SCIENTIFIC NOTEBOOK

170-8E

SCIENTIFIC NOTEBOOK NO. 170-8E

by

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10/12/98

Debugged PC vs.UNIX output differences (see *d:\from_bscr1* for these runs).

10/21/98

Modified the data_use FORTRAN program which read the tpa code **.res* files and generates **.plt* which can be used by the java plotting (see the ~rrice/mario directory for the latest *data_use.f* source code) - the code now writes only times when a WP failure occurs to the *wpsfail.plt* files for the histogram.

10/26/98

Modified and tested the FORTRAN code that generates the **.plt* files for the JAVA program that plots **.res* files from a TPA run (see these files in ~rrice/mario).

10/27/98

Prepared QA documentation for the PC version, parallel processing, and post-processing programs (see the SRDs for these programs).

10/29/98

Determined coordinates for the nfenv 12 rectangular regions based on the subarea coordinates defined in the *tpa.inp* file. The old coordinates in the *rectedge.dat* file were as follows:

```
TITLE="CNWRA - Composite areas."
 VARIABLES=easting,northing
 ZONE T="  1",F=POINT
     548367.4     4076234.2
     548457.0     4076506.6
     547649.7     4076772.4
     547560.0     4076500.0
     548367.4     4076234.2
 ZONE T="  2",F=POINT
     548468.9     4076501.1
     548578.6     4076834.4
     547609.7     4077153.3
```

```
    547500.0     4076820.0
    548468.9     4076501.1
ZONE T=" 3",F=POINT
    548444.8     4076876.1
    548565.3     4077241.9
    547520.4     4077585.8
    547400.0     4077220.0
    548444.8     4076876.1
ZONE T=" 4",F=POINT
    548489.8     4077264.8
    548605.4     4077615.8
    547465.5     4077991.0
    547350.0     4077640.0
    548489.8     4077264.8
ZONE T=" 5",F=POINT
    548514.8     4077643.5
    548622.0     4077969.0
    547387.1     4078375.5
    547280.0     4078050.0
    548514.8     4077643.5
ZONE T=" 6",F=POINT
    548544.8     4077993.5
    548652.9     4078321.9
    547418.1     4078728.3
    547310.0     4078400.0
    548544.8     4077993.5
ZONE T=" 7",F=POINT
    548537.3     4078359.2
    548646.4     4078690.4
    547459.0     4079081.2
    547350.0     4078750.0
    548537.3     4078359.2
ZONE T=" 8",F=POINT
    548539.8     4078724.8
    548638.7     4079025.1
    547498.9     4079400.3
    547400.0     4079100.0
    548539.8     4078724.8
ZONE T=" 9",F=POINT
    548544.8     4079056.1
```

```
    548624.9    4079299.2
    547580.0    4079643.2
    547500.0    4079400.0
    548544.8    4079056.1
ZONE T=" 10",F=POINT
    548587.4    4079311.7
    548639.8    4079470.9
    547642.4    4079799.2
    547590.0    4079640.0
    548587.4    4079311.7
ZONE T=" 11",F=POINT
    548589.9    4079487.3
    548649.2    4079667.5
    547699.3    4079980.2
    547640.0    4079800.0
    548589.9    4079487.3
ZONE T=" 12",F=POINT
    548649.9    4079667.3
    548705.1    4079835.2
    547755.3    4080147.9
    547700.0    4079980.0
    548649.9    4079667.3
```

The new coordinates are:

```
TITLE="CNWRA - Composite areas." - (modified 10/29/98 rwr)
 VARIABLES=easting,northing
 ZONE T="  1",F=POINT
    548360.1    4076229.3
    548449.6    4076514.9
    547663.0    4076754.8
    547580.8    4076468.7
    548360.1    4076229.3
 ZONE T="  2",F=POINT
    548433.7    4076521.1
    548524.6    4076810.6
    547581.7    4077100.5
    547491.8    4076810.1
    548433.7    4076521.1
```

```
ZONE T=" 3",F=POINT
    548461.1    4076830.3
    548550.1    4077122.1
    547496.6    4077441.4
    547407.7    4077154.8
    548461.1    4076830.3
ZONE T=" 4",F=POINT
    548477.5    4077144.7
    548571.7    4077431.3
    547413.9    4077790.4
    547327.9    4077502.0
    548477.5    4077144.7
ZONE T=" 5",F=POINT
    548496.7    4077454.8
    548586.6    4077751.5
    547346.1    4078136.6
    547256.2    4077840.0
    548496.7    4077454.8
ZONE T=" 6",F=POINT
    548512.5    4077779.9
    548595.7    4078064.5
    547370.6    4078440.0
    547280.7    4078156.3
    548512.5    4077779.9
ZONE T=" 7",F=POINT
    548525.1    4078087.1
    548622.7    4078385.2
    547407.7    4078749.6
    547318.7    4078457.3
    548525.1    4078087.1
ZONE T=" 8",F=POINT
    548534.2    4078443.6
    548624.1    4078698.2
    547436.5    4079062.6
    547346.6    4078772.7
    548534.2    4078443.6
ZONE T=" 9",F=POINT
    548553.4    4078719.8
    548640.4    4079003.5
    547469.2    4079367.0
```

```
    547387.5    4079078.5
    548553.4    4078719.8
ZONE T=" 10",F=POINT
    548578.9    4079023.7
    548663.0    4079294.9
    547538.9    4079638.6
    547455.3    4079370.4
    548578.9    4079023.7
ZONE T=" 11",F=POINT
    548590.0    4079317.5
    548671.7    4079587.7
    547630.3    4079905.0
    547549.5    4079635.8
    548590.0    4079317.5
ZONE T=" 12",F=POINT
    548598.1    4079610.8
    548679.9    4079881.0
    547718.7    4080172.8
    547637.0    4079904.5
    548598.1    4079610.8
```

Testing showed only a slight difference in the 2nd or 3rd significant digit (see printouts on file in Room A204).

11/2/98

Performed tests of the UNIX port code and the TPA 3.2 (dev) Version.

Summary of tests preformed:

1. basecase tpa.inp
2. basecase tpa.inp for 10 vectors
3. basecase tpa.inp with VOLCANO on
4. basecase tpa.inp with VOLCANO on and 10 vectors
5. basecase tpa.inp with FAULTO on
6. basecase tpa.inp with FAULTO on and 10 vectors
7. basecase tpa.inp with all append files generated
8. basecase tpa.inp with all append files generated and 10 vectors
9. bascase tpa.inp for 250 vectors, 50,000 yr, and all disruptive events on

In the comparison of results, all files matched using the UNIX 'diff' feature (see the 8 mm tape from 11/13/98 for these files).

Performed testing of the TPA 3.2 PC beta code that included the following. Installed the TPA 3.2 PC beta code on Cathy's machine, the 486 box in Room A241, and on the Pentium 200 ("cleric") in the lab downstairs using the self-extracting zip files in the 3 diskettes supplied to me by Michael Muller (this version was the same as the one Sitakanta took with him to the NRC and that was installed on the lap top). The files were extracted and the placed into the directory that I selected. I set the path (set TPA_DATA=d:\tpa and set TPA_TEST=d:\tpa) and ran the TPA code. The code ran with the precompiled executables, except on cleric
I had to get Jose to increase the virtual memory (swap size) from 100 MB to something much larger (I asked for 400 min and 500 max MB) and then the TPA code successfully ran on that machine and gave output consistent with the other machines and from bigbend (note that the tpa3.2 dev version of the code needed to be compiled for snllhs.f with -O3 and -r8 to give the same snllhs.f output in lhs.out)

11/4/98

Plotted results from TPA runs for 250, 500, 750 and 1000 vectors for EPA release and average total dose in an attempt to determine convergence based on number of realizations and found no significant difference in results (these results are archived on /project/tpa in the seeds subdirectory).

