FAILT Convergence

Tested By: R. Rice **Date:** November 7, 2005

Host Machine: Toshiba Laptop **Host OS:** XP Professional

Baseline Version: 5.0.1betaA **Test Version:** 5.0.1betaB

System Level (SL) Tests

SL-1. Name: Set Cm Rds Equal to Am Rds

Path for run directory: c:\SCR577\tpa501betaA\run
c:\SCR577\tpa501betaB\run

Path for archive of results: \SCR577\tpa501betaA\run\test1 (archived on CD "SCR#577 Testing")
\SCR577\tpa501betaB\run\test1 (archived on CD "SCR#577 Testing")

Environment variables: Baseline case
TPA_DATA=c:\SCR577\tpa501betaA
TPA_DATA=c:\SCR577\tpa501betaA

and

Test Case
TPA_DATA=c:\SCR577\tpa501betaB
TPA_DATA=c:\SCR577\tpa501betaB

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only and activate APPEND file flag)

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 test verifies that the Cm Rds for the unsaturated zone are determined from the file *coefkdeq.dat* instead of being specified in the *tpa.inp* file. Additionally, the test examines whether the Cm Rds are equal to the Am Rds by comparing the unsaturated zone NEFTRAN input file *nefiiuz.inp*.

- Objective: Verify that the TPA Version 5.0.1betaB code does not contain Cm UZ Rds in the *tpa.inp* file and that Cm and Am Rds for the UZ are equal in the NEFTRAN input file *nefiiuz.inp*.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *coefkdeq.dat, nefiiuz.inp*, and *tpa.inp*

- Step by step test procedure to be used:

1. Create "run" subdirectories in both the TPA Versions 5.0.1betaA and 5.0.1betaB main source code directories.
2. QModify the *tpa.inp* file according to the "Special input files or modifications to input files required" given above.
3. Execute the TPA Versions 5.0.1betaA and 5.0.1betaB code in the subdirectories created in #1 and capture the screenprint.
4. Create "test1" subdirectories in "run" subdirectories for both the TPA Versions 5.0.1betaA and 5.0.1betaB.
5. Copy the files *coefkdeq.dat, nefiiuz.inp*, and *tpa.inp* from the "run" subdirectories for TPA

Versions 5.0.1betaA and 5.0.1betaB code executions from #3 above.

6. In the “run\test1” subdirectory of TPA Version 5.0.1betaB, perform a file comparison between the files from #5 above. Name these file comparisons “fc_*” where * is the name of the files in #5 above.

- Pass/Fail criteria:

Criterion 1: Relative to the TPA Version 5.0.1betaA code, the Cm UZ Rds should be removed from the *tpa.inp* file in the TPA Version 5.0.1betaB code.

Criterion 2: The *coefkdeq.dat* file in the TPA Version 5.0.1betaB code should have data for Cm which is absent in the *coefkdeq.dat* file for the TPA Version 5.0.1betaA code.

Criterion 3: The Cm UZ Rds should be equal to the Am UZ Rds in the UZ NEFTRAN input file *nefiiuz.inp* for the TPA Version 5.0.1betaB code; while these values will be different in the UZ NEFTRAN input file *nefiiuz.inp* for the TPA Version 5.0.1betaA code.

Test Results: The files in the \SCR577\tpa501betaA\run\test1 and \SCR577\tpa501betaB\run\test1 subdirectories contain the files and file comparisons for this test. The file comparisons indicate that the Pass/Fail Criteria for all 3 criteria were met. (Note that the text for the file comparisons [“differences”] shown below are in the \SCR577\tpa501betaB\run\test1 subdirectory in files with names starting with “fc_”.)

<u>For Criterion 1,</u> visual inspection of the *fc_tpa.inp* file shows that the Cm UZ Rds have been commented out of the *tpa.inp* file. Therefore, <u>Criterion 1 is passed</u>.

<u>For Criterion 2,</u> the file comparison of the *coefkdeq.dat* files from the TPA Versions 5.0.1betaA and 5.0.1betaB code follows.

```
Comparing files coefkdeq.dat and
C:\SCR577\TPA501BETAA\RUN\COEFKDEQ.DAT
***** coefkdeq.dat
 of 5.5, but limited to 6.0)
```

```
# SCR 577 Add Cm with parameters identical to Am.  The actual
values for Cm are unknown, but are
# assumed to be similar to Am.  This will avoid great disparity
in values supplied to NEFTRAN.
# date: 6-3-2005 TPA 5.0.1betaB    <-- must have word "date" in
last header line only.
6     10    !Number of radioelements, Number of data rows for
each radioelement
Am(III)
***** C:\SCR577\TPA501BETAA\RUN\COEFKDEQ.DAT
 of 5.5, but limited to 6.0)
# date: 5-13-2005 TPA 5.0.0z    <-- must have word "date" in
last header line only.
5     10    !Number of radioelements, Number of data rows for
each radioelement
Am(III)
*****

***** coefkdeq.dat
Cm(III)
logPCO2(atm) pHLow pHhigh  a             b             c
  d            e           f
 -0.5  6.0  8.50  -3488.09627424  2629.51291541  -788.56176251
117.56073070  -8.70093305   0.25541926
 -1.0  6.0  8.50  -2773.90316917  2025.80503602  -588.12441063
84.82299722  -6.06673419   0.17183905
 -1.5  6.0  8.75  -2570.99868836  1798.94821209  -500.31232997
69.11860003  -4.73305712   0.12824036
 -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 10.00    130.72585800   -98.62225380    28.50975860
-3.95833162   0.27147852  -0.00743480
 -5.0  6.0 10.00     33.74073080   -25.65826470     6.78522964
-0.75797035   0.03813970  -0.00069526
***** C:\SCR577\TPA501BETAA\RUN\COEFKDEQ.DAT
*****
```

Note above that the differences in data between these files is the addition of the 6th element Cm. (Note that visual inspection of the contents of the *coefkdeq.dat* file from the TPA Versions 5.0.1betaB verifies the data for Cm and Am are equal). Therefore, Criterion 2 is passed.

For Criterion 3, the file comparison of the NEFTRAN UZ input file *nefiiuz.inp* from the TPA Versions 5.0.1betaA and 5.0.1betaB code follows.

```
Comparing files nefiiuz.inp and C:\SCR577\TPA501BETAA\RUN\NEFIIUZ.INP
***** nefiiuz.inp
INDEX    (KG/KG)    #                      MOD FACTOR
   1   0.000E+00    1   0.713E+06    0.000E+00      0.000E+00
                    2   0.713E+06    0.000E+00      0.000E+00
   2   0.000E+00    1   0.444E+02    0.000E+00      0.000E+00
***** C:\SCR577\TPA501BETAA\RUN\NEFIIUZ.INP
INDEX    (KG/KG)    #                      MOD FACTOR
   1   0.000E+00    1   0.192E+04    0.000E+00      0.000E+00
                    2   0.192E+04    0.000E+00      0.000E+00
   2   0.000E+00    1   0.444E+02    0.000E+00      0.000E+00
*****
```

Note that Cm is element #1. The Rd for element #3 (Am) in the NEFTRAN UZ input file *nefiiuz.inp* is provided below.

```
3   0.000E    1   0.713E    0.000E      0.000E
              2   0.713E    0.000E      0.000E
```

The Cm and Am UZ Rds are equal in the NEFTRAN UZ input file *nefiiuz.inp* for TPA Version 5.0.1betaB. Therefore, Criterion 3 is passed.

- Overall test status: PASS

SL-2. Name: Format Change in *nefiialluv.inp*

Path for run directory: c:\SCR577\tpa501betaA\run
c:\SCR577\tpa501betaB\run

Path for archive of results: \SCR577\tpa501betaA\run\test2 (archived on CD "SCR#577 Testing")
\SCR577\tpa501betaB\run\test2 (archived on CD "SCR#577 Testing")

Environment variables: Baseline case
TPA_DATA=c:\SCR577\tpa501betaA
TPA_DATA=c:\SCR577\tpa501betaA

and

Test Case
TPA_DATA=c:\SCR577\tpa501betaB
TPA_DATA=c:\SCR577\tpa501betaB

Special input files or modifications to input files required: *tpa.inp* (run Subarea 1 only; activate APPEND file flag; and set flag to separate NEFTRAN SZ legs equal 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: The test verifies that when the TPA code execution separates NEFTRAN SZ legs, an integer equal to zero is written for the diffusion flag instead of a floating point value into the *nefiizalluv.inp* file by using a modification introduced in the *szft.f* source code.

- Objective: Verify that the TPA Version 5.0.1betaB code correctly sets the diffusion flag equal to an integer value of zero in the *nefiialluv.inp* file by a using modification introduced in the *szft.f* source code.

- Assumptions: None, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *nefiialluv.inp* and *szft.f*

- Step by step test procedure to be used:

1. Create "run\test2" subdirectories in both the TPA Versions 5.0.1betaA and 5.0.1betaB main source code directories.
2. Modify the *tpa.inp* file according to the "Special input files or modifications to input files required" given above.
3. Execute the TPA Versions 5.0.1betaA and 5.0.1betaB code in the subdirectories created in #1 and capture the screenprint.
4. In the "run\test2" subdirectory of TPA Version 5.0.1betaB, perform a file comparison between the *szft.f* files from the TPA Versions 5.0.1betaA and 5.0.1betaB named *fc_szft.f*.

- Pass/Fail criteria:

Criterion 1: The file comparison between the *szft.f* files from the TPA Versions 5.0.1betaA and 5.0.1betaB code should show an integer instead of a floating point is written to the NEFTRAN SZ input file *nefiialluv.inp*.

Criterion 2: The file *nefiialluv.inp* from the TPA Version 5.0.1betaB code should show an integer for the diffusion flag.

Test Results: The files in the \SCR577\tpa501betaA\run\test2 and \SCR577\tpa501betaB\run\test2 subdirectories contain the files and file comparison for this test. The file comparisons indicate that the Pass/Fail

Criteria for all 2 criteria were met. (Note that the text for the file comparison ["differences"] shown below are in the \SCR577\tpa501betaB\run\test2 subdirectory in a file named *fc_szft.f*.)

For Criterion 1, the file comparison of the *szft.f* files from the TPA Versions 5.0.1betaA and 5.0.1betaB code follows.

```
Comparing files C:\SCR577\TPA501BETAB\szft.f and
C:\SCR577\TPA501BETAA\SZFT.F
***** C:\SCR577\TPA501BETAB\szft.f
c File Name:         szft.f
c File Date:        06/13/05
c Release Version:    5.0
***** C:\SCR577\TPA501BETAA\SZFT.F
c File Name:         szft.f
c File Date:        05/12/05
c Release Version:    5.0
*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005 SCR529; - no need to do this due to multiple
cc                  NEFTRAN simulations not a composite
***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005 - no need to do this due to multiple
cc                  NEFTRAN simulations not a composite
*****

***** C:\SCR577\TPA501BETAB\szft.f
cc TJM      write(i3,'(i5,5x,a)') nefleg+1,'NUMBER OF NETWORK LEGS'
cc   TJM  March 7, 2005  SCR529; revise input for 2 legs only
     write(i3,'(i5,5x,a)') 2,'NUMBER OF NETWORK LEGS'
***** C:\SCR577\TPA501BETAA\SZFT.F
cc TJM      write(i3,'(i5,5x,a)') nefleg+1,'NUMBER OF NETWORK LEGS'
cc   TJM  March 7, 2005  revise input for 2 legs only
     write(i3,'(i5,5x,a)') 2,'NUMBER OF NETWORK LEGS'
*****

***** C:\SCR577\TPA501BETAB\szft.f
cc TJM write(i3,'(i5,5x,a)') nefleg+1,'NUMBER OF MIGRATION PATH LEGS'
cc   TJM  March 7, 2005  SCR529; revise input for 2 legs only
     write(i3,'(i5,5x,a)') 2,'NUMBER OF MIGRATION PATH LEGS'
***** C:\SCR577\TPA501BETAA\SZFT.F
cc TJM write(i3,'(i5,5x,a)') nefleg+1,'NUMBER OF MIGRATION PATH LEGS'
cc   TJM  March 7, 2005  revise input for 2 legs only
     write(i3,'(i5,5x,a)') 2,'NUMBER OF MIGRATION PATH LEGS'
*****
```

```
***** C:\SCR577\TPA501BETAB\szft.f
    &                                0.0,0.0
cc  TJM  March 7, 2005  SCR529; No need for do-loops 900 & 901
cc  TJM              this is only TUFF so only need
***** C:\SCR577\TPA501BETAA\SZFT.F
    &                                0.0,0.0
cc  TJM  March 7, 2005  No need for do-loops 900 & 901
cc  TJM              this is only TUFF so only need
*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005     SCR529; do 900 ii=1,nefleg

***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005     do 900 ii=1,nefleg

*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005  SCR529; 900 continue

***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005  900 continue

*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005      SCR529; do 901 ii=1,nefleg

***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005      do 901 ii=1,nefleg

*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005  SCR529; 901 continue

***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005  901 continue

*****
```

```
***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM  March 7, 2005  SCR529; do not need to loop on 'kk'
cc  TJM                 only need one leg for TUFF
***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM  March 7, 2005  do not need to loop on 'kk'
cc  TJM                 only need one leg for TUFF
*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM  March 7, 2005      SCR529; if (kk .eq. 1) then
      write(i3,'(i5,3x,e10.3,2x,i5,3x,e10.3,5x,e10.3,8x,
***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM  March 7, 2005      if (kk .eq. 1) then
      write(i3,'(i5,3x,e10.3,2x,i5,3x,e10.3,5x,e10.3,8x,
*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM  March 7, 2005      SCR529; else
cc  TJM     write(i3,'(8x,10x,2x,i5,3x,e10.3,5x,e10.3,8x,e10.3)')
***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM  March 7, 2005      else
cc  TJM     write(i3,'(8x,10x,2x,i5,3x,e10.3,5x,e10.3,8x,e10.3)')
*****

***** C:\SCR577\TPA501BETAB\szft.f
c
cc  TJM  March 7, 2005      SCR529; endif

***** C:\SCR577\TPA501BETAA\SZFT.F
c
cc  TJM  March 7, 2005      endif

*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005 SCR529; - no need to do this due to multiple
cc                    NEFTRAN simulations not a composite
***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005 - no need to do this due to multiple
cc                    NEFTRAN simulations not a composite
*****
```

```
***** C:\SCR577\TPA501BETAB\szft.f
cc TJM      write(i3,'(i5,5x,a)') nefleg+1,'NUMBER OF NETWORK LEGS'
cc   TJM  March 7, 2005  SCR529; revise input for 2 legs only
     write(i3,'(i5,5x,a)') 2,'NUMBER OF NETWORK LEGS'
***** C:\SCR577\TPA501BETAA\SZFT.F
cc TJM      write(i3,'(i5,5x,a)') nefleg+1,'NUMBER OF NETWORK LEGS'
cc   TJM  March 7, 2005  revise input for 2 legs only
     write(i3,'(i5,5x,a)') 2,'NUMBER OF NETWORK LEGS'
*****

***** C:\SCR577\TPA501BETAB\szft.f
cc TJM write(i3,'(i5,5x,a)') nefleg+1,'NUMBER OF MIGRATION PATH LEGS'
cc   TJM  March 7, 2005  SCR529; revise input for 2 legs only
     write(i3,'(i5,5x,a)') 2,'NUMBER OF MIGRATION PATH LEGS'
***** C:\SCR577\TPA501BETAA\SZFT.F
cc TJM write(i3,'(i5,5x,a)') nefleg+1,'NUMBER OF MIGRATION PATH LEGS'
cc   TJM  March 7, 2005  revise input for 2 legs only
     write(i3,'(i5,5x,a)') 2,'NUMBER OF MIGRATION PATH LEGS'
*****

***** C:\SCR577\TPA501BETAB\szft.f
c   &                            0.0,0.0
cc  TJM  March 7, 2005  SCR529; No need for do-loops 900 & 901
cc  TJM              this is only ALLUVIUM so only need
***** C:\SCR577\TPA501BETAA\SZFT.F
c   &                            0.0,0.0
cc  TJM  March 7, 2005  No need for do-loops 900 & 901
cc  TJM              this is only ALLUVIUM so only need
*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005     SCR529; do 900 ii=1,nefleg

***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005     do 900 ii=1,nefleg

*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005  SCR529; 900 continue

***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005  900 continue

*****
```

```
***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005      SCR529; do 901 ii=1,nefleg

cc rwj 6-7-05 SCR577
c     write(i3,'(i3,x,e10.4,3x,f5.1,5x,i2,3x,e10.3,2x,e10.3,2x,e10.3,2x,
c    &  e10.3)') 2,nefdisper(2),spastp,0.0,por(2),
c    &          pori(2), 0.0,
c    &  nefvel(2)
      write(i3,'(i3,x,e10.4,3x,f5.1,5x,i2,3x,e10.3,2x,e10.3,2x,e10.3,2x,
     &  e10.3)') 2,nefdisper(2),spastp,  0,por(2),
     &          pori(2), 0.0,
***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005      do 901 ii=1,nefleg

      write(i3,'(i3,x,e10.4,3x,f5.1,5x,i2,3x,e10.3,2x,e10.3,2x,e10.3,2x,
     &  e10.3)') 2,nefdisper(2),spastp,0.0,por(2),
     &          pori(2), 0.0,
*****

***** C:\SCR577\TPA501BETAB\szft.f
     &  nefvel(2)

cc TJM write(i3,'(i3,x,e10.4,3x,f5.1,5x,i2,3x,e10.3,2x,e10.3,2x,e10.3,2x,
***** C:\SCR577\TPA501BETAA\SZFT.F
     &  nefvel(2)
cc TJM write(i3,'(i3,x,e10.4,3x,f5.1,5x,i2,3x,e10.3,2x,e10.3,2x,e10.3,2x,
*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM March 7, 2005  SCR529; 901 continue

***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM March 7, 2005  901 continue

*****

***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM  March 7, 2005  SCR529; do not need to loop on 'kk'
cc  TJM                 only need one leg for ALLUVIUM
***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM  March 7, 2005  do not need to loop on 'kk'
cc  TJM                 only need one leg for ALLUVIUM
*****
```

```
***** C:\SCR577\TPA501BETAB\szft.f

cc  TJM  March 7, 2005      SCR529; if (kk .eq. 1) then
      write(i3,'(i5,3x,e10.3,2x,i5,3x,e10.3,5x,e10.3,8x,
***** C:\SCR577\TPA501BETAA\SZFT.F

cc  TJM  March 7, 2005      if (kk .eq. 1) then
      write(i3,'(i5,3x,e10.3,2x,i5,3x,e10.3,5x,e10.3,8x,
*****

***** C:\SCR577\TPA501BETAB\szft.f
c
cc  TJM  March 7, 2005      SCR529; else
cc  TJM     write(i3,'(8x,10x,2x,i5,3x,e10.3,5x,e10.3,8x,e10.3)')
***** C:\SCR577\TPA501BETAA\SZFT.F
c
cc  TJM  March 7, 2005      else
cc  TJM     write(i3,'(8x,10x,2x,i5,3x,e10.3,5x,e10.3,8x,e10.3)')
*****

***** C:\SCR577\TPA501BETAB\szft.f
c
cc  TJM  March 7, 2005      SCR529; endif

***** C:\SCR577\TPA501BETAA\SZFT.F
c
cc  TJM  March 7, 2005      endif

*****
```

The above file comparison (see <u>**bold underline**</u> above) shows a write statement using an integer instead of a floating point (i.e., "0" instead of "0.0"). Therefore, <u>Criterion 1 is passed</u>.