11/9/98

Began to edit the JAVA program post-processor pre-processor (now called *fort_process.f* instead of *data_use.f* in ~rrice/mario/11_09) to add capabilities to create the expected dose plot and apply weighting factors for oso, vso, and osf .

11/12/98

Performed tpa runs to evaluate the impacts of using 32 and 42 GWd/MTU instead of 27.5 and 33 GWd/MTU mixture in invent (heat flux). The old and new values are identified in the "diff" file are listed below.

```
< cc rwr old values
< ccc    data pwr /  10582.389939929, 5740.4059300501, 3759.2845357583,
< ccc    1           2784.2817773404, 2265.6946703965, 1957.4006930445,
< ccc    1           1769.3467669287, 1641.4306331321, 1547.4025225008,
< ccc    1           1477.2287396442, 1231.4269507590, 1177.4945304798,
```

```
< ccc    1        1133.5847397631, 1026.9512899452, 941.70978796592,
< ccc    1        796.60789768898, 682.24662446097, 591.08154763896,
< ccc    1        518.10242850619, 458.53320081560, 410.13654369490,
< ccc    1        371.14193625678, 205.60656057384, 159.43532014065,
< ccc    1        134.23409933195, 116.03888758566, 65.483383518591,
< ccc    1        33.112898155448, 25.230178407012, 20.668519102596,
< ccc    1        15.006216017019, 5.9303606835181, 4.2836496141625,
< ccc    1        3.2613031113206, 1.2804850070161, 0.80268574640249,
< ccc    1        0.67173300459501, 0.48635580320226 /
< ccc
< ccc     data bwr /  6650.5169261958, 3654.3431759514, 2438.9422611497,
< ccc    1        1835.9420028648, 1523.5620327944, 1335.3417519340,
< ccc    1        1227.4091578069, 1143.3276141167, 1089.3615076925,
< ccc    1        1046.0607563246, 888.17707420479, 851.78225358829,
< ccc    1        818.39870974551, 745.23121906343, 682.85697217977,
< ccc    1        577.68720345550, 494.73023315482, 427.71253471103,
< ccc    1        373.74642409318, 329.94508801822, 294.55234513478,
< ccc    1        265.56020870350, 146.45889186333, 115.33666745622,
< ccc    1        98.330887010096, 85.677969272134, 50.267847133175,
< ccc    1        27.116131460830, 21.214642153317, 17.612610059280,
< ccc    1        12.709180897937, 4.9271948035521, 3.5342515845551,
< ccc    1        2.6736622459066, 1.0143060946416, 0.60492693949478,
< ccc    1        0.50807597001675, 0.37429115549995 /
--
(new values)
>     data pwr /  10582.389939929, 5740.4059300501, 3759.2845357583,
>     1        2784.2817773404, 2265.6946703965, 1957.4006930445,
>     1        1769.3467669287, 1641.4306331321, 1547.4025225008,
>     1        1477.2287396442, 1231.4269507590, 1177.4945304798,
>     1        1133.5847397631, 1026.9512899452, 941.70978796592,
>     1        796.60789768898, 682.24662446097, 591.08154763896,
>     1        518.10242850619, 458.53320081560, 410.13654369490,
>     1        371.14193625678, 205.60656057384, 159.43532014065,
>     1        134.23409933195, 116.03888758566, 65.483383518591,
>     1        33.112898155448, 25.230178407012, 20.668519102596,
>     1        15.006216017019, 5.9303606835181, 4.2836496141625,
>     1        3.2613031113206, 1.2804850070161, 0.80268574640249,
>     1        0.67173300459501, 0.48635580320226 /
>
>     data bwr /  6650.5169261958, 3654.3431759514, 2438.9422611497,
```

```
>    1        1835.9420028648, 1523.5620327944, 1335.3417519340,
>    1        1227.4091578069, 1143.3276141167, 1089.3615076925,
>    1        1046.0607563246, 888.17707420479, 851.78225358829,
>    1        818.39870974551, 745.23121906343, 682.85697217977,
>    1        577.68720345550, 494.73023315482, 427.71253471103,
>    1        373.74642409318, 329.94508801822, 294.55234513478,
>    1        265.56020870350, 146.45889186333, 115.33666745622,
>    1        98.330887010096, 85.677969272134, 50.267847133175,
>    1        27.116131460830, 21.214642153317, 17.612610059280,
>    1        12.709180897937, 4.9271948035521, 3.5342515845551,
>    1        2.6736622459066, 1.0143060946416, 0.60492693949478,
>    1        0.50807597001675, 0.37429115549995 /
<
1679,1681c1664
< cc rwr check values
< cc     qpermtu  = (0.65d0*qp + 0.35d0*qb)
<      qpermtu  = (0.6d0*qp + 0.40d0*qb)
```

Prepared plots of results from the basecase and the new invent data with 27.5/33 GWd/MTU (see printouts on file in Room A204). Note that the results differed slightly for the two cases.

11/19/98

prepared SCRs for the gap fraction data and invert properties (from Johnson and Tait, and Bobby Pabalan, respectively) and passed this information on to Ron Janetzke (see the SCRs on file)

11/20/98

performed installation testing for QA on the *fort_process.f* code using hornet and bigbend (these outputs are archived on aries in the d:\from_bscr0_1120 directory)

12/4/98

Ran the tpa code to identify a bug related to selecting to analyze only a few of the subareas (the same bug exists when the user analyzes only a few of the realizations). The bug exists because exec.f divides by the total number of subareas and realizations, instead of by the number of subareas or realizations being analyzed).

Prepared and tested a script file (*tparun*) that executes the TPA code and then runs *fort_process.e* to generate the *.*plt* files.

The script file is:

script file for running the TPA code and creating *.plt files for TPA3.2PPbeta
tpa.e
fort_process.e

After testing the script file *tparun*, this file was copied by Hollis Thomas onto his disk that will be delivered to the NRC and to QA (along with the *fort_process.f* source code and input file) - these files may be found at d:\fort_process on aries.

Modified exec.f to correctly determine the average values in *infilper.res*, *nearfld.res*, and the *r*a.tpa* files for the cases when the user sets start/stop for the subareas and realizations at something besides1 to 7 and 1 to the maxrealization and tested the changes. Also, completed the SCR and other paperwork for the *exec.f* modifications. See ~rrice/tpamods120398 for these changes.

12/7/98

Performed TPA runs and plotted results to examine the impacts of changing the time steps on release rates (looked at 100, 200, and 300 time steps in addition to others for the basecase data, with new gap fraction and invert kds). This testing was in response to results reported by J. Walton. Plotted results do not show the difference the time step dependency that J. Walton found. For these results, see printouts on file in Room A204 and files located on aries in d:\from_bscr0_1204.

Placed invert runs (with and without ebsfilt [bypass and no bypass]) in two /bscr0/rrice/invert/ directories (see these file on d:\from_bscr0_1211) and found that the invert calculations are not performed using the base case data set.

12/15/98

tested vulcan using the time step runs being performed on bigbend (so the cpu time and the results can be compared)

12/16/98

Tested vulcan using 10 tpa runs (performance was approx 2.2 times better than bigbend with a 50k yr run taking 1.6 min/real).

Scientific Notebook
Rob Rice
1/1/1999 - 3/31/99

(note: tapes and hard copy output contain the following work and are stored in my office)

1/4/99 - 1/8/99

Modified the tpa source code (e.g., exec.f) for cleanup of comments, etc. and placed these files in ~rrice/temp_vscr0/tpa2.

Prepared the 29 tpa.inp files for the testing suite in /project/tpa/suite subdirectories - also tested those files in tpa runs (to ensure there were no errors in the data entry) and the runs all completed without errors

1/11/99

Archived /bscr1 files onto tape because the limit 750 mB on vulcan was exceeded

1/14/99

Looked at the seismo module and worked with Gordon to explain the reasons why the seismo module results do not appear to be affected by changes to the hazard curve - these reasons are tied to the independence of the seismic hazard curve and computation that determine WP failures from seismic activity

Investigated whether changing the climato2.dat file to have increasing temperature instead of the dip in the first 10,000 years (i.e., basically shifting the infiltration) would be possible and not cause problems with other parts of the code - there were no problems found when this data file was modified (ran the TPA code on /vscr0)

1/25/99 - 1/27/99

Ran the chaint.f code on /vscr0 with the same input files, only modified for output, by using files that were archived from tape from ~baca. These plots will be used for Gordon's presentation to the board

2/1/99

prepared new *.bmp files for Gordon's animated

presentation (see /vscr2/rrice/vscr1/transfer2/bmp/*
for these files) and sent them to hank in visual presentations

2/2/99

Investigated the causes for the TPA code stopping - which
was found by Jim Weldy on Realization 50 for Subarea 6
(found that he was using a climato2.dat file that was
slightly different than the one the I placed into checkin
and that Ron moved into dev - there was not a 1000 yr
continuation of present-day conditions in Jim's file)

2/3/99

Generated more chaint.f plots for 50 times steps of 240 yrs
for Gordon's animated presentation

2/4/99 - 2/5/99

Completed the VA review for consistency in hydrology
scale and prepared a writeup summary of the results
(see the d:\ drive file va_hyrev.wpd) and gave it
to Sitakanta for his review

2/8/99

Prepared new figures 1 - 6 for Gordon's presentation
because hank could not get these figures to match
with the fifty new figures (see /vscr2/rrice/vscr1/albert/case1/
newrun/newrun2/newrun3/ for these 6 *.bmp files and see
/vscr2/rrice/vscr1/albert/case1/newrun/newrun2 for the last
fifty files)

2/17/99

Reviewed the TSPA VA for plots that would be useful
for generating (scanning and digitizing) plots of
TPA results and also plotting the DOE values

2/18/99

Continued the work from yesterday and prepared
a wpd file (d:\va_plots.wpd) which describes the
figures, page number, plots, and recommended
filenames and also included copies of the
pages from the TSPA VA report (labeled with
the plot number - both global and specific)

2/19/99

Generated TPA output files for a base case run
with the append option on and 250 realizations
and 100,000 yr archived these files (compressed)
on ~rrice/va_tpa/100kyr_append

2/22/99

Setup runs on ds9 (hornet) and foxtrot for the
for comparing with the DOE plots in the VA report
(11 runs on /project/tpa/doeva)

2/23/99 - 2/26/99

Prepared FORTRAN codes to process the
tpa output files for plotting with the
DOE data in the VA (see the file readplotdoeva.f
in ~rrice/read_va)

3/1/99 - 3/12/99

Continued to write and test a FORTRAN code to process
the tpa output files for plotting with the
DOE VA values including processing the
*.res files

Tested the file makeplotdoeva.f in ~rrice/read_va
and placed the output files into /project/tpa/doeva/va2/run*/plt_files
subdirectories

3/18/99

The following modifications should be made to the TPA source code
to enable the user to select 2500 vectors:

- change the maxrealizations in exec.f from 500 to 2500 (1 time)

- change NMAX in snllhs.f from 1000 to 2500 (36 times) and
  nmax from 1000 to 2500 (1 time)

With Ron Janetzke, merged the exec.f changes from 12/98
that were in the checkin subdirectory into the dev version
of the code (these modifications were to correctly weight
the tpa results by the number of subareas and number of
realizations when the "start at ..." and "stop at ..." options
were selected in the tpa.inp file for subareas and
realizations)

3/22/99 - 3/31/99

Prepared writeups for the multiple vector analysis and probabilistic
results for the sensitivity analysis, including plotting results
from the TPA runs in /project/tpa/doeva/va2/run11 using KaleidaGraph
and storing the plot and data files in c:\kgraph. Also used plots
previously generated in subdirectories of the /project/tpa/doeva/va2/run11
directory

Scientific Notebook
Rob Rice
4/1/1999 - 6/30/99

7/15/99

(note: tapes and hard copy output contain the following work and are stored in my office)

4/9/99
prepared plots of the run11 in /project/tpa/doeva/val/run11
(nominal case data set or dev tpa.inp) for 250 vectors with
all append flags on and developed a draft of the results

4/16/99
prepared the writeup of the sensitivity report - mean and sampled sections -
for delivery to the nrc (including figures)

4/30/99
prepared the writeup for chapter 2 of the sensitivity report
for the mean value 10k and 100k yr summary of results using
run11

prepared files with the scanned images of the figures in volume 1
from publications and placed them on a disk that will be shipped
with our changes to the nrc (see d:\vol1\figues for these files)

prepared 3 disks with the original volume 1 figures and converted then
to *.tif format (compressed the files to make them all fit onto 3 disks)

completed adding text describing the disruptive events to section 2
of the sensitivity report

prepared a writeup and plots of the results from analyzing the dependency of
the NEFTRAN mixing length on release rates (the plots are stored in c:\KGraph
in mix*.qpc files) - see hard copy printouts - the results were that the increased
Rds increase the dispersion and that there is also a dependency on the mixing
zone thickness

5/7/99
edited text and figures for section 2 of the sensitivity analysis report
in order to fit more of the figures on one page and thus reduce the
number of pages with figures (see the files 'sens_anal_fig ***.wpd' in
g:\mohanty and these files with the same file names are also archived
on the aries d:\ drive)

5/14/99
Performed TPA runs using the base case mean value data set for fifteen
alternative conceptual models. The results will be plotted and included
section 2 of the sensitivity analysis report. A write-up describing these
runs and the results was also prepared. The runs are stored in
/project/tpa/doeva/meanval/alt_models/ in 18 subdirectories. The
alternative models are:

1. backfill
2. matrix diffusion
3. cladding
4. higher flow
5. focused flow
6. flowthrough (imodel = 2)
7. flow through (imodel = 1)
8. bathtub (imodel = 3)
9. bathtub (imodel = 4)
10. immediate wp failure
11. no reterdation
12. faulting
13. volcano
14. no ebsfilt
15. base case
16. flow through (imodel = 3)
17. flow through (imodel = 4)
18. bathtub (imodel = 1)