<u>For Criterion 2,</u> the contents of the NEFTRAN SZ input file *nefiialluv.inp* for the TPA Version 5.0.1betaB code follows.

```
        AREA & PATH #S  1,   1  INFIL. =  0.000E  MASS FRC.=  0.100E
   GROUP 1 - OPTIONS, STANDARD PRINT, 0=NO PRINT
  1     LIST OF ALL THE  PARAMETERS
  1     THE NETWORK LEG PROPERTIES
  1     THE NETWORK JUNCTION PROPERTIES
  1     THE MIGRATION PATH PROPERTIES ARRAY
  1     THE DECAY CHAIN PROPERTIES ARRAY
  1     THE ELEMENT PROPERTIES ARRAY
  1     FLUID VELOCITIES & SOURCE/DISCH FLOWS
  1     SUBCHAINS, PRODUCTION & VELOCITIES
  1     SPACE & TIME STEPS AND SOURCE TYPE
```

1 TIME INDEPENDENT OUTPUT, IF +N, RATES/CONCS EVERY NTH TIME STEP
0 DISCHARGE SUMMARY
EXTERNAL FILES, NONZERO => FILE WRITTEN/READ
0 SRATE.DAT, SOURCE RATES (CI/Y) - WRITTEN TO UNIT 25
-1 nefii.dis, DISCHARGE RATES (CI/Y) - WRITTEN TO UNIT 30
1 EXTERNAL SOURCE FLAG (=1 =>READ UNIT 14)
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 CONTROLS
0 USE DVM (0) OR ANALYTIC SOLN (NONZERO)
1 SOLVE NETWORK (0) OR INPUT VELOCITIES (NONZERO)
0 LEACH (0), SOLUBILITIES (1), OR BOTH (2) FOR SOURCE RATES
0 FLOWTHRU (0), MIXCELL (1), OR CHOOSE (2) FOR SOURCE RATES
0 CONSTANT (0) OR EXPONENTIAL (1) LEACH RATE MODEL
0 FORCE (NONZERO) USE OF LEG-TO-LEG TRANSFER ALGORITHM
DEBUG PRINTS, NONZERO => PRINT
0 DVM MULTIPLIERS FOR TRANSPORT, DISCHARGE, AND SOURCE
0 DIAGNOSTIC INFO FOR SUBROUTINE BAND
0 DIAGNOSTIC INFO FOR FUNCTION GIT
0 MATRIX/VECTOR SYSTEM SOLVED FOR FLOW
0 THE DATA READ FROM UNIT 10, SAMP.DAT
1 CONC. FLAG (=1 => WRITE TO UNIT 29 IN CI/M**3)
1 INVENTORY AT RELEASE TIME
1 RESTRICTIONS PLACED ON THE TIME STEPS
0 LEG/JUNCTION & JUNCTION/LEG CONNECTIONS
1 VELOCITY FIELDS FROM UNIT 11
0 THE ATOM COUNT SUMMARY
0 JUNCTION PRESSURES & LEG FLOWRATES
0 LEG-TO-LEG TRANSFER FRACTIONS
0 TIME SPENT AS EACH ISOTOPE IN A SUBCHAIN
0 TIME DEPENDENT FLOWRATES THROUGH SOURCE REGIME
GROUP 2 - PROBLEM SIZE
2 NUMBER OF NETWORK LEGS
0 NUMBER OF NETWORK JUNCTIONS
2 NUMBER OF MIGRATION PATH LEGS
18 NUMBER OF DECAY CHAINS INPUT
20 NUMBER OF ELEMENTS INPUT
CHN1 CHN2 CHN3 CHN4 CHN5 - # PER CHAIN
2 5 2 1 4 1 1 1 1 1
1 1 1 2 3 2 1 3
CHN1 CHN2 CHN3 CHN4 CHN5 - TRANSPORT-0, SOURCE-1, NEITHER-2
0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0
GROUP 3 - SOURCE/FLOW PARAMETERS
0.100E FRACTION OF INVENTORY ACCESSED

0.000E PORE VOLUME CONTAINING SOURCE (M**3) USED FOR MIXING CELL
0.000E PORE AREA OF SOURCE (M**2)
0.100E-04 LEACH RATE (1/Y) IF LEACH LTD
1000.00 DENSITY OF SOURCE FLUID (KG/M**3)
0.000E PORE AREA AT DISCHARGE (M**2)
GROUP 4 - TIME PARAMETERS
0.100E TIME TO END OF SIMULATION (Y)
0.000E TIME OF ONSET OF MIGRATION (Y)
0.000E TIME OF ONSET OF LEACHING (Y)
0.000E TIME STEP FOR SOURCE (Y)
CHAIN1 CHAIN2 CHAIN3 CHAIN4 CHAIN5 TIME STEPS BY CHAIN (Y)
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
0.0 0.0 0.0 0.0 0.0 0.0 0.0 0.0
GROUP 5 - INCREMENT DETERMINATION
16 USE DEFAULTS (0) OR SUPPLY ALL 16 VALUES
0 # VELOCITY INTERVALS (DEFAULT = 7)
10.00 DTPAR(1) MINIMUM # OF SOURCE TIME STEPS ACROSS LEACH TIME (DEFAULT = 5)
20.00 DTPAR(2) ISOTOPE IMPORTANCE PARAMETER FOR SOURCE DT (DEFAULT = 20)
0.30 DTPAR(3) LOWER BOUND PARAMETER FOR SOURCE DT (DEFAULT = .5)
0.10 DTPAR(4) MIXING CELL PARAMETER FOR SOURCE DT (DEFAULT = .2)
0.10 DTPAR(5) PARAMETER TO DECIDE IF MIXING CELL USED (DEFAULT = .1)
0.80 DTPAR(6) PARAMETER TO ENSURE PEAK SOURCE FLOWRATE CAPTURE (DEFAULT = .8)
35.00 DTPAR(7) MINIMUM # OF TIME STEPS FOR SOURCE (DEFAULT = 20)
10.00 DXDTPA(1) ISOTOPE IMPORTANCE PARAMETER FOR TRANSPORT DT (DEFAULT = 10)
0.70 DXDTPA(2) CURVE RESOLUTION PARAMETER FOR TRANSPORT DT (DEFAULT = 1.5)
0.10 DXDTPA(3) MAX. RED. IN TRANS. DT FOR CURVE RESOLUTION DT (DEFAULT = 0.2)
5.00 DXDTPA(4) MINIMUM # OF TIME STEPS FOR TRANSPORT DT (DEFAULT = 30)
1.50 DXDTPA(5) THE INITIAL COURANT # TO FIND DX'S (1.0)
0.95 DXDTPA(6) MINIMUM COURANT # TO FIND DX'S (0.75)
100.00 DXDTPA(7) MINIMUM GRID BLOCKS FOR PATH-AVERAGED TRANSPORT (DEFAULT = 50)
15.00 DXDTPA(8) MINIMUM GRID BLOCKS/LEG FOR LEG-TO-LEG TRANSFER (DEFAULT = 7)
NETWORK LEG PROPERTIES ARRAY

LEG #	INLET JCT	OUTLET JCT	LENGTH (M)	AREA (M**2)	HYDRAULIC K (M/YR)	BRINE CONC.
1	1	2	50.0	0.0	0.0	0.0
2	2	3	2910.0	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 0.5000E    0.0     0   0.133E   0.000E   0.000E   0.237E
 2 0.2910E    0.0     0   0.133E   0.120E-07   0.000E   0.737E
                    DECAY CHAIN ARRAY
NAME      ATM#  ELE-   LOC  PAR  PAR  FRAC  FRAC     INVEN    HALF LIFE
WEIGH
 A6    (AMU)  MENT   NDX   #1   #2  FROM1 FROM2     (CI)      (Y)     FAC
'CM246 '  246.    1     1    0    0  0.000  0.000    0.000E 0.473E     0.100
'U238  '  238.    2     2    1    0  1.000  0.000    0.000E 0.447E     0.100
'CM245 '  245.    1     1    0    0  0.000  0.000    0.000E 0.850E     0.100
'AM241 '  241.    3     2    1    0  1.000  0.000    0.000E 0.432E     0.100
'NP237 '  237.    4     3    2    0  1.000  0.000    0.000E 0.214E     0.100
'U233  '  233.    2     4    3    0  1.000  0.000    0.000E 0.158E     0.100
'TH229 '  229.    5     5    4    0  1.000  0.000    0.000E 0.734E     0.100
'AM243 '  243.    3     1    0    0  0.000  0.000    0.000E 0.738E     0.100
'PU239 '  239.    6     2    1    0  1.000  0.000    0.000E 0.241E     0.100
'PU240 '  240.    6     1    0    0  0.000  0.000    0.000E 0.654E     0.100
'U234  '  234.    2     1    0    0  0.000  0.000    0.000E 0.244E     0.100
'TH230 '  230.    5     2    1    0  1.000  0.000    0.000E 0.770E     0.010
'RA226 '  226.    7     3    2    0  1.000  0.000    0.000E 0.160E     0.100
'PB210 '  210.    8     4    3    0  1.000  0.000    0.000E 0.223E     1.000
'CS135 '  135.    9     1    0    0  0.000  0.000    0.000E 0.230E     1.000
'I129  '  129.   10     1    0    0  0.000  0.000    0.000E 0.157E     0.100
'TC99  '   99.   11     1    0    0  0.000  0.000    0.000E 0.213E    10.000
'NI59  '   59.   12     1    0    0  0.000  0.000    0.000E 0.800E     1.000
'C14   '   14.   13     1    0    0  0.000  0.000    0.000E 0.573E     0.100
'SE79  '   79.   14     1    0    0  0.000  0.000    0.000E 0.110E     1.000
'NB94  '   94.   15     1    0    0  0.000  0.000    0.000E 0.203E     1.000
'CL36  '   36.   16     1    0    0  0.000  0.000    0.000E 0.301E     1.000
'JC246 '  246.   17     1    0    0  0.000  0.000    0.000E 0.473E     0.000
'U238  '  238.    2     2    1    0  1.000  0.000    0.000E 0.447E     0.100
'JC245 '  245.   17     1    0    0  0.000  0.000    0.000E 0.850E     0.000
'JA241 '  241.   18     2    1    0  1.000  0.000    0.000E 0.432E     0.000
'NP237 '  237.    4     3    2    0  1.000  0.000    0.000E 0.214E     0.100
'JA243 '  243.   18     1    0    0  0.000  0.000    0.000E 0.738E     0.000
'JP239 '  239.   19     2    1    0  1.000  0.000    0.000E 0.241E     0.000
'JP240 '  240.   19     1    0    0  0.000  0.000    0.000E 0.654E     0.000
'JT230 '  230.   20     1    0    0  0.000  0.000    0.000E 0.770E     0.000
'RA226 '  226.    7     2    1    0  1.000  0.000    0.000E 0.160E     0.100
'PB210 '  210.    8     3    2    0  1.000  0.000    0.000E 0.223E     1.000
               ELEMENT PROPERTIES ARRAY
ELEM.   SOLUBILITY   LEG   MOBIL RD      IMMOBILE RD      MASS XFER
INDEX     (KG/KG)     #                              MOD FACTOR
   1    0.000E     1    0.100E      0.100E        0.000E
                 2    0.105E      0.100E        0.000E
   2    0.000E     1    0.100E      0.100E        0.000E
                 2    0.361E      0.100E        0.000E
   3    0.000E     1    0.100E      0.100E        0.000E
                 2    0.105E      0.100E        0.000E
   4    0.000E     1    0.100E      0.100E        0.000E
```

```
                2   0.783E    0.100E      0.000E
     5   0.000E    1   0.100E    0.100E      0.000E
                2   0.700E    0.100E      0.000E
     6   0.000E    1   0.100E    0.100E      0.000E
                2   0.253E    0.100E      0.000E
     7   0.000E    1   0.100E    0.100E      0.000E
                2   0.358E    0.100E      0.000E
     8   0.000E    1   0.100E    0.100E      0.000E
                2   0.195E    0.100E      0.000E
     9   0.000E    1   0.100E    0.100E      0.000E
                2   0.473E    0.100E      0.000E
    10   0.000E    1   0.100E    0.100E      0.000E
                2   0.100E    0.100E      0.000E
    11   0.000E    1   0.100E    0.100E      0.000E
                2   0.100E    0.100E      0.000E
    12   0.000E    1   0.100E    0.100E      0.000E
                2   0.650E    0.100E      0.000E
    13   0.000E    1   0.100E    0.100E      0.000E
                2   0.100E    0.100E      0.000E
    14   0.000E    1   0.100E    0.100E      0.000E
                2   0.200E    0.100E      0.000E
    15   0.000E    1   0.100E    0.100E      0.000E
                2   0.357E    0.100E      0.000E
    16   0.000E    1   0.100E    0.100E      0.000E
                2   0.100E    0.100E      0.000E
    17   0.000E    1   0.100E    0.100E      0.000E
                2   0.532E    0.100E      0.000E
    18   0.000E    1   0.100E    0.100E      0.000E
                2   0.532E    0.100E      0.000E
    19   0.000E    1   0.100E    0.100E      0.000E
                2   0.532E    0.100E      0.000E
    20   0.000E    1   0.100E    0.100E      0.000E
                2   0.532E    0.100E      0.000E
```

Note above that the diffusion flag equals 0. See **bold and underlined** above. Therefore, Criterion 2 is passed.

- Overall test status: PASS

SL-3. Name: FAILT Convergence

Path for run directory: c:\SCR577\tpa501betaA\run
c:\SCR577\tpa501betaB\run

Path for archive of results: \SCR577\tpa501betaA\run\test3 (archived on CD "SCR#577 Testing")
\SCR577\tpa501betaB\run\test3 (archived on CD "SCR#577 Testing")

Environment variables:

Baseline case
TPA_DATA=c:\SCR577\tpa501betaA
TPA_DATA=c:\SCR577\tpa501betaA

and

Test Case
TPA_DATA=c:\SCR577\tpa501betaB
TPA_DATA=c:\SCR577\tpa501betaB

Special input files or modifications to input files required: FAILT input files *chlrdmf.dat*, *deltaec.inp*, *ebsfail.inp,* and *ebsrhc.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 FAILT standalone code is executed in standalone mode using input files form a TPA code in which the FAILT calculations did not converge.

- Objective: Verify convergence of calculations from the FAILT standalone code.

- Assumptions: use FAILT input files from an eariler TPA code simulation in which FAILT calculations did not converge. Otherwise, there are no assumptions, other than the assumptions made in the TPA code

- Constraints: None

- Output files to compare or examine: *failt.out*

- Step by step test procedure to be used:

1. Create "run\test3\run_failt" and "run\test3\failt_input_files" subdirectories in both the TPA Versions 5.0.1betaA and 5.0.1betaB main source code directories.
2. Copy the FAILT input files *chlrdmf.dat*, *deltaec.inp*, *ebsfail.inp,* and *ebsrhc.inp* into the subdirectories created in #1 above. .
3. Copy the FAILT executable *failt.exe* from the TPA Versions 5.0.1betaA and 5.0.1betaB code subdirectories into the "run\test3\run_failt" subdirectories from #1 above.
4. In the "run\test3\run_failt" subdirectories, execute FAILT in standalone mode.
5. Examine the FAILT screenprint in the file *failt.out* for both the TPA Versions 5.0.1betaA and 5.0.1betaB codes

- Pass/Fail criteria:

Criterion 1: For the TPA Version 5.0.1betaA, there should be statements regarding convergence in the *failt.out* file.

Criterion 2: For the TPA Version 5.0.1betaB, using the same input files as for Criteria 1, there should not be statements regarding convergence in the *failt.out* file.

Test Results: The files in the \SCR577\tpa501betaA\run\test3 and \SCR577\tpa501betaB\run\test3 subdirectories contain the files for this test.

For Criterion 1, the FAILT screenprint in the *failt.out* file for the TPA Version 5.0.1betaA code follows.