(note that these alternative conceptual models match, for the most part those analyzed in nureg-1668, vol.2)

The figure, text and table that was prepared in wordperfect is in file name: d:\alt_models.wpd

began a TPA run that is equivalent to run11 (base case, 100,000 yrs, 250 vectors) with SEISMO off in the /project/tpa/doeva/disruptive_events/no_seismic directory

with R. Janetzke, examined the reasons why run14, with initial failures set at 1,000 years was having releases at 500 years - found that the cause was for realizations 216 (SA7) and 139 (SA5) there was zero release at 500 yr but nonzero release at 1000 yr (note: 500 yr releaset.f time steps in ebsnef.dat) so that when the values are mapped back to TPA time steps it is indeed possible to have releases before wp failure (just as we have found instances when sz releases occur before ebs releases) - again, the TPA mapping of results to TPA time steps should be modified in subsequent versions of the code

5/18/99
tested the tpa code using the modifications in neftran for the mixing zone length (see printout of results and file in /project/tpa/doeva/meanval/run2sa7/ subdirectories - also see files in the c:\kgraph directory called neftranfixed*)

5/21/99
prepared figures that will be included in the NRC/DOE Tech Exchange next week using run11, run18, and the meanval2 output in /project/tpa/doeva/

as part of preparing the figures and testing the code modifications to correct for EBS releases before WP failure or before releases in the input data (UZ and SZ), new tpa runs were performed using the modified tpa code (neftran fixed and early releases fixed) - see /vscr0/rrice/run and /project/tpa/doeva/meanval2/ for these results - note that these files were moved to /project/tpa/doeva/va2/run18)

6/4/99
performed tpa runs for the alternative conceptual model section of section 2 in the sensitivity analysis report (see /project/tpa/doeva/meanval2)

modified the tpa code in ~smohanty/A_yichi to have the same seismo events in a set of realizations (used for the sensitivity analysis) - see the testseismo subdirectory in ~smohanty/A_yichi for this run and a subdirectory with the basecase in the ~smohanty/A_yichi/testseismo/basecase directory

7/15/99

Scientific Notebook No. 170
Rob Rice
4/1/1999 - 6/30/99

7/15/99

(note: tapes and hard copy output contain the following work and are stored in my office)

4/9/99
prepared plots of the run11 in /project/tpa/doeva/val/run11
(nominal case data set or dev tpa.inp) for 250 vectors with
all append flags on and developed a draft of the results

4/16/99
prepared the writeup of the sensitivity report - mean and sampled sections -
for delivery to the nrc (including figures)

4/30/99
prepared the writeup for chapter 2 of the sensitivity report
for the mean value 10k and 100k yr summary of results using
run11

prepared files with the scanned images of the figures in volume 1
from publications and placed them on a disk that will be shipped
with our changes to the nrc (see d:\vol1\figues for these files)

prepared 3 disks with the original volume 1 figures and converted them
to *.tif format (compressed the files to make them all fit onto 3 disks)

completed adding text describing the disruptive events to section 2
of the sensitivity report

prepared a writeup and plots of the results from analyzing the dependency of
the NEFTRAN mixing length on release rates (the plots are stored in c:\KGraph
in mix*.qpc files) - see hard copy printouts - the results were that the increased
Rds increase the dispersion and that there is also a dependency on the mixing
zone thickness

5/7/99
edited text and figures for section 2 of the sensitivity analysis report
in order to fit more of the figures on one page and thus reduce the
number of pages with figures (see the files 'sens_anal_fig ***.wpd' in
g:\mohanty and these files with the same file names are also archived
on the aries d:\ drive)

5/14/99
Performed TPA runs using the base case mean value data set for fifteen
alternative conceptual models. The results will be plotted and included
section 2 of the sensitivity analysis report. A write-up describing these
runs and the results was also prepared. The runs are stored in
/project/tpa/doeva/meanval/alt_models/ in 18 subdirectories. The
alternative models are:

Post-it® Fax Note 7671
To Ron Janke
Co./Dept.
Phone # 210-522-3338
Fax # 210-522-5155
Date 10/11/99
From R. Rice
Co.
Phone # 915-581-0853
Fax # 915-581-0853
# of pages ▶ 2

Rob Rice
Scientific Notebook No. 170

Initials

1. backfill
2. matrix diffusion
3. cladding
4. higher flow
5. focused flow
6. flowthrough (imodel = 2)
7. flow through (imodel = 1)
8. bathtub (imodel = 3)
9. bathtub (imodel = 4)
10. immediate wp failure
11. no retardation
12. faulting
13. volcano
14. no ebsfilt
15. base case
16. flow through (imodel = 3)
17. flow through (imodel = 4)
18. bathtub (imodel = 1)

(note that these alternative conceptual models match, for the most part those analyzed in nureg-1668, vol.2)

The figure, text and table that was prepared in wordperfect is in file name: d:\alt_models.wpd

began a TPA run that is equivalent to run11 (base case, 100,000 yrs, 250 vectors) with SEISMO off in the /project/tpa/doeva/disruptive_events/no_seismic directory

with R. Janetzke, examined the reasons why run14, with initial failures set at 1,000 years was having releases at 500 years - found that the cause was for realizations 216 (SA7) and 139 (SA5) there was zero release at 500 yr but nonzero release at 1000 yr (note: 500 yr releaset.f time steps in cbsnef.dat) so that when the values are mapped back to TPA time steps it is indeed possible to have releases before wp failure (just as we have found instances when sz releases occur before ebs releases) - again, the TPA mapping of results to TPA time steps should be modified in subsequent versions of the code

5/18/99
tested the tpa code using the modifications in neftran for the mixing zone length (see printout of results and file in /project/tpa/doeva/meanval/run2sa7/ subdirectories - also see files in the c:\kgraph directory called neftranfixed*)

5/21/99
prepared figures that will be included in the NRC/DOE Tech Exchange next week using run11, run18, and the meanval2 output in /project/tpa/doeva/

as part of preparing the figures and testing the code modifications to correct for EBS releases before WP failure or before releases in the input data (UZ and SZ), new tpa runs were performed using the modified tpa code (neftran fixed and early releases fixed) - see /vaer0/rrice/run and /project/tpa/doeva/meanval2/ for these results - note that these files were moved to /project/tpa/doeva/va2/run18)

6/4/99
performed tpa runs for the alternative conceptual model section of section 2 in the sensitivity analysis report (see /project/tpa/doeva/meanval2)

modified the tpa code in ~smohanty/A_ylchi to have the same seismo events in a set of realizations (used for the sensitivity analysis) - see the testseismo subdirectory in ~smohanty/A_ylchi for this run and a subdirectory with the basecase in the ~smohanty/A_ylchi/testseismo/basecase directory

Entries into Scientific Notebook No. 170 for pages 1 and 2 have been made by Robert W. Rice 10/11/99

7/15/99

No original text entered into this Scientific Notebook has been removed. 10/11/99

INITIAL ENTRIES

Scientific Notebook: #170

Issued to: S. Mohanty

Issue Date: Apr. 3,1996

Account Number: 20-1402-761

Title: TPA Code

Participant: Robert W. Rice

7/12/99

Looked into the UTM coordinates and whether they
were in NAD27 or NAD83 (it looks like NAD27 from Randy Fedors), so
there is a question of whether the subarea coordinates, the
NEFENV coordinates in rectedge.dat, and the UZFLOW coordinates
in the *dem.dat data file are consistent (and whether these
coordinates are consistent with the DOE coordinates) - Randy determined
there was apparently an inconsistency which he will address in the future.

7/14/99

Prepared testing documentation for the SCR
related to early releases (prior to WP failures
and with no UZ and SZ travel time) - see /project/tpa/doeva/run14/test
directory for this run and ~rrice/testing_scr_early_releases for
this file.

7/15/99

Plotted results from the mean values runs in
/project/tpa/doeva/meanval2/alt_models (subdirectories for
model 1 and 4 [9_* and 18_*]) to compare the results for
the model 1 and model 4 cases

7/26/99

Ran the TPA code and prepared pots of results showing the differences
between models 1, 2, and 4 (see /project/tpa/doeva/meanval3/).

7/27/99

Prepared a figure for the annual report showing the
parameter tree approach in color (see d:\g_drive_072999\gordon3.cdr).

7/28/99

Wrote a FORTRAN code to post-process results
from TPA runs (see /project/tpa/doeva/plt*/rel*/* files)

7/29/99

Revised figures for the sensitivity analysis report
(see d:\g_drive_072999\sens_anal_figs.ppt)

8/17/99

Tested the TPA Version 3.2.3 code on CD using
a Windows 98 and an NT machine and found that
the results were compatible with the Sun and NT output in Division 20

Also found a problem with the TPA executable on the CD

and requested for R. Janetzke to send a new executable to me
via an email attachment (in compiling the code, a flag that allowed
for the redirection of the TPA output was not activated)

9/1/99 - 9/9/99

Prepared test plans for SCRs 273 - 277:

SCR-273	Importance Analysis Flag
SCR-274	Modify test for zero release in uzft.f
SCR-275	Add time and date to ashplume.f and snllhs.f output
SCR-276	Change to double precision in the cp.tpa file
SCR-277	Automate generation of the tpanames.dbs file

9/9/99

Test plans for SCRs 271 through 277 were submitted to R. Janetzke
for review via email attachments.

9/16/99

Test plans for SCRs 273 through 277 were approved by
R. Janetzke, who signed and dated the test plans.
R. Janetzke has custody of the original test plans

9/21/99

Prepared a CD with data from three TPA 3.2.3 simulations
for 10,000, 50,000, and 100,000 yr to evaluate time steps
on the TPA output. This CD has been placed with the SCR
and testing performed for the releaset.f time step modifications
made by D. Codell. The documentation was prepared by
R. Janetzke.

9/24/99

Prepared four CDs with the data from TPA simulations which were used in the Sensitivity Analysis Report. One CD contained the results from the mean value simulations and the other three CDs contained data from the multiple realization simulation (i.e., the files are from /project/tpa/doeva/meanval3 and /project/tpa/doeva/va4/run24, respectively).

10/26/99 - 11/5/99

Began to perform test according to the Test Plans for SCRs 273 - 277. A directory structure described in the test plans was created on the "c:\" partition in the subdirectory "testing_3.2.3e". The tests will be conducted in the same order provided in the test plans with the first being

Prior to testing, the following was noted.
****
Source Code Correction Recommended: (1) With the APPEND option ON (all files) for both the v3.2.3 and v3.2.3e codes, there is a message printed to the screen stating "The name specified is not recognized as an internal or external command, operable program or batch file." After examining the output files, it is clear that this message indicates that the three *.cum files (which are created to "cat" the NEFTRAN UZ, FAILT, and RELEASET output files) are not written when the append file is activated. These files should be written. (2) In the screenprint, the first letter of information written to the screen is left off. This is results in a confusing and unclear message being provided to the user. The source code that writes this information to the screen should be modified to write all the information. (3) The standalone code executables require about 130 Mb of disk space. If possible, it would be useful for the size of these files to be smaller. (4) A screen message stating that the importance analysis is activated and which barriers have been removed would be very useful.
****

TESTING FOR SCR273

Note: (1) the file comparisons [filecomp.bat and filecomp.out] are located in the v3.2.3 subdirectories for all tests unless otherwise noted).

(2) contrary to the information stated on the test plans, the v3.2.3 and v3.2.3 source codes were delivered on a single CD prepared by R. Janetzke on 9/24/99.

SCR273\flag1\test1\10k - Expected Results: The filecomp.out file shows no differences in the output files when compared to the results in the SCR273\flag1\test1\10k\v3.2.3 subdirectory(*.res,

*.tpa [except spquery.tpa, see below], *.rlt, *.ech, and *.cum), except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision) and the time, date ad header of the run. A comparison between the v3.2.3 and v3.2.3e cp.tpa files performed using an EXCEL spreadsheet indicates no differences except those attributable to precision. It is also noted that the 15 new flags for the importance analysis are present in the cp.tpa file from v3.2.3e. Additionally, there are a handful (10 or so) parameter names that are queried for a value one more time in version 3.2.3e than in version 3.2.3. The reasons for these differences are identified below for the 100k-yr run.

SCR273\flag1\test1\100k - Unexpected Results: The filecomp.out file in the v3.2.3 subdirectory shows many differences in the output files when compared to the results in the SCR273\flag1\test1\100k\v3.2.3 subdirectory in addition to the expected differences noted in the test plan for the cp.tpa file (single vs. double precision) and the time, date, and header of the run. As mentioned earlier, there are a handful (10 or so) parameter names that are queried for a value one more time in version 3.2.3e than in version 3.2.3. The reasons for this difference are attributable to a different methodology used to determine the WP_Stiffness in the two versions. In version 3.2.3e, the following approach is used (from seismo.f):

```
cc rwj 7-2-99 importance analysis
cc      Calculate package stiffness.
cc      (Page 4-41 of 3.1.4 User's Guide)
cc      3.14159d0 is pi

      WPWall = OuterWPThickness + AInnerWPThickness
      Rave = WPDiameter - WPWall/2.0d0
      Package_Stiffness = 48.d0 * Package_Modulus * 3.14159d0 *
     &              Rave**3 * WPWall /  WPLength**3
```

and the screen print shows the following:

(v3.2.3):

```
xec: calling seismo
xec: failed WPs from INITIAL   event =    16 at time =     0.0 yr
xec: failed WPs from CORROSION event =  1647 at time =  20525.6 yr
```

(v3.2.3):

```
xec: calling seismo
xec: failed WPs from INITIAL   event =    16 at time =     0.0 yr
xec: failed WPs from SEISMIC   event =     4 at time =  4169.3 yr
xec: failed WPs from CORROSION event =  1643 at time =  20525.6 yr
```

The results, as documented in filecomp.out, before the execution of SEISMO are the same for both versions, however after SEISMO the results are inconsistent.

To verify that the additional code in SEISMO was causing this difference, TPA runs were performed with the SEISMO flag OFF in "test" subdirectories located below the v3.2.3 and v3.2.3e subdirectories. A comparison of the output from these two runs verifies that the differences in the output were caused by the additional code in SEISMO. All other results were expected and consistent between the v3.2.3 and v.3.2.3e runs. Furthermore, the increased number of times certain parameters were queried for a value (as identified in the 10k-yr analysis) is solely attributable to the additional code in SEISMO.