```
ebspac (engineering barrier system performance assessment code)
this is the part of the code that computes wp failure time
version= 1.0
Tue Nov 01 07:37:25 2005
nhist3= 5001
nhist= 5001

**Calculation of Weld Failure Time**
 Case II: RH transitioned to aqueous
 Localized corrosion intitiated at   2235.22   years
Weld failure time =   2364.57  yr
**End of Weld Failure Calculation**

            calculation of waste package failure time
=================================================================
=====================
                end of simulation time [yr]:    1000000.
      no. of rows of data to pass to release.f:        5001
-------------------------------------------------------------------------------------
ilayer  tstop    tcan     ecrit     ecorr   chloride   rthick     mode
      [yr]      [C]     [vshe]    [vshe]    flag        [m]
=================================================================
=====================
1       2.31     59.73    0.0000    0.0000    0    7.0000000E-02  dry oxd
1       4.67     65.86    0.0000    0.0000    0    7.0000000E-02  dry oxd
1       7.09     68.36    0.0000    0.0000    0    7.0000000E-02  dry oxd
1       9.57     69.56    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      12.10     70.21    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      14.70     70.54    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      17.35     70.65    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      20.07     70.60    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      22.85     70.44    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      25.69     70.14    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      28.61     69.48    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      31.59     68.71    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      34.63     67.90    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      37.76     67.08    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      40.95     66.26    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      44.22     65.45    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      47.56     64.66    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      50.99    146.38    0.0000    0.0000    0    7.0000000E-02  dry oxd
1      54.49    188.34    0.0000    0.0000    0    7.0000000E-02  dry oxd
```

1	58.08	198.75	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	61.75	202.63	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	65.50	204.06	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	69.35	204.23	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	73.28	203.65	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	77.31	202.64	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	81.43	201.38	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	85.64	199.92	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	89.96	198.33	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	94.37	196.65	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	98.89	194.92	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	103.52	193.15	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	108.25	191.37	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	113.10	189.58	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	118.06	206.89	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	123.13	345.03	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	128.32	389.13	0.0000	0.0000	0	6.9872276E-02	dry oxd
1	133.64	407.84	0.0000	0.0000	0	6.9744553E-02	dry oxd
1	139.08	416.05	0.0000	0.0000	0	6.9616829E-02	dry oxd
1	144.64	418.92	0.0000	0.0000	0	6.9489106E-02	dry oxd
1	150.34	418.75	0.0000	0.0000	0	6.9361382E-02	dry oxd
1	156.17	411.93	0.0000	0.0000	0	6.9233659E-02	dry oxd
1	162.13	404.07	0.0000	0.0000	0	6.9105935E-02	dry oxd
1	168.24	396.45	0.0000	0.0000	0	6.8978211E-02	dry oxd
1	174.49	389.05	0.0000	0.0000	0	6.8850488E-02	dry oxd
1	180.88	383.59	0.0000	0.0000	0	6.8722764E-02	dry oxd
1	187.43	378.53	0.0000	0.0000	0	6.8595041E-02	dry oxd
1	194.13	373.60	0.0000	0.0000	0	6.8467317E-02	dry oxd
1	200.98	368.81	0.0000	0.0000	0	6.8339594E-02	dry oxd
1	208.00	364.14	0.0000	0.0000	0	6.8211870E-02	dry oxd
1	215.18	359.58	0.0000	0.0000	0	6.8084147E-02	dry oxd
1	222.52	355.13	0.0000	0.0000	0	6.8005265E-02	dry oxd
1	230.04	350.77	0.0000	0.0000	0	6.8004909E-02	dry oxd
1	237.74	346.52	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	245.62	342.36	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	253.68	338.29	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	261.93	334.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	270.37	330.43	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	279.01	326.63	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	287.85	322.94	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	296.90	319.34	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	306.16	315.80	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	315.64	312.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	325.34	308.93	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	335.26	305.61	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	345.42	302.35	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	355.82	299.16	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	366.46	296.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	377.35	292.95	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	388.49	289.95	0.0000	0.0000	0	6.8004905E-02	dry oxd

1	399.90	287.00	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	411.57	284.10	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	423.52	281.26	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	435.74	278.47	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	448.25	275.72	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	461.06	273.05	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	474.16	270.42	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	487.57	267.17	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	501.30	263.91	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	515.35	260.70	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	529.72	257.54	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	544.43	254.44	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	559.49	251.39	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	574.90	248.42	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	590.67	245.49	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	606.80	242.63	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	623.32	239.81	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	640.22	237.04	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	657.52	234.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	675.23	231.66	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	693.34	229.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	711.89	226.44	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	730.86	223.91	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	750.28	221.43	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	770.16	218.99	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	790.50	216.59	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	811.32	214.24	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	832.62	211.92	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	854.42	209.64	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	876.74	207.38	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	899.57	205.16	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	922.94	202.98	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	946.86	200.83	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	971.34	198.71	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	996.39	196.34	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1022.03	193.95	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1048.26	191.60	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1075.12	189.30	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1102.60	187.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1130.72	184.78	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1159.50	182.56	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1188.96	180.36	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1219.10	178.18	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1249.95	176.04	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1281.53	173.92	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1313.84	171.83	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1346.91	169.76	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1380.75	167.72	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1415.39	165.70	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1450.83	163.68	0.0000	0.0000	0	6.8004905E-02	dry oxd

```
1    1487.11    161.69    0.0000    0.0000    0   6.8004905E-02  dry oxd
1    1524.23    159.72    0.0000    0.0000    0   6.8004905E-02  dry oxd
1    1562.23    157.77    0.0000    0.0000    0   6.8004905E-02  dry oxd
1    1601.11    155.84    0.0000    0.0000    0   6.8004905E-02  dry oxd
1    1640.91    153.94    0.0000    0.0000    0   6.8004905E-02  dry oxd
1    1681.63    152.06    0.0000    0.0000    0   6.8004905E-02  dry oxd
1    1723.31    150.20    0.0000    0.0000    0   6.8004905E-02  dry oxd
1    1765.97    148.36    0.0000    0.0000    0   6.8004905E-02  dry oxd
1    1809.62    146.51    0.0000    0.0000    0   6.8003814E-02  hmd oxd
1    1854.30    144.67    0.0000    0.0000    0   6.8002697E-02  hmd oxd
1    1900.02    142.85    0.0000    0.0000    0   6.8001554E-02  hmd oxd
1    1946.81    141.05    0.0000    0.0000    0   6.8000384E-02  hmd oxd
1    1994.70    139.45    0.0000    0.0000    0   6.7999187E-02  hmd oxd
1    2043.71    138.18    0.0000    0.0000    0   6.7997961E-02  hmd oxd
1    2093.87    136.92    0.0000    0.0000    0   6.7996708E-02  hmd oxd
1    2145.20    135.68    0.0000    0.0000    0   6.7995424E-02  hmd oxd
1    2197.73    134.46    0.0000    0.0000    0   6.7994111E-02  hmd oxd
failt: Outer overpack LC initiated at 2251.489900000000  years
failt: Outer overpack LC initiated at 2217.888650000000  years
failt: Outer overpack LC initiated at 2214.528525000000  years
failt: Outer overpack LC initiated at 2212.848462500001  years
failt: Outer overpack LC initiated at 2212.008431250000  years
1    2251.49    133.24    0.2730    0.4099    1   5.7841544E-02  local
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    2306.51    132.06    -9.9599   -10.3811    1   -6.9455288E+01  general
=================================================================
====================
               wp wetting time [yr]:       2198.
               wp failure time [yr]:       2251.
      penetration by dry oxidation [m]:       2.006E-03
               echoed input data in:      echo_fail.dat
            output data are in files:      ebstrh.dat and corrode.out
=================================================================
====================
```

The above file (see **<u>bold underline</u>** above) contains statements about FAILT calculations converging. Therefore, <u>Criterion 1 is passed</u>.

<u>For Criterion 2,</u> the FAILT screenprint in the *failt.out* file for the TPA Version 5.0.1betaB code follows.

```
ebspac (engineering barrier system performance assessment code)
this is the part of the code that computes wp failure time
version= 1.0
```

Tue Nov 01 07:39:03 2005
nhist3= 5001
nhist= 5001

Calculation of Weld Failure Time
Case II: RH transitioned to aqueous
Localized corrosion intitiated at 2235.22 years
Weld failure time = 2364.57 yr
End of Weld Failure Calculation

calculation of waste package failure time

===

end of simulation time [yr]: 1000000.
no. of rows of data to pass to release.f: 5001

----

ilayer	tstop [yr]	tcan [C]	ecrit [vshe]	ecorr [vshe]	chloride flag	rthick [m]	mode
1	2.31	59.73	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	4.67	65.86	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	7.09	68.36	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	9.57	69.56	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	12.10	70.21	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	14.70	70.54	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	17.35	70.65	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	20.07	70.60	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	22.85	70.44	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	25.69	70.14	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	28.61	69.48	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	31.59	68.71	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	34.63	67.90	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	37.76	67.08	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	40.95	66.26	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	44.22	65.45	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	47.56	64.66	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	50.99	146.38	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	54.49	188.34	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	58.08	198.75	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	61.75	202.63	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	65.50	204.06	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	69.35	204.23	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	73.28	203.65	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	77.31	202.64	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	81.43	201.38	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	85.64	199.92	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	89.96	198.33	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	94.37	196.65	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	98.89	194.92	0.0000	0.0000	0	7.0000000E-02	dry oxd

1	103.52	193.15	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	108.25	191.37	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	113.10	189.58	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	118.06	206.89	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	123.13	345.03	0.0000	0.0000	0	7.0000000E-02	dry oxd
1	128.32	389.13	0.0000	0.0000	0	6.9872276E-02	dry oxd
1	133.64	407.84	0.0000	0.0000	0	6.9744553E-02	dry oxd
1	139.08	416.05	0.0000	0.0000	0	6.9616829E-02	dry oxd
1	144.64	418.92	0.0000	0.0000	0	6.9489106E-02	dry oxd
1	150.34	418.75	0.0000	0.0000	0	6.9361382E-02	dry oxd
1	156.17	411.93	0.0000	0.0000	0	6.9233659E-02	dry oxd
1	162.13	404.07	0.0000	0.0000	0	6.9105935E-02	dry oxd
1	168.24	396.45	0.0000	0.0000	0	6.8978211E-02	dry oxd
1	174.49	389.05	0.0000	0.0000	0	6.8850488E-02	dry oxd
1	180.88	383.59	0.0000	0.0000	0	6.8722764E-02	dry oxd
1	187.43	378.53	0.0000	0.0000	0	6.8595041E-02	dry oxd
1	194.13	373.60	0.0000	0.0000	0	6.8467317E-02	dry oxd
1	200.98	368.81	0.0000	0.0000	0	6.8339594E-02	dry oxd
1	208.00	364.14	0.0000	0.0000	0	6.8211870E-02	dry oxd
1	215.18	359.58	0.0000	0.0000	0	6.8084147E-02	dry oxd
1	222.52	355.13	0.0000	0.0000	0	6.8005265E-02	dry oxd
1	230.04	350.77	0.0000	0.0000	0	6.8004909E-02	dry oxd
1	237.74	346.52	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	245.62	342.36	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	253.68	338.29	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	261.93	334.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	270.37	330.43	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	279.01	326.63	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	287.85	322.94	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	296.90	319.34	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	306.16	315.80	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	315.64	312.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	325.34	308.93	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	335.26	305.61	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	345.42	302.35	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	355.82	299.16	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	366.46	296.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	377.35	292.95	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	388.49	289.95	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	399.90	287.00	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	411.57	284.10	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	423.52	281.26	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	435.74	278.47	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	448.25	275.72	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	461.06	273.05	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	474.16	270.42	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	487.57	267.17	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	501.30	263.91	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	515.35	260.70	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	529.72	257.54	0.0000	0.0000	0	6.8004905E-02	dry oxd

1	544.43	254.44	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	559.49	251.39	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	574.90	248.42	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	590.67	245.49	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	606.80	242.63	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	623.32	239.81	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	640.22	237.04	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	657.52	234.32	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	675.23	231.66	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	693.34	229.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	711.89	226.44	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	730.86	223.91	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	750.28	221.43	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	770.16	218.99	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	790.50	216.59	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	811.32	214.24	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	832.62	211.92	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	854.42	209.64	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	876.74	207.38	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	899.57	205.16	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	922.94	202.98	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	946.86	200.83	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	971.34	198.71	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	996.39	196.34	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1022.03	193.95	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1048.26	191.60	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1075.12	189.30	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1102.60	187.02	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1130.72	184.78	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1159.50	182.56	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1188.96	180.36	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1219.10	178.18	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1249.95	176.04	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1281.53	173.92	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1313.84	171.83	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1346.91	169.76	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1380.75	167.72	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1415.39	165.70	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1450.83	163.68	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1487.11	161.69	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1524.23	159.72	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1562.23	157.77	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1601.11	155.84	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1640.91	153.94	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1681.63	152.06	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1723.31	150.20	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1765.97	148.36	0.0000	0.0000	0	6.8004905E-02	dry oxd
1	1809.62	146.51	0.0000	0.0000	0	6.8003814E-02	hmd oxd
1	1854.30	144.67	0.0000	0.0000	0	6.8002697E-02	hmd oxd
1	1900.02	142.85	0.0000	0.0000	0	6.8001554E-02	hmd oxd