****

Source Code Correction Recommended: Because of the different methodologies employed to determine the WP_Stiffness in v3.2.3 and v3.2.3e, which causes a different WP failure history, either the v3.2.3 methodology should be adopted in v3.2.3e, or the v3.2.3 methodology should be maintained and an SCR specific to that change should be written and tested. Also, if the new methodology is kept, because the WP_Stiffness is now calculated, the parameter "WPStiffnessforSEISMO[Pa*m]" should be removed from tpa.inp and tpanames.dbs.

****

SCR273\flag1\test2\10k - Expected Results: The filecomp.out file in the SCR273\flag1\test2\10k\v3.2.3e subdirectory shows no differences in the output files when compared to the results in the SCR273\flag1\test1\10k\v3.2.3 subdirectory(*.res, *.tpa, *.rlt, *.ech, and *.cum), except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. Based on the previous testing, there are no unexpected results.

SCR273\flag1\test2\100k - Expected Results: The filecomp.out file in the SCR273\flag1\test2\100k\v3.2.3e subdirectory shows no differences in the output files when compared to the results in the SCR273\flag1\test1\100k\v3.2.3 subdirectory(*.res, *.tpa, *.rlt, *.ech, and *.cum), except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date, and header of the run, and differences described and explained earlier in this report. To remove the differences in results attributable to modifications in the SEISMO methodology that was identified in test1 at 100 kyr, the "test" subdirectory below the SCR273\flag1\test2\100k\v3.2.3e subdirectory contains a TPA run performed without SEISMO. The TPA results in this subdirectory (specifically, refer to the filecomp.out file) verify that the output from v3.2.3 and v3.2.3e are consistent. Thus, based on the previous testing, there are no unexpected results.

SCR273\flag1\test3\10k - Expected Results: The filecomp.out file in the SCR273\flag1\test3\10k\v3.2.3e subdirectory shows no differences in the output files when compared to the results in the SCR273\flag1\test1\10k\v3.2.3 subdirectory(*.res, *.tpa, *.rlt, *.ech, and *.cum), except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. Based on the previous testing, there are no unexpected results.

SCR273\flag1\test3\100k - Expected Results: The filecomp.out file in the SCR273\flag1\test3\100k\v3.2.3e subdirectory shows no differences in the output files when compared to the results in the SCR273\flag1\test1\100k\v3.2.3 subdirectory (*.res, *.tpa, *.rlt, *.ech, and *.cum), except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date, and header of the run, and differences described and explained earlier in this report. To remove the differences in results attributable to modifications in the SEISMO methodology that was identified in test1 at 100 kyr, the "test" subdirectory below the SCR273\flag1\test2\100k\v3.2.3e subdirectory contains a TPA run performed without SEISMO. The TPA results in this subdirectory (specifically, refer to the filecomp.out file) verify that the output from v3.2.3 and v3.2.3e are consistent. Thus, based on the previous testing, there are no unexpected results.

****

Two notes in the output from flag1: (1) C14 is zeroed out after the EBS. If it is zeroed out, why is the TPA code modeling it in the first place (i.e., it will not contribute to GW dose and note the large contribution of C14 to dose in the DOE VA and EIS results)? and (2) if a WP fails at t=0 it is classified as an initial failure even though the fraction of initial failures may be specified at 0.0 in tpa.inp.

****

SCR273\flag1\test4\10k and SCR273\flag1\test4\100k: The v3.2.3e subdirectories in the SCR273\flag1\test4\10k and SCR273\flag1\test4\100k directories contain the preliminary output from these runs. Final testing for SCR273\flag1\test4\10k and SCR273\flag1\test4\100k will be conducted after the changes identified in this report are addressed to verify that all flags can be activated and the results are reasonable. The preliminary testing indicated that all flags could be activated and that the 10-kyr and 100-kyr results are reasonable (i.e., all WPs fail at t=0; EBS, UZ, and SZ releases are equal; and peak doses and doses at the end of the simulation time are high). These results are reasonable because with all flags activated the groundwater dose directly arises from EBS release rates.

SCR273\flag2\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag2\test1\10k\v3.2.3_modified subdirectory shows no differences in the output files (*.res, *.tpa, *.rlt, *.ech, and *.cum) compared to the v3.2.3e subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and

header of the run, and differences described and explained earlier in this report. Based on the previous testing, there are no unexpected results.

SCR273\flag2\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag2\test1\100k\v3.2.3_modified subdirectory shows no differences in the output files (*.res, *.tpa, *.rlt, *.ech, and *.cum) compared to the v3.2.3e subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. Based on the previous testing, there are no unexpected results.

SCR273\flag3\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag3\test1\10k\v3.2.3_modified subdirectory shows no differences in the output files (*.res, *.tpa, *.rlt, *.ech, and *.cum) compared to the v3.2.3e subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. Based on the previous testing, there are no unexpected results.

SCR273\flag3\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag3\test1\100k\v3.2.3_modified subdirectory shows no differences in the output files (*.res, *.tpa, *.rlt, *.ech, and *.cum) compared to the v3.2.3e subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. Based on the previous testing, there are no unexpected results.

SCR273\flag4\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag4\test1\10k\v3.2.3e subdirectory shows no differences in the output files when compared to the results in the SCR273\flag1\test1\10k\v3.2.3 subdirectory(*.res, *.tpa, *.rlt, *.ech, and *.cum), except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. Based on the previous testing, there are no unexpected results.

SCR273\flag4\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag4\test1\100k\v3.2.3e subdirectory shows no differences in the output files when compared to the results in the SCR273\flag1\test1\100k\v3.2.3 subdirectory (*.res, *.tpa, *.rlt, *.ech, and *.cum), except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date, and header of the run, and differences described and explained earlier in this report. To remove the differences in results attributable to modifications in the SEISMO methodology that was identified in test1 at 100 kyr, the "test" subdirectory below the SCR273\flag4\test1\100k\v3.2.3e subdirectory contains a TPA run performed without SEISMO. The TPA results in this subdirectory (specifically, refer to the filecomp.out file) verify that the output from v3.2.3 and v3.2.3e are consistent. Thus, based on the previous testing, there are no unexpected

results.

SCR273\flag5\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag5\test1\10k\v3.2.3e subdirectory shows many differences in the output files when compared to the results in the SCR273\flag1\test1\10k\v3.2.3 subdirectory(*.res, *.tpa, *.rlt, *.ech, and *.cum), including the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report.

SCR273\flag5\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag5\test1\100k\v3.2.3e subdirectory shows many differences in the output files when compared to the results in the SCR273\flag1\test1\100k\v3.2.3 subdirectory(*.res, *.tpa, *.rlt, *.ech, and *.cum), including the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report.

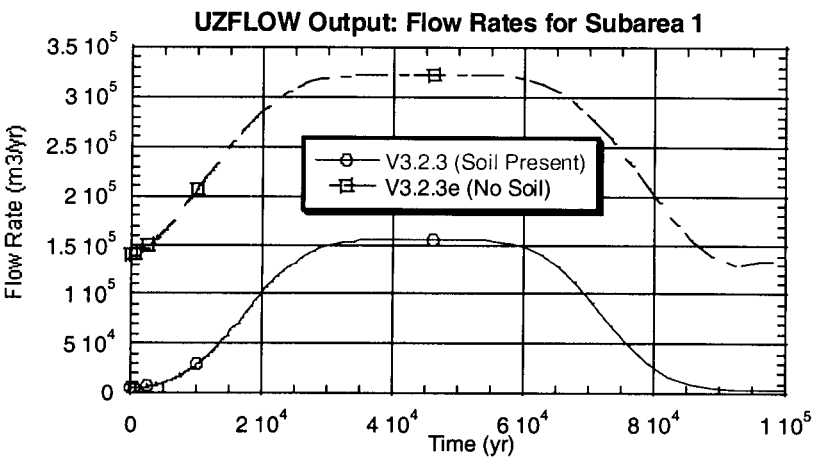
For flag5 testing, to explain the results and understand whether the behavior is reasonable the following hand calculations were conducted and plots prepared.

To compute the area of subarea 1, the following EXCEL was used (note that the area of subarea 1 is 791,564 m^2) using the methodology in subarea.f.

Subarea 1			
x	y	d1 625.8528	
547472	4079324	d2 1338.817	
548069.2	4079137	d3 114641.5	area1 415011.4
547847.3	4077816		
547318.4	4077934	d1 541.8598	
		d2 1398.163	
		d3 82467.62	area2 376553.2
			total area 791564.6

From the dcagw.ech file, the AAP (average annual precipitation) at a representative time (i.e., t = 0) is 6.4094 in/yr [or 0.1628 m/yr]. Since subarea has an area of about 792,000 m^2, the volumetric flow rate of year in subarea 1 is 129,000 m^3/yr. This value is reasonable when compared to the volumetric flow rate in uzflow.rlt, which is 141,320 m^3/yr. The differences appear to be attributable to subarea dependencies and the differences are reasonable.

The following plot shows the difference between v3.2.3 and v3.2.3e flow rates if the soil is removed. As expected, when the soil is removed, the flow rate shows a large increase.



To further explore these results and whether the flow rates are reasonable, additional TPA runs for 100 kyr were performed with the SEISMO flag OFF using v3.2.3e and v3.2.3 (see the SCR273\f lag5\test1\100k\v3.2.3e\test and lag5\test1\100k\v3 SCR273\f .2.3_modified subdirectories). The v3.2.3 subdirect run using modified code was data in soildem.dat soil depth the soil thicknesses with all to zero. Using the set equal filecomp.bat file, the results in these two directories were found to be the same. Thus, based on this run and the plot and hand calculation presented previously, the flag in v3.2.3e is correctly setting the soil thicknesses to zero.

SCR273\flag6\test1\10k and SCR273\flag6\test1\100k - Unexpected Results: The filecomp.out

file in the SCR273\flag6\test1\10k\v3.2.3e and SCR273\flag6\test1\100k\v3.2.3e subdirectories shows many differences in the output files when compared to the results in the SCR273\flag1\test1\10k\v3.2.3 and SCR273\flag1\test1\100k\v3.2.3 subdirectories and the SCR273\flag6\test1\10k\v3.2.3_modified and SCR273\flag6\test1\100k\v3.2.3_modified subdirectories (*.res, *.tpa, *.rlt, *.ech, and *.cum). The results from these runs are quite different because of what appears to be two inconsistencies in the implementation of the UUL presence flag. The other changes (i.e., factors affecting the repository temperature, FOW, FMULT, removal of near-field reflux and losses, and the subarea wet fraction) appear to be correctly implemented. The inconsistencies are related to setting the SF wet fraction equal to 0.5 and the chloride concentration equal to zero. It appears that the parameters are not being reset to these values. The following example shows that the SF wet fractions are not set equal to 0.5 (in ebsrel.inp):

```
Comparing files ebsrel.inp and
C:\TESTING_3.2.3E\SCR273\FLAG6\TEST1\10K\V3.2.3E\EBSREL.INP
***** ebsrel.inp
\Fuel leaching model paramters
 4.99398E-01          ! wetfrac(1): ht. fraction of wet SF in initially def. WPs
 5.00519E-01          ! wetfrac(2): ht. fraction of wet SF in faulting failure WPs
 4.99327E-01          ! wetfrac(3): ht. fraction of wet SF in volcanic failure WPs
 5.00899E-01          ! wetfrac(4): ht. fraction of wet SF in seismt1 failure WPs
 4.99908E-01          ! wetfrac(5): ht. fraction of wet SF in seismt2 failure WPs
 4.99330E-01          ! wetfrac(6): ht. fraction of wet SF in seismt3 failure WPs
 5.00520E-01          ! wetfrac(7): ht. fraction of wet SF in seismt4 failure WPs
 5.00618E-01          ! wetfrac(8): ht. fraction of wet SF in corrosion failure WPs
***** C:\TESTING_3.2.3E\SCR273\FLAG6\TEST1\10K\V3.2.3E\EBSREL.INP
\Fuel leaching model paramters
 1.99136E-01          ! wetfrac(1): ht. fraction of wet SF in initially def. WPs
 7.59571E-01          ! wetfrac(2): ht. fraction of wet SF in faulting failure WPs
 1.63517E-01          ! wetfrac(3): ht. fraction of wet SF in volcanic failure WPs
 9.49294E-01          ! wetfrac(4): ht. fraction of wet SF in seismt1 failure WPs
 4.53967E-01          ! wetfrac(5): ht. fraction of wet SF in seismt2 failure WPs
 1.64902E-01          ! wetfrac(6): ht. fraction of wet SF in seismt3 failure WPs
 7.60013E-01          ! wetfrac(7): ht. fraction of wet SF in seismt4 failure WPs
 8.08787E-01          ! wetfrac(8): ht. fraction of wet SF in corrosion failure WPs
*****
```

The next example shows that the screen message has a different WP corrosion time for the v3.2.3 and v3.2.3e simulations. This difference can most likely be attributed to the chloride concentrations (note the expected results of an later failure time for v3.2.3, with [Cl] = 0, than for v3.2.3e, which has a nonzero [Cl]):

```
v3.2.3: ----------------------------------------------------------------
          subarea  1 of  7        realization   1 of   1
        ----------------------------------------------------------------
        xec: calling uzflow
        xec: calling nfenv
        xec: calling ebsfail
           ebsfail: time of WP failure =   26840.6  yr
        xec: calling seismo
        xec: failed WPs from INITIAL   event =    16 at time =     0.0 yr
        xec: failed WPs from CORROSION event =  1647 at time =  26840.6 yr


v3.2.3e----------------------------------------------------------------
          subarea  1 of  7        realization   1 of   1
        ----------------------------------------------------------------
        xec: calling uzflow
        xec: calling nfenv
        xec: calling ebsfail
           ebsfail: time of WP failure =   19756.2  yr
        xec: calling seismo
        xec: failed WPs from INITIAL   event =    16 at time =     0.0 yr
        xec: failed WPs from SEISMIC   event =     4 at time =  4169.3 yr
        xec: failed WPs from CORROSION event =  1643 at time =  19756.2 yr
         *** failed WPs: all WPs failed ***
        xec: calling ebsrel
```

****

Source Code Correction Recommended: Because of the different results, the following two changes should be implemented: (1) the failt.f code should be modified to read in the data contained in chlrdmf.dat, instead of reading multiflo.dat and overwriting chlrdmf.dat with this data, and (2) when the UUL presence flag is activated, the SF wet fractions should be reset to 0.5, instead of using the sampled values from SNLLHS.F

****

Note: For the following tests (flags 7 to 14) which remove hydrostratigraphic units from the UZ or SZ, the test procedure was streamlined from that described in the Test Plan, in that for v3.2.3e, the

flag was activated, while for v3.2.3 the hydrostratigraphic unit thickness was set equal to zero in tpa.inp (i.e., instead of forcing the hydrostratigraphic unit to be considered, the unit was removed using the flag in v3.2.3e and the thicknesses were set equal to zero in v3.2.3; thus, the results should be the same). For these tests, the filecomp.out file should be the same, whereas a useful file, filecom2.out, (comparison between v3.2.3e runs with the different hydrostratigraphic units removed and the base case runs of v3.2.3 in SCR273\flag1\test1 for 10 kyr and 100 kyr) should be different.