```
1    1946.81    141.05    0.0000    0.0000    0   6.8000384E-02  hmd oxd
1    1994.70    139.45    0.0000    0.0000    0   6.7999187E-02  hmd oxd
1    2043.71    138.18    0.0000    0.0000    0   6.7997961E-02  hmd oxd
1    2093.87    136.92    0.0000    0.0000    0   6.7996708E-02  hmd oxd
1    2145.20    135.68    0.0000    0.0000    0   6.7995424E-02  hmd oxd
1    2197.73    134.46    0.0000    0.0000    0   6.7994111E-02  hmd oxd
failt: Outer overpack LC initiated at 2251.489900000000  years
failt: Outer overpack LC initiated at 2217.888650000000  years
failt: Outer overpack LC initiated at 2214.528525000000  years
failt: Outer overpack LC initiated at 2212.848462500001  years
failt: Outer overpack LC initiated at 2212.008431250000  years
1    2251.49    133.24    0.2730    0.4099    1   5.7841544E-02  local
failt: Inner overpack LC initiated at 2251.489900000000  years
2    2306.51    132.06   -9.9599   -5.1751    1  -5.4970700E+01  local
=================================================================
=====================
             wp wetting time [yr]:      2198.
             wp failure time [yr]:      2251.
     penetration by dry oxidation [m]:      2.006E-03
             echoed input data in:      echo_fail.dat
          output data are in files:      ebstrh.dat and corrode.out
=================================================================
=====================
```

The above file does not contains statements about FAILT calculations converging. Therefore, <u>Criterion 2 is passed</u>.

- Overall test status: <u>PASS</u>

11/28/05 - Prepared the following two tables which summarize results from the TPA Version 5.0.1betaG code for the Peak Mean Dose (PMD) and the percent contribution of individual radionuclides to that PMD. This information was passed on to Oleg Povetko.

TPA501betaG - 364 realizations and 1,000,000 yr				
Time of Peak Dose (yr)	**10,825**		**Time of Peak Dose (yr)**	**3,549**
Total Dose (mrem/yr)	**173.24**		**Total Dose (mrem/yr)**	**11.26**
	BASECASE		**NO IRREVERSIBLE COLLOIDS**	
Radionuclide	**% of Total Dose**		**% of Total Dose**	
Cm246	0.03%		0.00%	
U238	0.01%		0.01%	
Cm245	0.16%		0.00%	
Am241	0.15%		0.00%	
Np237	0.11%		0.00%	
U233	0.02%		0.01%	
Th229	0.00%		0.00%	
Am243	8.25%		0.00%	
Pu239	61.19%		0.00%	
Pu240	29.44%		0.00%	
U234	0.03%		0.02%	
Th230	0.07%		0.00%	
Ra226	0.00%		0.00%	
Pb210	0.00%		0.00%	
Cs135	0.00%		0.00%	
I129	0.07%		22.46%	
Tc99	0.47%		76.71%	
Ni59	0.00%		0.00%	
C14	0.00%		0.00%	
Se79	0.01%		0.48%	
Nb94	0.00%		0.00%	
Cl36	0.00%		0.31%	

TPA501betaG - 1024 realizations and 1,000,000 years			
Time of Peak	**12,062**	**yr**	
Peak Dose	**106**	**mrem/yr**	
	Basecase		**No Cm245 and Am241**
	% of Total Dose		**% of Total Dose**
Cm246	0.03%		0.03%
U238	0.03%		0.03%
Cm245	0.18%		REMOVED
Am241	0.18%		REMOVED
Np237	0.19%		0.09%
U233	0.05%		0.04%
Th229	0.00%		0.00%
Am243	6.08%		6.08%
Pu239	62.84%		63.15%
Pu240	29.73%		29.87%
U234	0.10%		0.10%
Th230	0.10%		0.10%
Ra226	0.00%		0.00%
Pb210	0.00%		0.00%
Cs135	0.00%		0.00%
I129	0.08%		0.08%
Tc99	0.41%		0.41%
Ni59	0.00%		0.00%
C14	0.00%		0.00%
Se79	0.01%		0.01%
Nb94	0.00%		0.00%
Cl36	0.00%		0.00%

12/05/05 - Prepared a summary of results from the TPA Version 5.0.2 code. The work was conducted based on a request from Oleg Povetko. Results were also discussed with R. Janetzke and J. Winterle and passed on to F. Osidele and S. Mohanty who were out of town on travel.

The results look at the peak expected dose, time of the peak expected dose, run and time for 10k, 100k, and 1,000k year TPA code maximum simulations using (a) the basecase radionuclide list and decay chains and (b) a modified list with 9 radionuclides and no chains. See the table below for a list of these input parameters.

Comparison of TPA Results
TPA Version 5.0.2
362 Realizations

Scenario	PMD = Peak Expected Dose TPMD = Time of PMD PMD in mrem/yr (TPMD in yr)	Maximum Simulation Time 10,000 years	 100,000 years	 1,000,000 years*
Basecase Radionuclides (22 aqueousnuclides - 4 chains w/ 2, 2, 4, & 5 members)	PMD in mrem/yr (TPMD in yr)	84 (9,323)	89 (9,769)	88 (9,769)*
(11 colloidalnuclides - 4 chains w/ 2, 2, 3, & 3 members)	Run Time on TPA/GOLDSIM	2h 36 m	5h 56m	67h 16m
Tim's List of 9 Aqueousnuclides w/ No Chains (Np237, U238, Pu239, Th230, Pu240, I129, Tc99, Cs135, & Pu242)	PMD (TPMD)	78 (9,323)	82 (9,543)	81 (9,543)* **
(colloidalnuclides are Jp239, Jp240, & Jp242)	Run Time on TPA/GOLDSIM	2h 6m	3h 55m	41h 16m ***
	Change in Performance (i.e., % decrease in run time achieved by reducing number of radionuclides and no chains)	-19%	-34%	-39%

* = UZ Courant number set equal to 0.15
** = note that PMD and TPMD are the same w/ UZ Courant Number of 1.50 for the Reduced List
*** = note that runtime decreases 3% (i.e., 1h 15m in a 42h 31m run) when UZ Courant Number changes from 1.50 to 0.15

12/11/05 - At the request of Oleg Povetko, performed follow-up analysis with the TPA Version 5.0.2 code for a long simulation (1e6 yr), a list of 9 radionuclides above minus U238, and 362 realizations. The following table contains the follow-up results.

Comparison of TPA Results

TPA Version 5.0.2

362 Realizations

PMD = Peak Expected Dose
TPMD = Time of PMD
PMD in mrem/yr (TPMD in yr)

Scenario		Maximum Simulation Time		
		10,000 years	100,000 years	1,000,000 years*
Basecase Radionuclides (22 aqueousnuclides - 4 chains w/ 2, 2, 4, & 5 members)	PMD in mrem/yr (TPMD in yr)	84 (9,323)	89 (9,769)	88 (9,769)*
(11 colloidalnuclides - 4 chains w/ 2, 2, 3, & 3 members)	Run Time on TPA/GOLDSIM	2h 36 m	5h 56m	67h 16m
Tim's List of 9 Aqueousnuclides w/ No Chains (Np237, U238, Pu239, Th230, Pu240, I129, Tc99, Cs135, & Pu242)	PMD (TPMD)	78 (9,323)	82 (9,543)	81 (9,543)* **
(colloidalnuclides are Jp239, Jp240, & Jp242)	Run Time on TPA/GOLDSIM	2h 6m	3h 55m	41h 16m *** ****
	Change in Performance (i.e., % decrease in run time achieved by reducing number of radionuclides and no chains)	-19%	-34%	-39%

* = UZ Courant number set equal to 0.15

** = note that PMD and TPMD are the same w/ UZ Courant Number of 1.50 for the Reduced List

*** = note that runtime decreases 3% (i.e., 1h 15m in a 42h 31m run) when UZ Courant Number changes from 1.50 to 0.15

**** = (follow-up analysis) removal of U238 from Tim's list of 9 radionuclides reduces PMD by 0.02% with essentially no difference in runtime (i.e., decrease by 2 minutes out of 2476 minutes)

12/12/05 - Performed TPA Version 5.0.2 code runs for the 9 radionuclides above (no chains), 362 realizations, and 1e6yr maximum simulation time (4,800 time steps following 10,000 yr compliance time). Also, the *uzft.f* source code was modified for *gwttmin* = 5.0 yr (instead of 20.0 yr) and there was no CHnv reset to zero if the sampled value was from 0 to 2 m. The PMD and TPMD were 68 mrem/yr and 10,825 yr and NEFTRAN was not skipped (compare this to 88 skips out of 2,896 subarea calculations). Note that these values are comparable to 81 mrem/yr and 9,543 yr, respectively. This is a 16% decrease in PMD and a 1,282 yr increase in the TPMD. An interpretation of these results is that, by not skipping NEFTRAN and using any sampled value for CHnv (i.e., not setting equal to zero) satisfying criteria in UZFT, the TPA code releases are spread out more in time. Thus, the PMD is decreased and the TPMD is shifted to a larger value.

12/13/05 - Prepared the following information.

INFORMATION - Plots from results of the TPA Version 5.0.2 code

Basecase run with the following exceptions:

362 realizations

1,000,000 yr maximum simulation time
4,800 time steps following the 10,000 yr simulation time

9 aqueousnuclides with no chains
(Np237, U238, Pu239, Th230, Pu240, I129, Tc99, Cs135, and Pu242)
Colloidal nuclides are Jp239, Jp240, and Jp242

As a result of modifying uzft.f by changing gwttmin, minimum groundwater travel time which is hardcoded in the uft.f file, from 20 yrs to 5 yrs, there was no skipping of UZ NEFTRAN.

In the basecase, UZ NEFTRAN is skipped for 88 of the 2,896 subarea calculations. These 88 times UZ NEFTRAN is skipped corresponds to 84 different realizations.

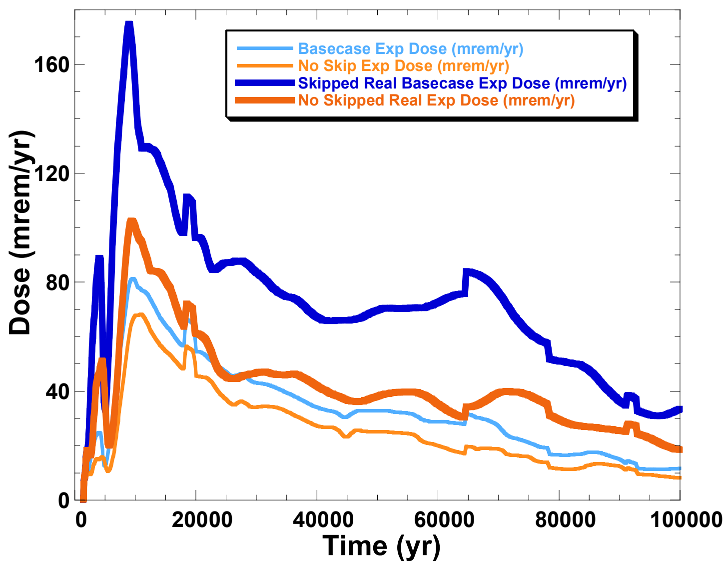
Five hair diagrams which follow are total dose for each of the 84 realizations. Each hair diagram shows 16 or 17 individual realizations. The blue lines represent realizations with UZ NEFTRAN skipped for at least one of the subareas. The orange lines represent corresponding realizations without skipping UZ NEFTRAN.

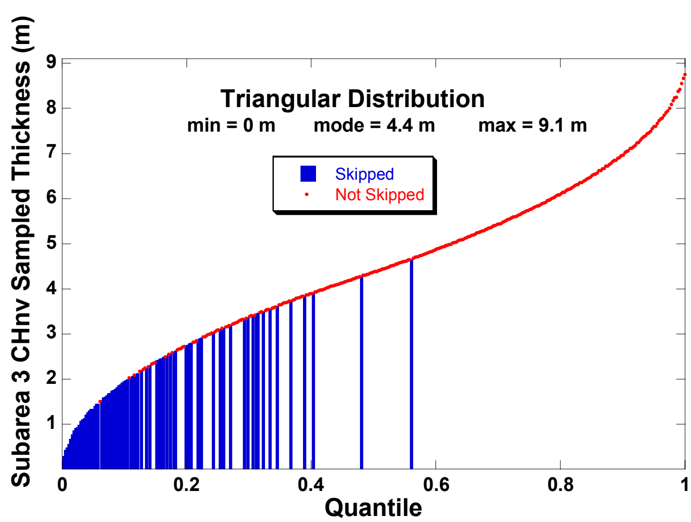
	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
Basecase	81	9,543
No skip of UZ NEFTRAN	68	10,825

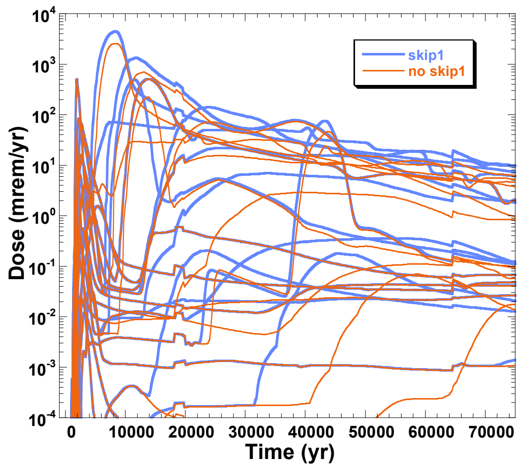
Note that for the 88 subarea calculations with UZ NEFTRAN skipped, Subarea 1 was skipped 3 times, Subarea 2 was skipped 8 times, and Subarea 5 was skipped 1 time. Subarea 3 was skipped the most of any subarea (i.e., 76 times or about 1 in 5 realizations).

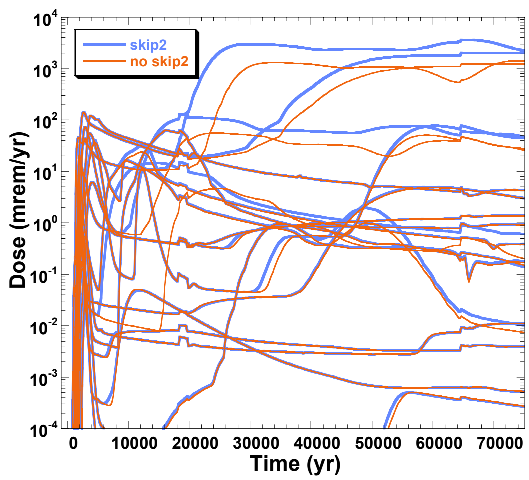
Subarea CHnv distribution (min, mode, max of a triangular distribution)

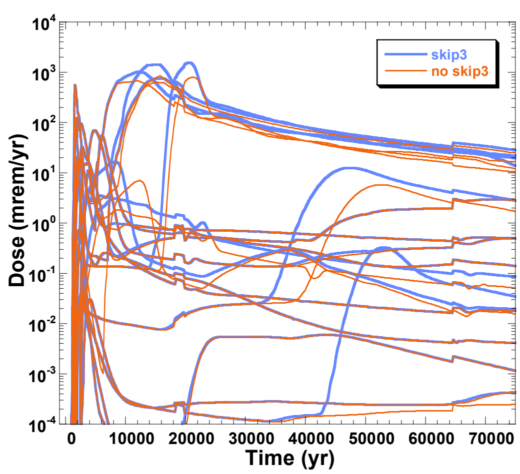
1	0.0	27.7	66.9	(mean = 31.5 m)
2	0.0	16.4	77.8	(mean = 31.4 m)
3	0.0	4.2	9.1	(mean = 4.4 m)
4	51.7	55.5	62.1	(mean = 56.4 m)
5	3.2	49.5	62.7	(mean = 38.5 m)
6	2.4	16.7	71.2	(mean = 30.1 m)
7	2.4	38.5	104.0	(mean = 48.3 m)
8	3.9	65.0	96.0	(mean = 55.0 m)

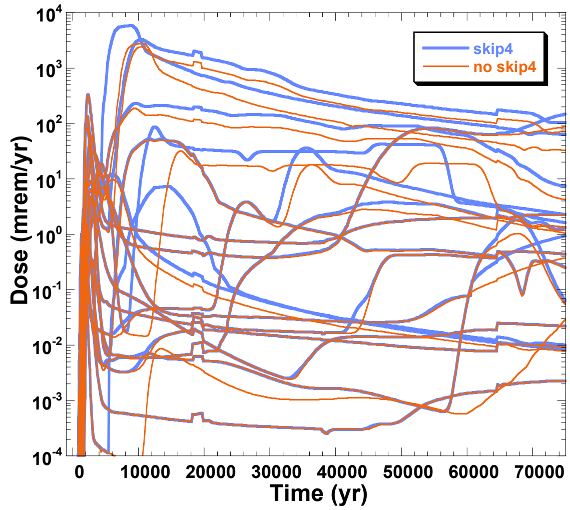




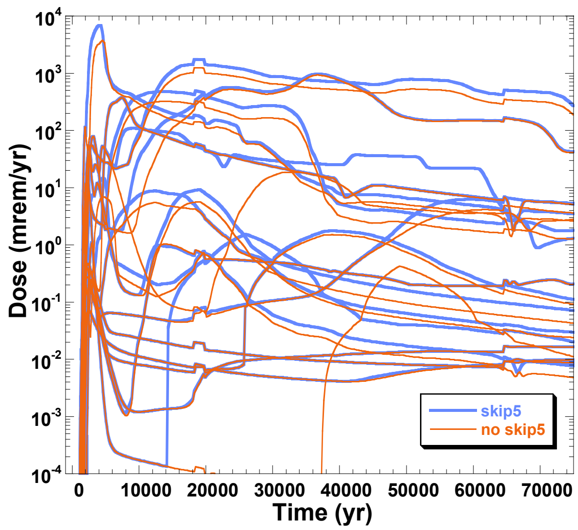

skip1
no skip1
Dose (mrem/yr)
Time (yr)
0
10000
20000
30000
40000
50000
60000
70000


skip2
no skip2
Dose (mrem/yr)
Time (yr)
0
10000
20000
30000
40000
50000
60000
70000


skip3
no skip3
Dose (mrem/yr)
Time (yr)
0
10000
20000
30000
40000
50000
60000
70000



skip4
no skip4
Dose (mrem/yr)
Time (yr)



skip5
no skip5
Dose (mrem/yr)
Time (yr)

12/15/05 - Performed a number of TPA Version 5.0.1betaF code simulations to investigate the effects of the Courant number (values of 1.5 [basecase] and 0.15) on the Peak Mean Dose (PMD) and Time of the Peak Mean Dose (TPMD) for maximum simulation times of 1e4 yr, 1e5 yr, and 1e6yr and different realizations. The time required to complete the simulations is also noted in order to determine whether Courant numbers of 1.5 and 0.15 impact the execution time. The "TPA" computer was used for these simulations.

			PMD (TPMD)**	
			Courant Number	
# Realizations	**Max Time**	**Difference in RunTime***	**1.5**	**0.15**
363	1,000,000		stopped sa1 real3 U234	410.8 (11,238)
364	10,000	+4m/2hr 41m	382.5 (10,000)	382.5 (10,000)
364	100,000	-35m/5hr 55m	404.2 (11,350)	404.3 (11,350)
364	1,000,000		stopped sa1 real3 U234	-
366	100,000		181.1 (19,450)	181.5 (19,450)
1,020	100,000	-1.5h/16hr	309.5 (7,914)	309.7 (7,914)
1,024	10,000	+11m/7hr 34m	285.4 (10,000)	285.6 (10,000)
1,024	100,000		stopped sa6 real154 Cm245	285.2 (10,450)
1,024	1,000,000		stopped sa6 real154 Cm245	285.2 (10,450)

* difference in run time is relative to the basecase run time for Courant number of 1.5
**note: PMD units are mrem/yr and TPMD units are yr)

12-30-05 During testing involving the TPA Version 5.0.2d code and SCR607 testing with the TPA Version 5.0.2 and 5.0.2 codes, noticed that when the thickness of the OuterOverPack is zero, WP corrosion by humid oxidation continued until the InnerOverPack was completely corroded. At that time, WP failure by corrosion was considered to occur. Note that Localized Corrosion only needs to penetrate the OuterOverPack for WP corrosion. I thought that there was no credit taken for (i.e., no protection offered by) the InnerOverPack. I spoke with O. Pensado on 12-29-05 about this. He thought that currently the TPA code should not take credit for the InnerOverPack. He also pointed out that for future barrier analysis, it was important to have the capability to set the OuterOverPack thickness to zero in order to force WP failure.

To avoid taking credit for the InnerOverPack (as protection for corrosion of the WP) and for future barrier analysis, we decided that a minimal approach in terms of TPA code modification should be examined. Preferably, without adding input parameter(s) or many lines of code additions/modifications.

I looked into this with the TPA Version 5.0.2d code and found the following fix as is documented using the PC "fc" (file comparison) utility.

```
Comparing files failt.f and FAILT.F.ORIGINAL
***** failt.f

cc rwr debug 12/31/05 take no credit for the InnerThickness (hmd ox is configured
cc                to corrode the InnerThickness before failing the WP by corrosion)
cc        thicktot = cthick1 + cthick2
      thicktot = cthick1

***** FAILT.F.ORIGINAL

      thicktot = cthick1 + cthick2

*****
```

I did preliminary testing and found that this change did not impact temperatures (the InnerOverPack thickness is used in the NFENV). The change did force humid oxidation to fail the WP by corrosion if the OuterOverPack was penetrated (i.e., no credit was taken for the InnerOverPack).

This change is simple and may be considered (or something similar) for implementation in the TPA code.

1-4-6 Composed and sent the following email to R. Janetzke and G. Adams.

1/03/06

Ron,

After talking with George, I am following-up my email from the previous week to help focus what we see.

Note that I did finish checking the transfer of WPs in SF and glass to the "ebsrel.inp" file, which I said in my previous email still needed to be done. To do this, I needed to modify EBSREL to avoid overwriting the "ebsrel.inp" file from the SF RELEASET calculations.

George and I agree that the following 2 items should be addressed.

1. The corrosion failures reported to "wpsfail.res" are incorrectly written at SEISMIC times and that value is repeated until a new value for a corrosion failure is written (which after that time is repeated also). It looks like the corrosion number needs to be zeroed out.

2. For a VOLCANIC event, the number of WPs failed is written to the screenprint, as is the number of WPs ejected. The "wpsfail.res" contains the number of WPs failed by intrusive volcanism. RELEASET calculations (through EBSREL) sees the number of intrusive volcanic failures. The problem is that the "wpsfail.res" contains CORROSION failures that include accounting for EXTRUSIVE volcanism too. I thought that we agreed it was OK to double count extrusive volcanism failures. Therefore, the number of CORROSION failures in "wpsfail.res" needs to be increased by the number of WPs ejected. Note that (a) RELEASET/EBSREL are receiving/contain correct and (b) CORROSION failures in "wpsfail.res" (that occur after a volcanic event in a subarea with WPs ejected) is under-represented by the number of WPs ejected. As a fix, I'd recommend only writing the number of INTRUSIVE VOLCANO failures in the screenprint (since the number ejected is written to the screenprint on one of the next lines) - otherwise, increase the number of WPs failed from CORROSION by the number of ejected WPs in both the screenprint (in which case the total number of WPs won't add up) and the "wpsfail.res" file.

The next items are somewhat related and also need to be addressed, I believe.

1. The total number of Subarea 10 WPs is 1,747 (screenprint). The number of SF WPs is 1,258 (from "ebsrel.inp" for SF) and the number of glass WPs is 490 (from "ebsrel.inp" for glass) for a total of 1,748 WPs. The extra 1 WP is from rounding. For the other subareas, the total number of WPs equals the sum of the SF and glass WPs. I know that we are trying to ensure that these WP totals add up. I think that a simple check/adjustment could be added to catch this - either that, or not using "IDINT" (i.e., rounding) until the end of this calculation of the number of SF and glass WPs.

2. Currently, in EBSREL, the TPA code zeros out all releases that occur prior to WP failure. This occurs when there are zero initial failures, but there is a weld failure and all RELEASET releases are zeroed out until the first time of WP failure. I noticed this in a subarea calculation which showed zero initial failures, no WP failures, and releases from the EBS; however, in this case, even though there were EBS releases, there were no UZ and SZ releases. There was a weld failure, but these releases were zeroed out. As a fix, I think that we could zero out all releases that occurred before EITHER a WP or a weld failure.

The next item is an observation/note that needs to be documented and still a question in my mind at least.

1. The time of SEISMIC/ROCKFALL events is tied to the midpoint of the SEISMIC interval (which is written to "wpsfail.res" and passed on to EBSREL and RELEASET) and NOT the time reported in the screenprint. I've mentioned this before as something we need to be aware of and agree that this is OK (i.e., SEISMIC/ROCKFALL can only occur at these midpoint times of 1,000 yr; 3,500 yr; 7,500 yr; and 10,000 yr.

I'll talk to you and do some preliminary looking around the code, not spending much time, for where to fix some of these items.

Please contact me if you have any questions.

Thanks,

Rob

1–04-06 Also sent the following email to R. Janetzke.

1/04/06

From: rwrice@aol.com
To:
Cc:
Bcc:
Subject:

Ron,

In the last few days that I was looking through the TPA code, I thought that the following two items would be useful and help make the code easier to follow. (Maybe this information is already present, but I couldn't find it.)

I was trying to track down information and couldn't find it.

1. It would be useful to have a *.ech and *.rlt file for ASHREMOB, especially to see the # of ejected WPs, (or maybe put this into a VOLCANO *.ech/*.rlt file) instead of just in the screenprint. We used to put this into ashout.res, but that doesn't contain any information when ASHREMOB is used

2. It would be useful have with the number of WPs that RELEASET uses in its release calculations - maybe in a file like "rel_flow.out" - since RELEASET computes the number of CORROSION failed WPs

based in information in "ebsrel.inp".

Please contact me if I've been unclear or if you've questions.

Thanks,

Rob

01/17/06 - Performed a number of TPA code simulations and those results are summarized below for the PMD and TPMD.

TPA Version 5.0.2d
398 realizations

Peak Mean Dose - mrem/yr (Time of Peak Mean Dose - yr)

	Max. Simulation Time		
Run Description	**10,000 yr**	**100,000 yr**	**1,000,000 yr**
Subareas 3, 4, 5 only	38.2 (7,551)	42.4 (14,500)	41.9 (14,538)
All 10 Subareas[1]	51.3 (10,000)	65.5 (18,550)	65.3 (18,456)[2]
Subarea 3 (lumped)	44.2 (7,551)	57.1 (18,550)	57.1 (18,662)
All 8 Subareas	55.7 (7,551)	81.7 (18,550)	81.5 (18,456)[3]
UZ Steady-State	50.8 (10,000)	63.3 (14,950)	63.1 (14,950)

[1] approximately 50% increase in execution time for 10 Subareas compared with 8 Subareas
[2] UZ NEFTRAN skipped 239 times out of 3,980 total (6%)
[3] UZ NEFTRAN skipped 102 times out of 3,184 total (3%)

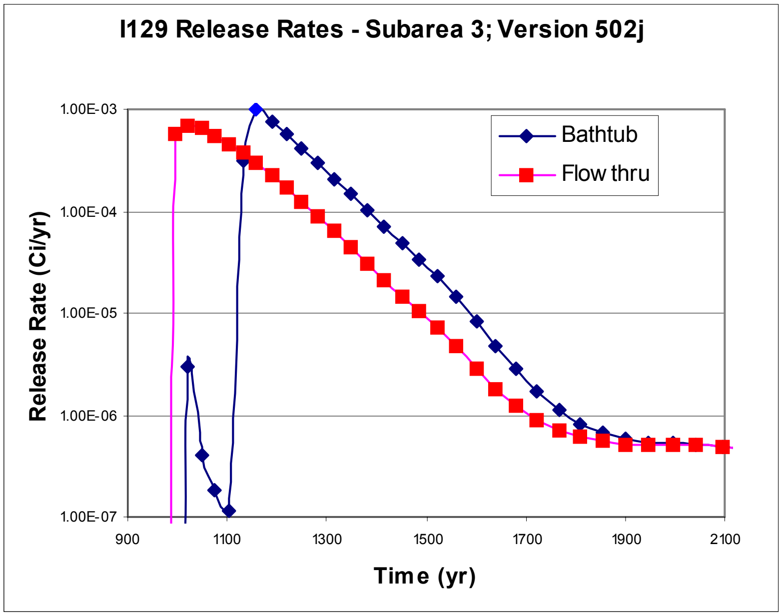
TPA Version 5.0.2
362 realizations
8 Subareas
Maximum Simulation Time = 1,000,000 yr

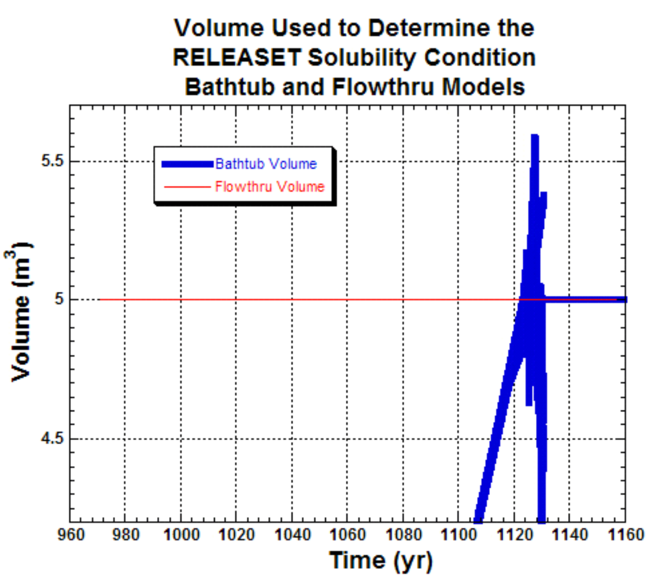
Run Description	**Courant Number (TPMD in yr)**	**PMD in mrem/yr**
Basecase - skip UZ NEFTRAN	0.15	88.3 (9,769)
Basecase - Steady-State [1]	1.5	84.4 (11,856)
Reset Length - no skip UZ NEFTRAN	0.15	75.8 (10,000)
Reset Length - Steady-State	1.5	72.3 (10,206)

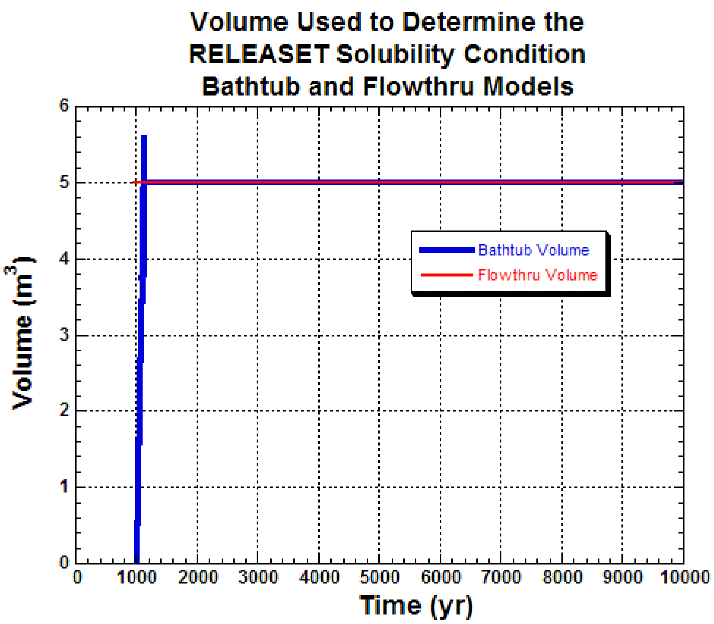
(Note that resetting *gwttmin* at Steady-State to either 0 yr or 5 yr yields an error in reading the NEFTRAN output file in UZFT because the number of rates in *nefii.dis* is greater than 999,999.)

[1] approximately equal execution time with Steady-State compared to the Basecase

3/16/06 - Ran RELEASET in standalone mode for I129 only and high release rates. Plotted the following results from TPA Version 5.0.2j. Investigated high release rates, cladding in versions 4.1 and 5.0, and the volume used in the flow thru and bathtub models to determine solubility-limited releases.







<u>RELEASET variables</u>

The following are variables contained in the cumrel.out file and also the ebsrel.rlt file.

xnoloss [Ci] - for a radionuclide, the number of Curies present in a WP; calculated based in the initial inventory available for release; accounting only for decay/ingrowth; and assuming no EBS release

amwp [Ci] - for a radionuclide, at a time corresponding to the maximum TPA code simulation time, the number of Curies that have accumulated in a WP from SF dissolution, but have not been released from the EBS; (note that this inventory may accumulate because of solubility limits)

xmass [Ci] - for a radionuclide, at a time corresponding to the maximum TPA code simulation time, the cumulative number of Curies that have been released from the EBS; this value may be found be integrating the releases in ebsnef.dat (a RELEASET output file that the TPA code reads) over the entire TPA code simulation time

<u>Others</u>

claddingcorfact - a tpa.inp file parameter (constant equal to 1); this factor has a proportionate affect on amwp, but no impact on xnoloss and a small impact on xmass (less than 0.5%); That is, if the factor is decreased from 1.0 to 0.5, amwp decreases by 50%. This value is included in the RELEASET input file ebsrel.inp.

sawetfrac - a tpa.inp file parameter (uniform from 0 to 1); this factor used to scale the calculated RELEASET values to reflect the inventory available for release; any change in this parameter results in a proportionate change in the three variables described above for the relcum.out file. This value is included in the RELEASET input file ebsrel.inp.

<u>For high release rates and I129 only</u>

In version 4.1jpd, found:
7. Sfwetfraction is proportional to the available inventory
8. Cladding correction factor is proportional to the amount that can be released
(so there appears to be mass balance)

In version 5.0.2j, found:
1. Can change Sfwetfraction and get all mass released (xnoloss changes and can be greater than xmass)
2. Cladding correction factor at 1.0 an 0.5 can give all mass released (i.e., no mass protected from release)
3. Cladding velocity enhancement factor (from 1 to 240) is proportional to the release rate but at extremes can not protect mass from releases

With SCR608 changes in TPA Version 5.0.2f, obtained the following PMD and TPMD:
(450 realizations)

basecase	147 mrem/yr at 7,038 yr
protection	173 mrem/yr at 7,038 yr
basecase	172 mrem/yr at 7,038 yr

3/28/06 - Ran the TPA Version 502o code and obtained the following results.
(note that this version has MECHFAIL, Seepage, and UZFT modifications included)

<u>Basecase</u>
10,000 yr and 460 realizations

Peak mean dose = 12.9 mrem/yr
Time of peak mean dose = 8,293 yr

MECH failed WPs	65/4600 or **1.4% of subarea calculations**
	failure times 996 - 7,380 yr (using seismic intervals)
	# WPs failed = 65,085/56,014,200 = **0.1% of all WPs**
CORR failed WPs	348/4600 or **7.6% of subarea calculations**
	failure times 591 - 2,600 yr
	# WPs failed = 436,040/56,014,200 = **0.8% of all WPs**

3/20/06 - Began to implement through SCR614 the suggested changes to UZFT supplied by T. McCartin. Those changes are provided below.

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
```

Additionally, the following information was prepared and implementation began for this SCR.

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 614	**2. Software Title and Version:** TPA 5.1	**3. Project No:** 20.06002.01.354

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

5. Change Requested by: O. Osidele Date: 11-4-2005	**6. Change Authorized by** (*Software Developer*): Date:

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

* No need to loop over all matrix layers at every time step when checking "highestmatrixfraction" because it will be same matrix layer at all time steps.
* adjust tpatime_infil(itime) proportionally whenever "fracturefraction" GT 0.0 (e.g., multiply by highestmatrixfraction).
*make sure adjusted flux gets carried forward and used toe calculate velocity in neftran run.
* only when a run for a subarea has fracturefraction GT 0, remember what layer that was and force it to be a matrix leg in neftran, regardless of conductivity.

****

* If no UZ layer has travel time greater than 20 years. Find the matrix layer had the highest travel time and reset the thickness so that travel time is equal to 20 years for that layer.

****

* For colloid filtration: more than one option (check with D. Pickett)
    1. we could calculate a composite filtration factor based on all layers with nonzero thickness regardless of whether they are included in the neftran run. But, if some layers are not present, composite values may not be applicable.
    2. (Recommended) we could just take the filtration factor for the nonzero thickness layer that had the highest value. In this case filtration factors need to be specific to each layer, not dependent on the filtration in the preceding layer.

****

Miscellaneous:
* Get rid of line of code that set Chnv thickness to zero if a value less than 2m is sampled.
* Reformat output from neftran to have more precision in output times (currently only 4 significant figures).
* Add check for UZ layers with zero thickness so they are not used in flux splitting or colloid filtration.

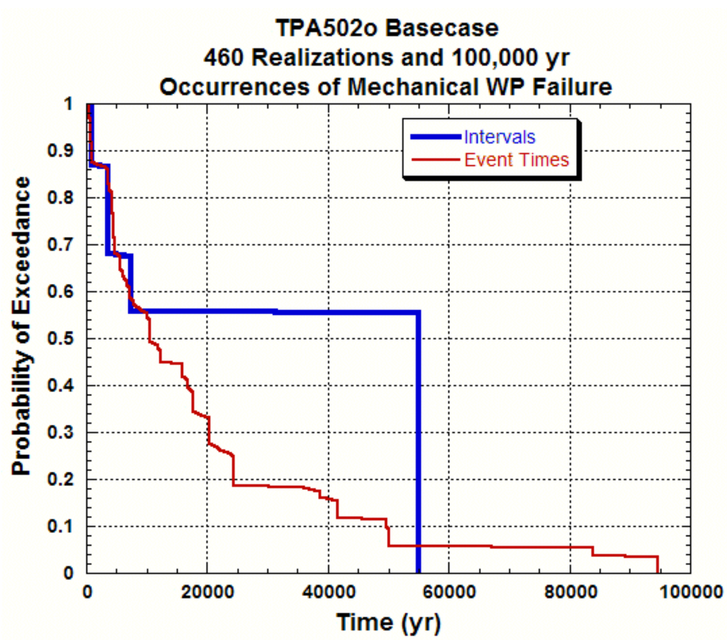
8. Implemented by:	**Date:**
9. Description of Acceptance Tests:	
10. Tested by:	**Date:**

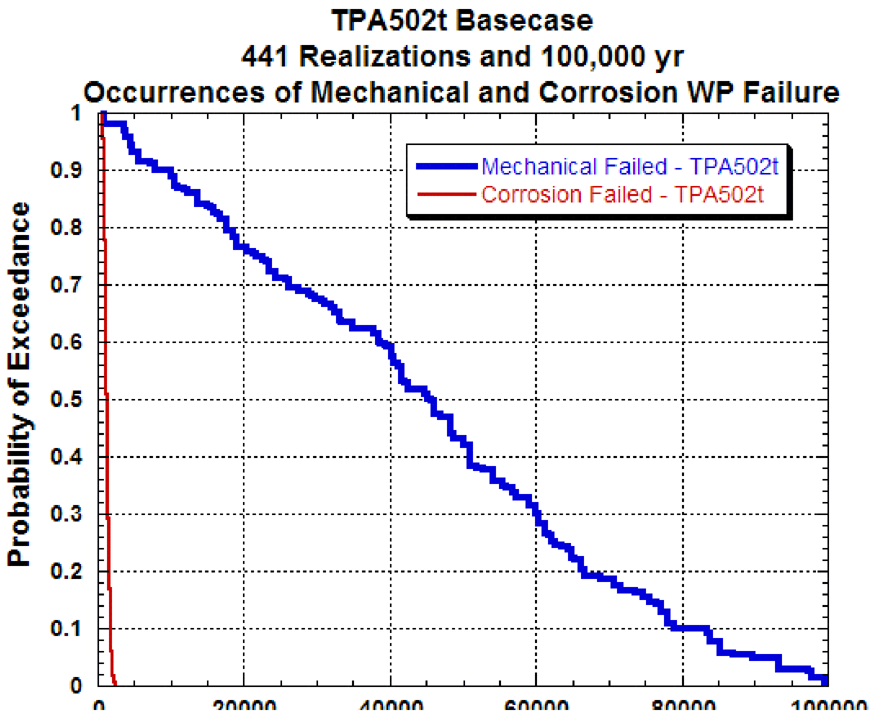
CNWRA Form TOP-5 (05/2000)

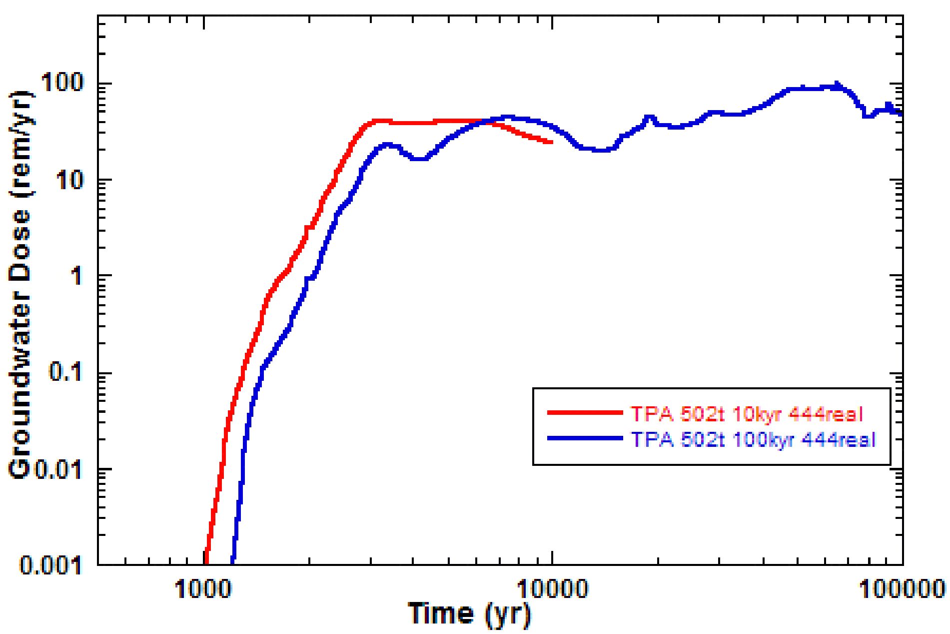
3/29/06 - Performed TPA Version 502o runs and plotted the results for number of failed WPs. See the following plot.

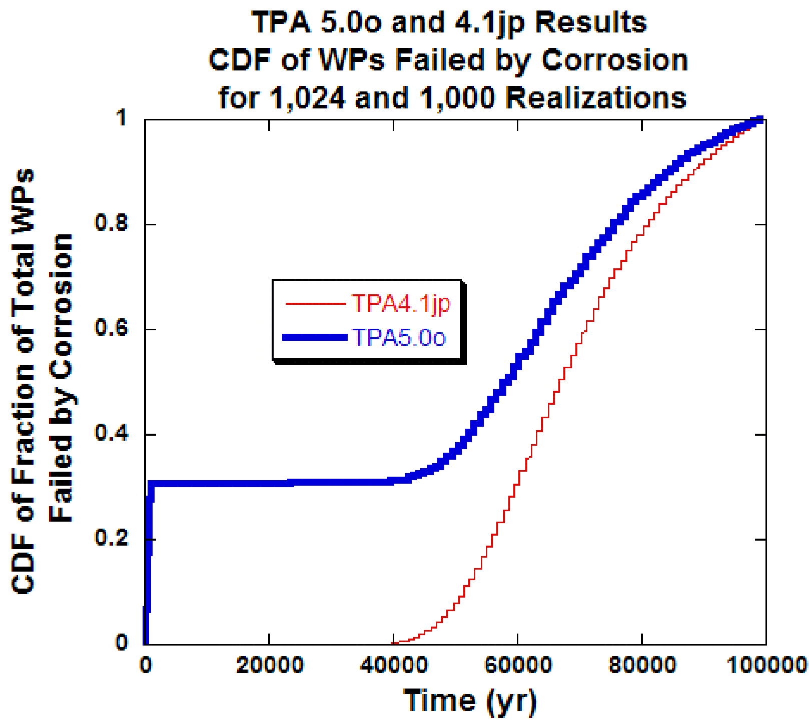
		TPA502t 441real		WP failures					
				number	total		number	total	
		min time	max time	sa calcs	sa calcs	%	WPs	WPs	% WPs
1e5 yr	Corrosion	658	2,602	237	4410	5.4%	286,154	5,370,057	5.3%
1e5yr	Mechanical	791	100,000	484	4410	11.0%	582,565	5,370,057	10.8%

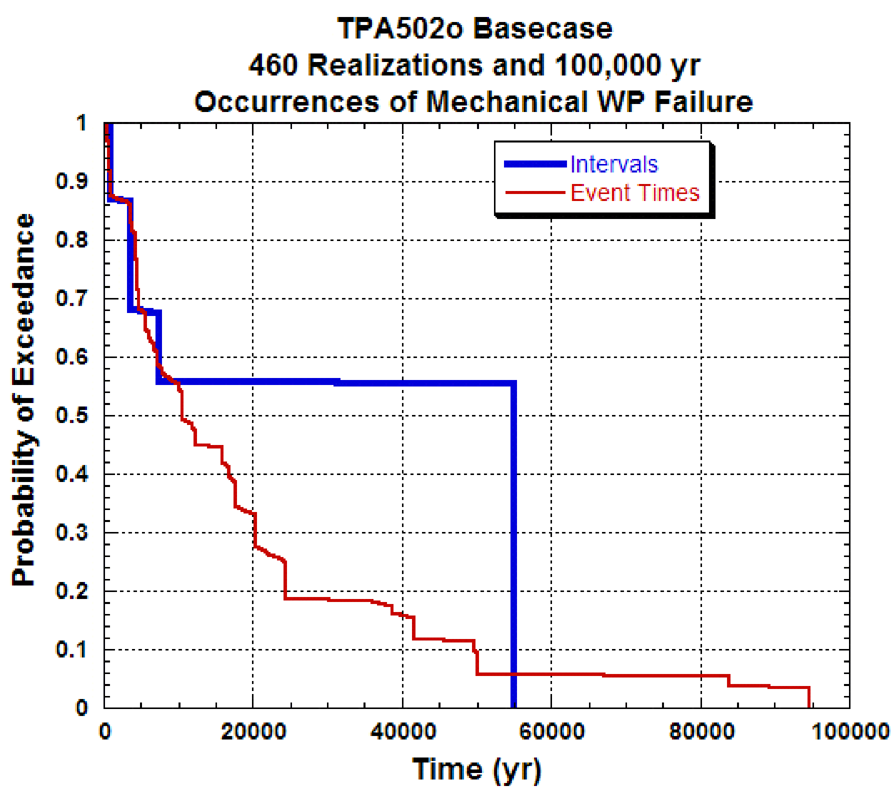
4/10/06 - Analyzed TPA Version 502t code output files and other TPA code results to examine dose and the number of WP failures by corrosion and mechanical processes. The results are summarized below in a table and plots.



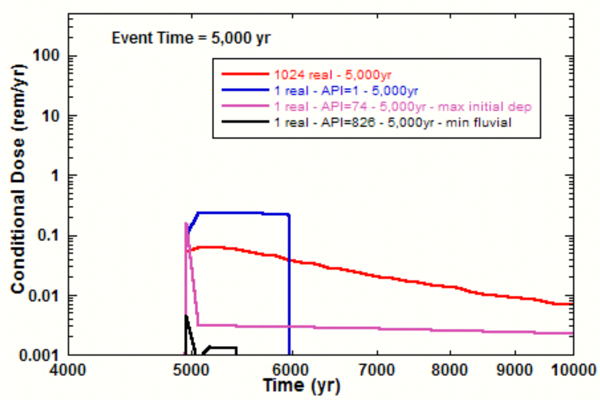

TPA502t Basecase
441 Realizations and 100,000 yr
Occurrences of Mechanical and Corrosion WP Failure
Probability of Exceedance
Mechanical Failed - TPA502t
Corrosion Failed - TPA502t
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
20000
40000
60000
80000
100000

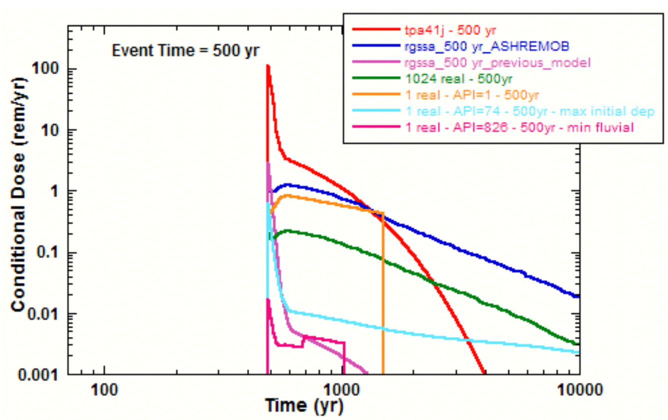

Groundwater Dose (rem/yr)
Time (yr)
TPA 502t 10kyr 444real
TPA 502t 100kyr 444real
0.001
0.01
0.1
1
10
100
1000
10000
100000

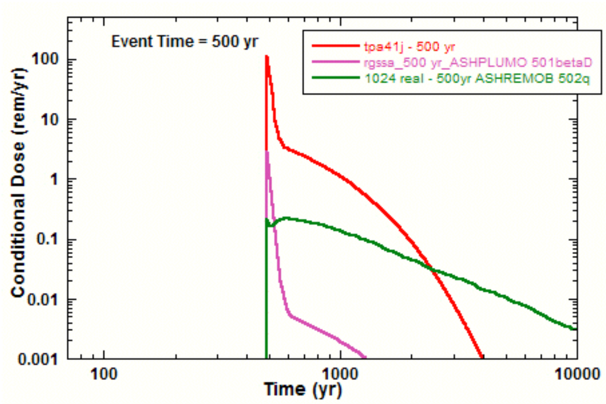

TPA 5.0o and 4.1jp Results
CDF of WPs Failed by Corrosion
for 1,024 and 1,000 Realizations
CDF of Fraction of Total WPs
Failed by Corrosion
TPA4.1jp
TPA5.0o
Time (yr)
0
0.2
0.4
0.6
0.8
1
0
20000
40000
60000
80000
100000

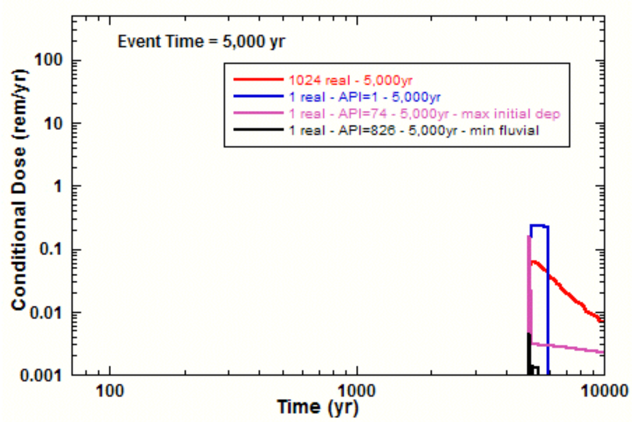

TPA502o Basecase
460 Realizations and 100,000 yr
Occurrences of Mechanical WP Failure
Probability of Exceedance
Intervals
Event Times
Time (yr)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
20000
40000
60000
80000
100000

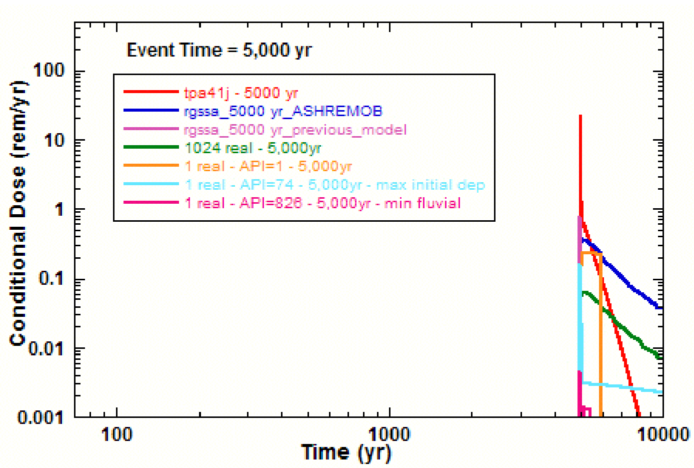
4/11/06 - Prepared plots of results associated with the ASHREMOB model. These plots are provided below.

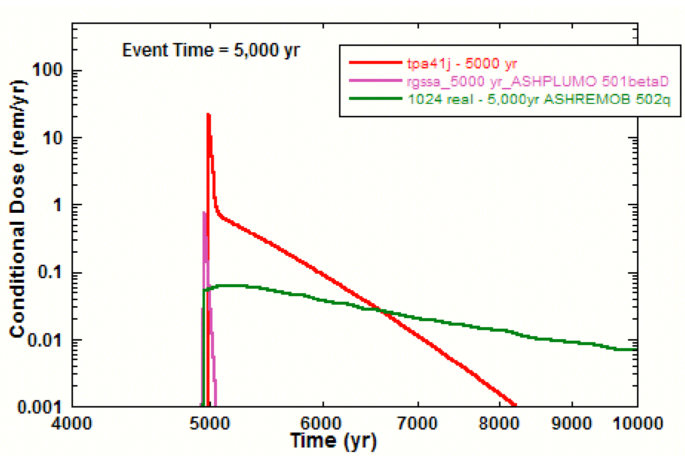


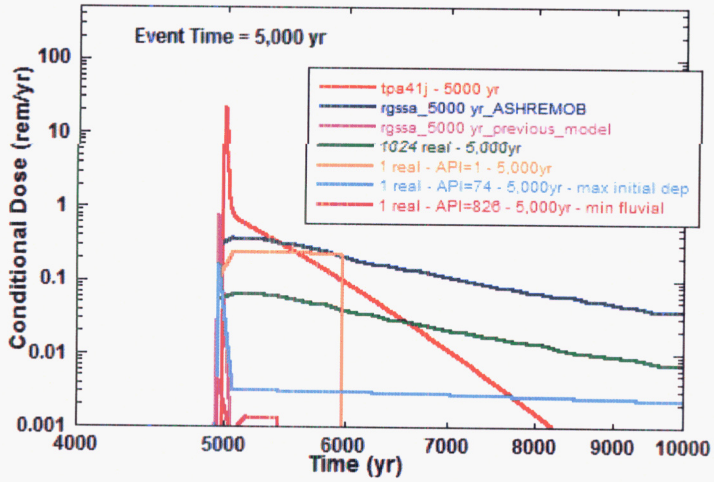


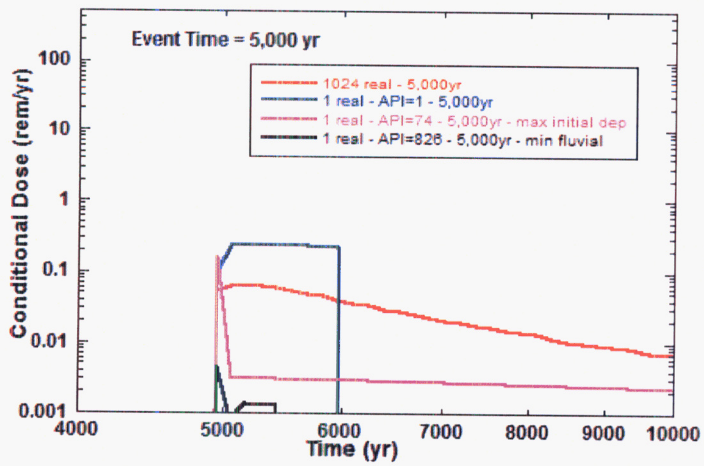



Event Time = 5,000 yr
1024 real - 5,000yr
1 real - API=1 - 5,000yr
1 real - API=74 - 5,000yr - max initial dep
1 real - API=826 - 5,000yr - min fluvial
Conditional Dose (rem/yr)
Time (yr)


Event Time = 5,000 yr
tpa41j - 5000 yr
rgssa_5000 yr_ASHREMOB
rgssa_5000 yr_previous_model
1024 real - 5,000yr
1 real - API=1 - 5,000yr
1 real - API=74 - 5,000yr - max initial dep
1 real - API=826 - 5,000yr - min fluvial
Conditional Dose (rem/yr)
Time (yr)


Event Time = 5,000 yr
tpa41j - 5000 yr
rgssa_5000 yr_ASHPLUMO 501betaD
1024 real - 5,000yr ASHREMOB 502q
Conditional Dose (rem/yr)
Time (yr)





5/18/06 - Performed and completed TPA code simulations to investigate the impacts of the WP internal volume on results. The following table summarizes the results for 10,000 years.

TPA51betaA - 445 realizations (WP Internal Volume is sampled paramete

Peak Mean Dose (mrem/yr) and Time of Peak Mean Dose (yr)

	10,000 yr simulation time		
Scenario	**SF and Glass**	**SF only**	**Glass Only**
Basecase	33.4 @ 10,000	32.0 @10,000	2.0 @10,000
Min WP Int Vol (~ 0 m3)	56.5 @ 3,466	49.2 @ 3,635	8.8 @3,151
Max WP Int Vol (~11 m3)	26.1 @ 10,000	25.2 @ 10,000	1.6 @ 3,227
Sampled WP Int Vol (uniform 0 - 11 m3)	33.0 @ 10,000	31.7 @ 10,000	2.4 @ 3,305

7/13/06 - Performed and completed TPA code simulations to investigate the impacts of the water contact mode and the WP temperature on results. The following email, which summarizes the results, was sent to the Center staff.

Hello.

Osvaldo asked me to do some scoping analyses
for two cases:

(1) water does not enter the WP, if the WP temperature
is above boiling (specified at 97 deg C in the tpa.inp file)

(2) make all water contact modes flow-thru

The first required TPA code modifications to "ebsrel.f" and the
second required a data change in the " tpa.inp" file.

I performed TPA code runs with these changes and also with
the basecase, for comparison purposes. The results follow:

TPA Version 5.1betaC
500 realizations

(the peak mean dose and time of the peak mean dose are listed)

```
                         TPA code Simulation Time
Scenario                     10,000 yr           100,000 yr
*******                   *******           ********
```

Basecase	21.6 mrem/yr at 2,363 yr	28.7 mrem/yr at 18,550 yr
No flow into WP if WP temp is >= Tboil	17.0 mrem/yr at 3,076 yr	28.3 mrem/yr at 18,550 yr
Flow-thru only	21.5 mrem/yr at 2,363 yr	26.5 mrem/yr at 64,900 yr

These runs are available in subdirectories on GOLDSIM in "rrice\Scope_betaC\tpa51betaC\run\500real".

Please contact me if you have any questions.

Thanks,

Rob

9/18/06 - Performed and completed TPA Version 51betaD code (with SCR658) simulations to investigate the system behavior of the TPA code.. The following email and plots/tables, which summarizes the results, was sent to the Center staff.

Subj: Sampled Parameters Contributing to Peak Mean GW Dose
Date: 9/18/2006
To: jwinterle@cnwra.swri.edu, opensado@cnwra.swri.edu, rjanetzke@cnwra.swri.edu, oosidele@cnwra.swri.org, jmancillas@cnwra.swri.edu, smohanty@cnwra.swri.edu
CC: rwrice@aol.com
File:
C:\SRT_Inc\SWRI\TPA51betaD_results\results\readsp\parameter_ranking\summary_results.pdf (1977557 bytes) DL Time (32000 bps): < 17 minutes

Hello.

I have finished putting together a ranking of sampled parameters from 13 separate multiple realization TPA51betaD (with SCR658) executions over 10,000 yrs.

These parameters were identified by ranking the correlation between the values

of a parameter and the peak mean GW doses for a particular TPA code execution
and then averaging those ranks and also finding the median rank over the 13 executions.

It was interesting that 7 parameters standout when looking at the average rank. These parameters are:

1 Preexponential_SFDissolutionModel2
2 SubAreaWetFraction
3 AA_1_1[C/m2/yr]
4 ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
5 KD_Soil_Tc[cm3/g]
6 MatrixPermeability_TSw_[m2]
7 PlantUptakeScaleFactor

For the median rank, these same seven parameters, in addition to "EnvironmentII_pH_Subarea_3[]",
standout apart from the other 490 or so parameters.

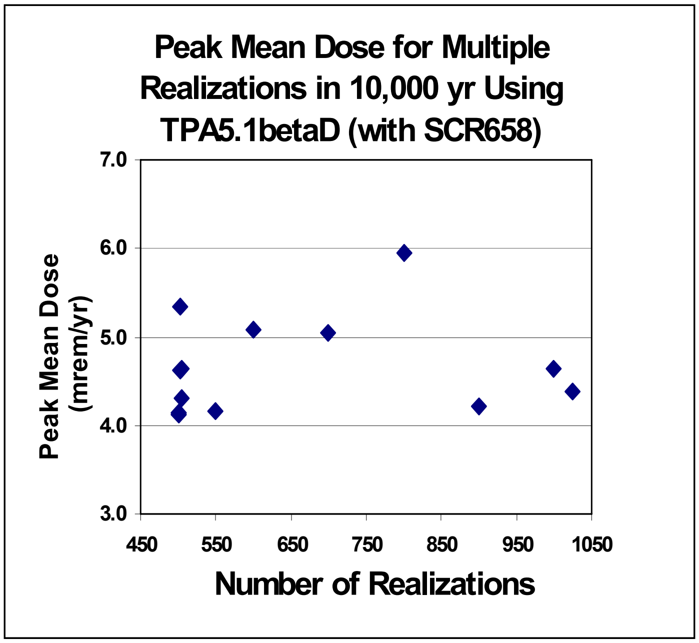
I have more detailed information and have provided a summary of 10,000 yr results in the file
attachment (I have sent some of these results to you previously).

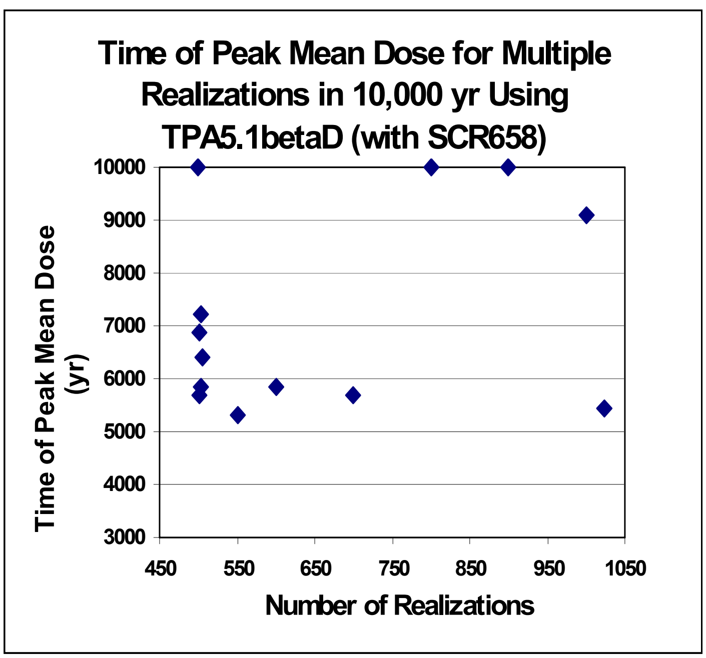
I am currently also preparing the same kind of plots/results for 13 100,000 yr simulations.

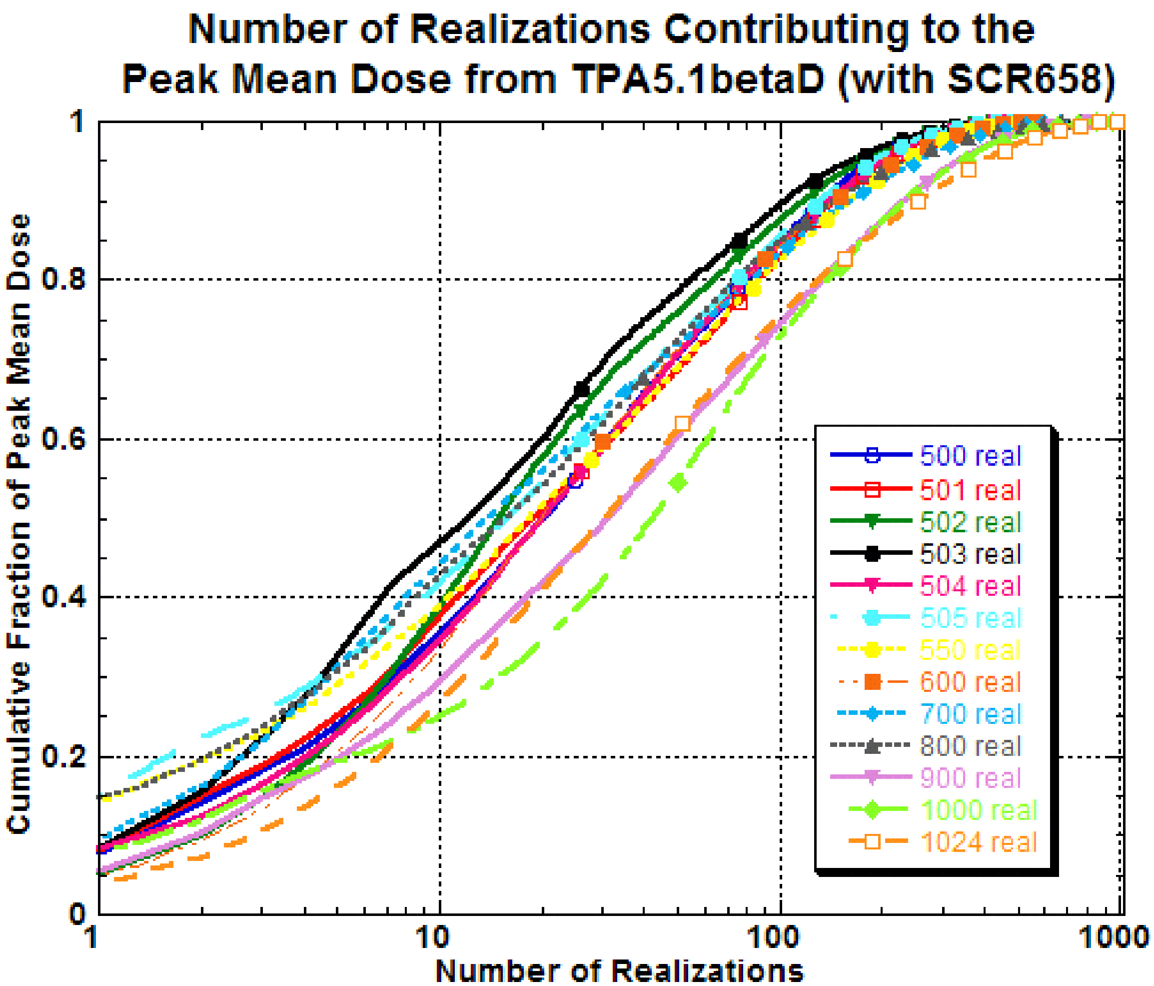
Please contact me if you have any questions.

Thanks,

Rob


Peak Mean Dose for Multiple Realizations in 10,000 yr Using TPA5.1betaD (with SCR658)
Peak Mean Dose (mrem/yr)
7.0
6.0
5.0
4.0
3.0
450
550
650
750
850
950
1050
Number of Realizations

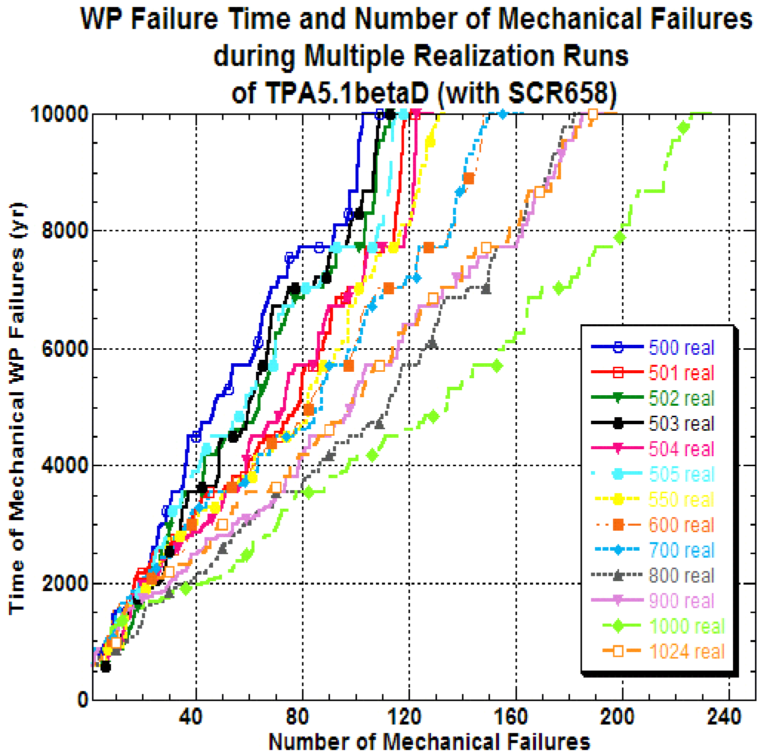

Time of Peak Mean Dose for Multiple Realizations in 10,000 yr Using TPA5.1betaD (with SCR658)
Time of Peak Mean Dose (yr)
10000
9000
8000
7000
6000
5000
4000
3000
450
550
650
750
850
950
1050
Number of Realizations

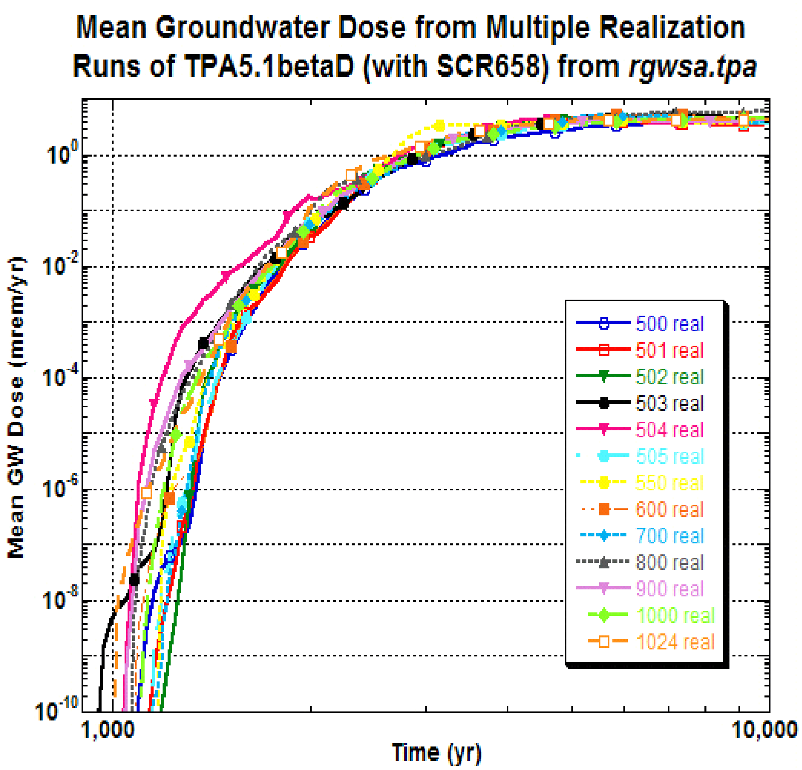

Number of Realizations Contributing to the
Peak Mean Dose from TPA5.1betaD (with SCR658)
Cumulative Fraction of Peak Mean Dose
Number of Realizations
0
0.2
0.4
0.6
0.8
1
1
10
100
1000
500 real
501 real
502 real
503 real
504 real
505 real
550 real
600 real
700 real
800 real
900 real
1000 real
1024 real

TPA Version 5.1betaD - Basecase (with SCR658 included)

Maximum Time = 10,000 yr

Realizations	% WPs Mechanically Failed	% Subarea Calculations with Mechanically Failed WPs	Mechanical Failure Times Minimum (yr)	Mechanical Failure Times Maximum (yr)	Mechanical Failure Times Average (yr)
500	2.00	2.28	575	10,000	5,590
501	2.14	2.55	575	10,000	4,820
502	1.95	2.35	575	10,000	5,060
503	1.98	2.35	575	10,000	5,150
504	2.16	2.56	575	10,000	4,720
505	2.10	2.46	575	10,000	5,350
550	1.82	2.44	575	10,000	4,690
600	2.22	2.48	575	10,000	4,880
700	2.10	2.33	575	10,000	5,310
800	1.99	2.48	575	10,000	5,000
900	1.87	2.18	575	10,000	5,230
1000	1.76	2.34	854	10,000	4,900
1024	1.55	1.93	575	10,000	5,340


WP Failure Time and Number of Mechanical Failures
during Multiple Realization Runs
of TPA5.1betaD (with SCR658)
Time of Mechanical WP Failures (yr)
Number of Mechanical Failures
0
2000
4000
6000
8000
10000
40
80
120
160
200
240
500 real
501 real
502 real
503 real
504 real
505 real
550 real
600 real
700 real
800 real
900 real
1000 real
1024 real

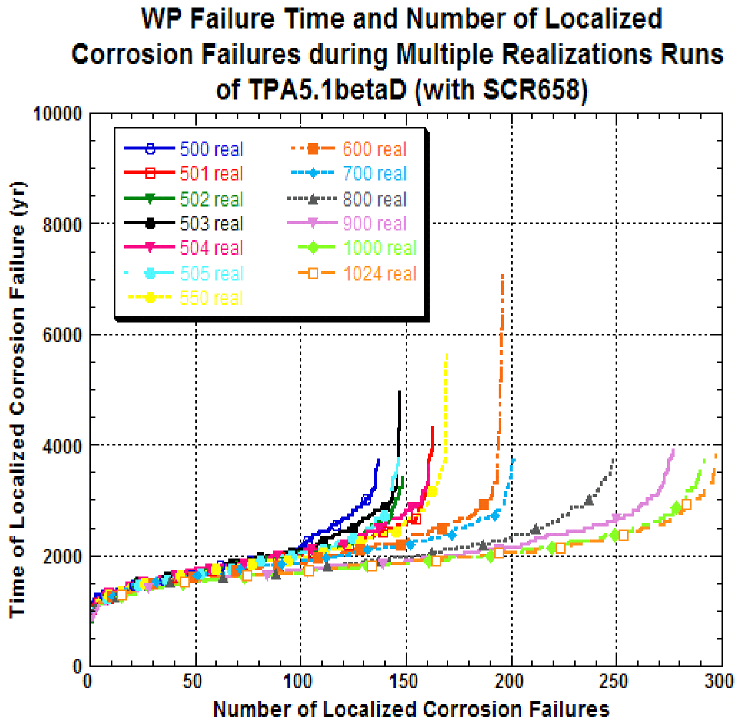

Mean Groundwater Dose from Multiple Realization
Runs of TPA5.1betaD (with SCR658) from rgwsa.tpa
Mean GW Dose (mrem/yr)
Time (yr)
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
1,000
10,000
500 real
501 real
502 real
503 real
504 real
505 real
550 real
600 real
700 real
800 real
900 real
1000 real
1024 real

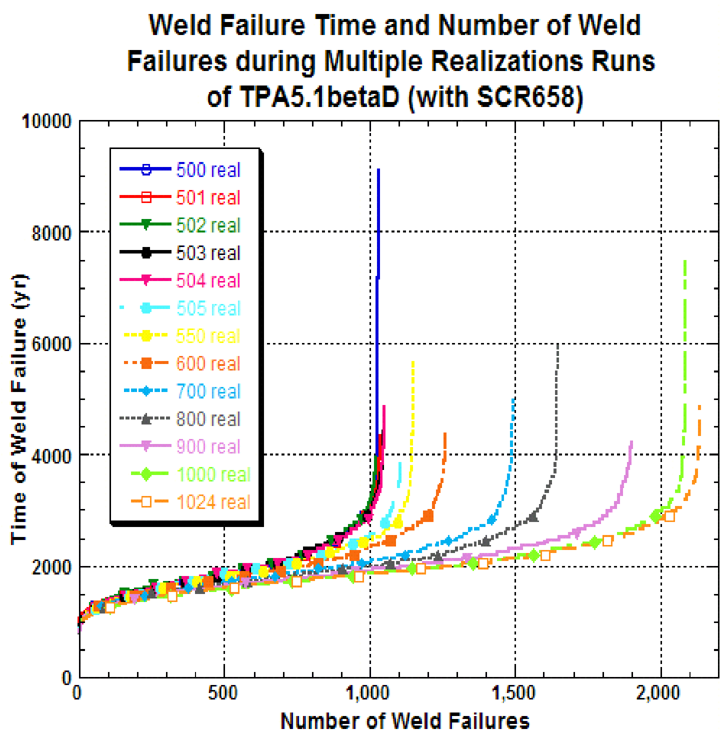
time of localized corrosion failure

	# real												
	500	501	502	503	504	505	550	600	700	800	900	1000	1024
min	**1,103**	**1,075**	**791**	**971**	**923**	**854**	**996**	**971**	**877**	**996**	**811**	**900**	**923**
max	**3,722**	**4,291**	**3,384**	**4,945**	**3,635**	**3,812**	**5,696**	**7,038**	**3,722**	**3,812**	**3,903**	**3,722**	**3,812**
ave	**1,949**	**1,947**	**1,889**	**1,973**	**1,983**	**1,897**	**1,987**	**1,986**	**1,953**	**1,947**	**1,956**	**1,918**	**1,928**
count	137	163	149	147	161	147	170	196	202	249	277	292	297
frequency	**2.74%**	**3.25%**	**2.97%**	**2.92%**	**3.19%**	**2.91%**	**3.09%**	**3.27%**	**2.89%**	**3.11%**	**3.08%**	**2.92%**	**2.90%**

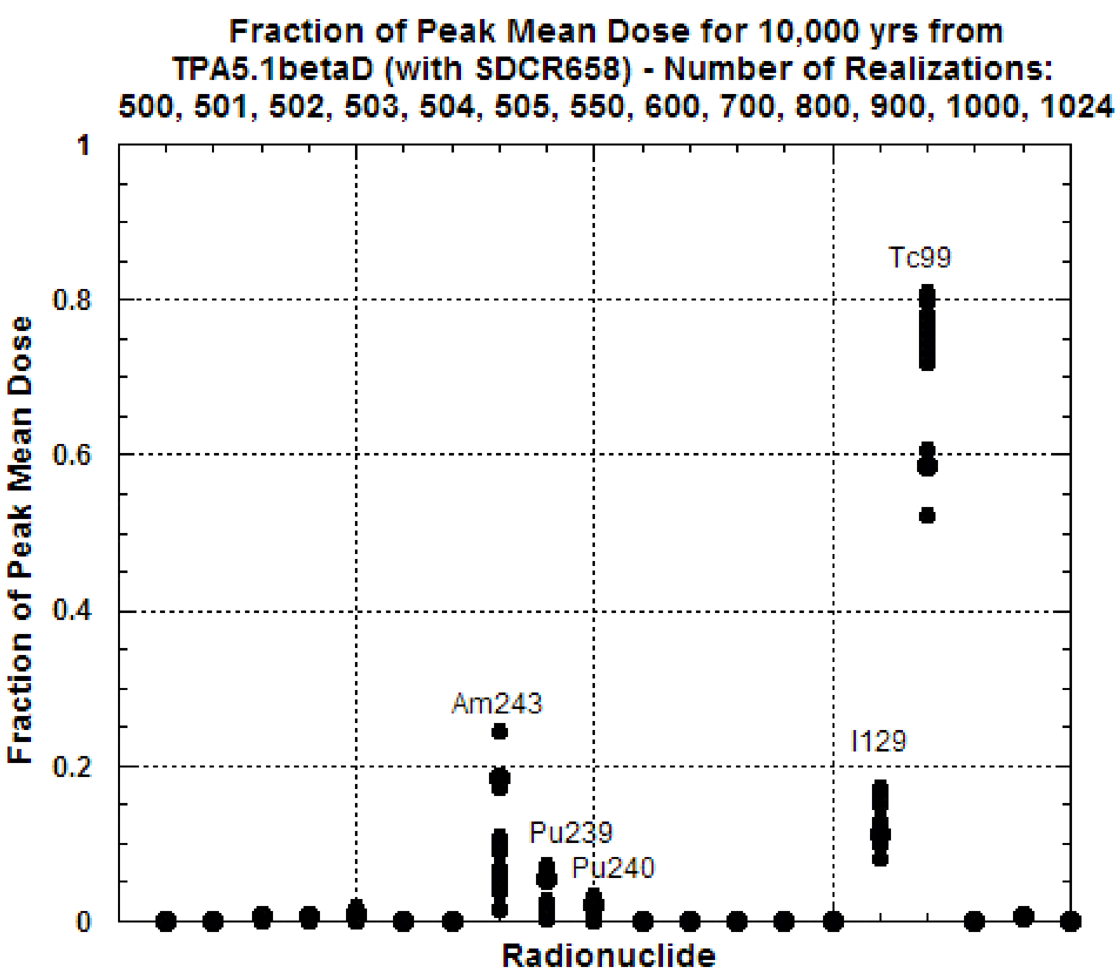
time of weld failure

	# real												
	500	501	502	503	504	505	550	600	700	800	900	1000	1024
min	**840**	**968**	**782**	**902**	**860**	**860**	**860**	**881**	**880**	**782**	**820**	**801**	**801**
max	**9,089**	**4,320**	**3,935**	**4,421**	**4,851**	**3,846**	**5,708**	**4,420**	**4,964**	**5,948**	**4,219**	**7,461**	**4,850**
ave	**1,960**	**1,957**	**1,956**	**1,967**	**1,964**	**1,936**	**1,950**	**1,963**	**1,953**	**1,961**	**1,964**	**1,950**	**1,967**
count	1029	1037	1021	1045	1049	1107	1150	1261	1491	1646	1902	2085	2138
frequency	**20.58%**	**20.70%**	**20.34%**	**20.78%**	**20.81%**	**21.92%**	**20.91%**	**21.02%**	**21.30%**	**20.58%**	**21.13%**	**20.85%**	**20.88%**


WP Failure Time and Number of Localized Corrosion Failures during Multiple Realizations Runs of TPA5.1betaD (with SCR658)
Time of Localized Corrosion Failure (yr)
Number of Localized Corrosion Failures
500 real
501 real
502 real
503 real
504 real
505 real
550 real
600 real
700 real
800 real
900 real
1000 real
1024 real
0
2000
4000
6000
8000
10000
0
50
100
150
200
250
300


Weld Failure Time and Number of Weld Failures during Multiple Realizations Runs of TPA5.1betaD (with SCR658)
Time of Weld Failure (yr)
Number of Weld Failures
500 real
501 real
502 real
503 real
504 real
505 real
550 real
600 real
700 real
800 real
900 real
1000 real
1024 real
0
2000
4000
6000
8000
10000
0
500
1,000
1,500
2,000

					Percent Contribution to the Peak Mean Dose for 10,000 yr													
					Number of Realizations													
	500	**501**	**502**	**503**	**504**	**505**	**550**	**600**	**700**	**800**	**900**	**1000**	**1024**		Min	Max	**Average**	
Cm246	0.0970%	0.0151%	0.0555%	0.0830%	0.0704%	0.0646%	0.0357%	0.0659%	0.0244%	0.1195%	0.1236%	0.1354%	0.0213%		0.02%	0.14%	**0.07%**	**Cm246**
U238	0.0090%	0.0023%	0.0032%	0.0056%	0.0046%	0.0032%	0.0025%	0.0022%	0.0042%	0.0110%	0.0220%	0.0094%	0.0014%		0.00%	0.02%	**0.01%**	**U238**
Cm245	0.5682%	0.0673%	0.2643%	0.4075%	0.3253%	0.3013%	0.1551%	0.3050%	0.1087%	0.7041%	0.7245%	0.7496%	0.0930%		0.07%	0.75%	**0.37%**	**Cm245**
Am241	0.5488%	0.0972%	0.2947%	0.4206%	0.4346%	0.3401%	0.3956%	0.3857%	0.1531%	0.7007%	0.6890%	0.7582%	0.2330%		0.10%	0.76%	**0.42%**	**Am241**
Np237	0.0704%	0.0069%	0.0065%	0.3421%	0.0393%	0.0499%	0.0027%	0.0066%	0.0053%	1.8988%	0.9992%	1.0520%	0.0069%		0.00%	1.90%	**0.35%**	**Np237**
U233	0.0650%	0.0166%	0.0200%	0.0379%	0.0106%	0.0126%	0.0106%	0.0228%	0.0094%	0.0676%	0.0786%	0.0864%	0.0188%		0.01%	0.09%	**0.04%**	**U233**
Th229	0.0001%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0001%	0.0001%	0.0000%		0.00%	0.00%	**0.00%**	**Th229**
Am243	10.1304%	1.6711%	9.1649%	11.0291%	6.5535%	6.9518%	4.9624%	6.0997%	1.8697%	24.5337%	17.2605%	18.3183%	3.8151%		1.67%	24.53%	**9.41%**	**Am243**
Pu239	2.6112%	0.3085%	2.4700%	1.8151%	0.8784%	1.5259%	0.8774%	0.8756%	0.3585%	7.1921%	6.2034%	5.5948%	0.9526%		0.31%	7.19%	**2.44%**	**Pu239**
Pu240	0.6891%	0.1295%	1.2761%	0.6748%	0.1945%	1.0202%	0.4435%	0.3306%	0.2278%	3.1927%	2.0954%	2.2466%	0.7699%		0.13%	3.19%	**1.02%**	**Pu240**
U234	0.0331%	0.0084%	0.0117%	0.0206%	0.0170%	0.0113%	0.0091%	0.0080%	0.0154%	0.0417%	0.0819%	0.0343%	0.0051%		0.01%	0.08%	**0.02%**	**U234**
Th230	0.0759%	0.0121%	0.0485%	0.1651%	0.0681%	0.0383%	0.0111%	0.1053%	0.0100%	0.3193%	0.2048%	0.1521%	0.0180%		0.01%	0.32%	**0.09%**	**Th230**
Ra226	0.0001%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0005%	0.0004%	0.0000%	0.0000%		0.00%	0.00%	**0.00%**	**Ra226**
Pb210	0.0002%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0012%	0.0006%	0.0000%	0.0000%		0.00%	0.00%	**0.00%**	**Pb210**
Cs135	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%		0.00%	0.00%	**0.00%**	**Cs135**
I129	12.1855%	17.1235%	11.3965%	11.2908%	15.7562%	12.9350%	15.1269%	15.8986%	15.3898%	8.1499%	10.0627%	11.2545%	15.1235%		8.15%	17.12%	**13.21%**	**I129**
Tc99	72.0490%	79.6669%	74.0989%	72.9044%	74.8304%	75.9745%	77.1929%	74.9675%	81.0091%	52.4281%	60.6131%	58.7567%	78.1306%		52.43%	81.01%	**71.74%**	**Tc99**
Ni59	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%		0.00%	0.00%	**0.00%**	**Ni59**
Se79	0.7036%	0.6728%	0.7215%	0.6580%	0.6368%	0.6069%	0.5730%	0.7300%	0.6199%	0.5209%	0.6937%	0.7107%	0.6191%		0.52%	0.73%	**0.65%**	**Se79**
Nb94	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%	0.0000%		0.00%	0.00%	**0.00%**	**Nb94**
Cl36	0.1637%	0.2018%	0.1677%	0.1452%	0.1803%	0.1644%	0.2016%	0.1966%	0.1947%	0.1183%	0.1463%	0.1408%	0.1917%		0.12%	0.20%	**0.17%**	**Cl36**



Average ranks over 13 TPA5.1betaD (with SCR658) executions for 10,000 years (500, 501, 502, 503, 504, 505, 550, 600, 700, 800, 900, 1000, and 1024 realizations)		Rank (average)		Median ranks over 13 TPA5.1betaD (with SCR658) executions for 10,000 years (500, 501, 502, 503, 504, 505, 550, 600, 700, 800, 900, 1000, and 1024 realizations)	
	Sampled Parameter Name				Sampled Parameter Name
1	Preexponential_SFDissolutionModel2	1.85		1	Preexponential_SFDissolutionModel2
2	SubAreaWetFraction	2.00		2	SubAreaWetFraction
3	AA_1_1[C/m2/yr]	4.77		3	AA_1_1[C/m2/yr]
4	ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]	5.23		4	ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
5	KD_Soil_Tc[cm3/g]	9.92		5	KD_Soil_Tc[cm3/g]
6	MatrixPermeability_TSw_[m2]	16.15		6	PlantUptakeScaleFactor
7	PlantUptakeScaleFactor	19.69		7	EnvironmentII_pH_Subarea_3[]
8	EnvironmentII_pH_Subarea_3[]	67.77		8	MatrixPermeability_TSw_[m2]
9	EnvironmentII_CO3_Subarea_3[mol/L]	69.08		9	WeldAdvectiveFraction[]
10	WeldAdvectiveFraction[]	77.15		10	EnvironmentII_CO3_Subarea_3[mol/L]
11	OuterOverpackErpIntercept	111.77		11	InitialRadiusOfSFParticle[m]
12	InitialSeepageReductionFractionByMechFailedDS	116.77		12	OuterOverpackErpIntercept
13	InitialRadiusOfSFParticle[m]	125.69		13	MeanAnnualPrecipitationMultiplierAtGlacialMaximum
14	SFWettedFraction_SEISMO1_5	132.46		14	MatrixColloidRetardationFactor_PPw_[]
15	CladdingVelocityEnhancementFactor[]	134.15		15	CladdingVelocityEnhancementFactor[]
16	EnvironmentII_pH_Subarea_10[]	135.77		16	InitialSeepageReductionFractionByMechFailedDS
17	MatrixColloidRetardationFactor_PPw_[]	137.46		17	EnvironmentII_Cl_Subarea_3[mol/L]
18	SeepageThresholdT[C]	138.54		18	SeepageThresholdT[C]
19	MeanAnnualPrecipitationMultiplierAtGlacialMaximum	152.46		19	EnvironmentII_pH_Subarea_10[]
20	EnvironmentII_SO4_Subarea_8[mol/L]	152.92		20	EnvironmentII_NO3_Subarea_2[mol/L]
21	FractureColloidRetardationFactor_CHnv[]	156.69		21	SFWettedFraction_SEISMO1_5
22	EnvironmentII_FI_Subarea_6[mol/L]	158.15		22	SFWettedFraction_SEISMO3_7
23	SorptionCapacity[moles/m3]	159.77		23	SorptionCapacity[moles/m3]
24	KdOfSeleniumInVolcanicAsh[cm3/g]	163.85		24	HenFeedIrrigationTimePB[mo/yr]
25	DefectiveFractionOfWPs/cell	168.69		25	KdOfSeleniumInVolcanicAsh[cm3/g]

Ordered listed of TPA51betaD (with SCR658) parameters having the largest linear correlation with peak GW dose for 10,000 years
(average rank for 500, 501, 502, 503, 504, 505, 550, 600, 700, 800, 900, 1000, and 1024 realizations)

1 Preexponential_SFDissolutionModel2
2 SubAreaWetFraction
3 AA_1_1[C/m2/yr]
4 ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
5 KD_Soil_Tc[cm3/g]
6 MatrixPermeability_TSw_[m2]
7 PlantUptakeScaleFactor
8 EnvironmentII_pH_Subarea_3[]

There are no additional entries by Robert W. Rice into this Scientific Notebook for the period from 10/1/06 through 3/8/07.

There are no additional entries by Robert W. Rice into this Scientific Notebook for the period from 3/8/07 through 9/17/07.

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

______________________ 1/29/10

Jim Winterle
Manager, PA Group