****

ALSO NOTE: Source Code Correction Recommended. It appears that all legs are used to determine the GWTT for the UZ, even if the leg is not used in the NEFTRAN calculation (leg is skipped). See the following example (v3.2.3e zeros out the values with the flag, while v3.2.3 does not call NEFTRAN for every realization yet has a different GWTT) - note that there is a 5 yr difference in these values indicating that the nonzero leg in the tpa.inp file is counted (5 yr is the minimum GWTT):

```
v3.2.3e***** gwttuzsz.res
          yr
           1      2.3018E+01     2.1307E+01     2.4378E+01     2.0479E+01     1.7280E+03
        1.9634E+03     1.9106E+01
         5.4281E+02      5.0860E+03      5.0794E+03      2.3381E+03      2.3349E+03
      2.3794E+03     2.3758E+03     2.3743E+03
         3.1383E+03      5.1090E+03      5.1007E+03      2.3625E+03      2.3554E+03
      4.1074E+03     4.3392E+03     2.3934E+03
        3.6811E+03
v3.2.3  ***** C:\TESTING_3.2.3E\SCR273\FLAG1\TEST1\10K\V3.2.3\GWTTUZSZ.RES
          yr
           1      2.8018E+01     2.6307E+01     2.9378E+01     2.5479E+01     1.7330E+03
        1.9684E+03     2.4106E+01
         5.4781E+02      5.0860E+03      5.0794E+03      2.3381E+03      2.3349E+03
      2.3794E+03     2.3758E+03     2.3743E+03
         3.1383E+03      5.1140E+03      5.1057E+03      2.3675E+03      2.3604E+03
      4.1124E+03     4.3442E+03     2.3984E+03
        3.6861E+03
*****
**********
```

SCR273\flag7\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag7\test1\10k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag7\test1\10k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. As expected, filecom2.out file

(comparison between SCR273\flag7\test1\10k\v3.2.3e and SCR273\flag1\test1\10k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag7\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag7\test1\100k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag7\test1\100k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. (Note that for the 100-kyr simulations the SEISMO flag was not activated, because of reasons described previously.) As expected, filecom2.out file (comparison between SCR273\flag7\test1\100k\v3.2.3e and SCR273\flag1\test1\100k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag8\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag8\test1\10k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag8\test1\10k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. As expected, filecom2.out file (comparison between SCR273\flag8\test1\10k\v3.2.3e and SCR273\flag1\test1\10k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag8\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag8\test1\100k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag8\test1\100k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. (Note that for the 100-kyr simulations the SEISMO flag was not activated, because of reasons described previously.) As expected, filecom2.out file (comparison between SCR273\flag8\test1\100k\v3.2.3e and SCR273\flag1\test1\100k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag9\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag9\test1\10k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag9\test1\10k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. As expected, filecom2.out file (comparison between SCR273\flag9\test1\10k\v3.2.3e and SCR273\flag1\test1\10k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag9\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag9\test1\100k\v3.2.3e subdirectory shows no differences in the output files compared

to the SCR273\flag9\test1\100k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. (Note that for the 100-kyr simulations the SEISMO flag was not activated, because of reasons described previously.) As expected, filecom2.out file (comparison between SCR273\flag9\test1\100k\v3.2.3e and SCR273\flag1\test1\100k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag10\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag10\test1\10k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag10\test1\10k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. As expected, filecom2.out file (comparison between SCR273\flag10\test1\10k\v3.2.3e and SCR273\flag1\test1\10k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag10\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag10\test1\100k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag10\test1\100k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. (Note that for the 100-kyr simulations the SEISMO flag was not activated, because of reasons described previously.) As expected, filecom2.out file (comparison between SCR273\flag10\test1\100k\v3.2.3e and SCR273\flag1\test1\100k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag11\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag11\test1\10k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag11\test1\10k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. As expected, filecom2.out file (comparison between SCR273\flag11\test1\10k\v3.2.3e and SCR273\flag1\test1\10k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag11\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag11\test1\100k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag11\test1\100k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. (Note that for the 100-kyr simulations the SEISMO flag was not activated, because of reasons described previously.) As

expected, filecom2.out file (comparison between SCR273\flag11\test1\100k\v3.2.3e and SCR273\flag1\test1\100k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag12\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag12\test1\10k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag12\test1\10k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. As expected, filecom2.out file (comparison between SCR273\flag12\test1\10k\v3.2.3e and SCR273\flag1\test1\10k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag12\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag12\test1\100k\v3.2.3e subdirectory shows no differences in the output files compared to the SCR273\flag12\test1\100k\v3.2.3_modified subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. (Note that for the 100-kyr simulations the SEISMO flag was not activated, because of reasons described previously.) As expected, filecom2.out file (comparison between SCR273\flag12\test1\100k\v3.2.3e and SCR273\flag1\test1\100k\v3.2.3 results) shows differences in the results, which indicates the unit was removed from the calculations.

SCR273\flag13\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag13\test1\10k\v3.2.3e subdirectory shows no differences through the UZ release rates in the output files compared to the SCR273\flag1\test1\10k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The differences in the results begin after the SZ computation when the STFF layer is removed. The following information shows that the STFF layer was removed from nefiisz.inp and that the GWTT was affected. Moreover, the SZ release rates with STFF removed began at 2,800 yr, whereas these releases began at 3,200 yr with the STFF layer present. It was not possible to readily modified the data to generate v3.2.3 results that matched v3.2.3e results with the STFF layer removed.

SCR273\flag13\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag13\test1\100k\v3.2.3e subdirectory shows no differences through the UZ release rates in the output files compared to the SCR273\flag1\test1\100k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The differences in the results begin after the SZ computation when the STFF layer is removed. The following information shows that the STFF layer was removed from nefiisz.inp. Moreover, the SZ

release rates with STFF removed began at 2,800 yr, whereas these releases began at 3,200 yr with the STFF layer present. It was not possible to readily modified the data to generate v3.2.3 results that matched v3.2.3e results with the STFF layer removed. (Note that for the 100-kyr simulations the SEISMO flag was not activated, because of reasons described previously.)

```
***** nefiisz.inp
 1    1    2    187.2     0.0     0.0     0.0
 2    2    3   8039.0     0.0     0.0     0.0
              MIGRATION PATH PROPERTIES ARRAY
***** C:\TESTING_3.2.3E\SCR273\FLAG1\TEST1\10K\V3.2.3\NEFIISZ.INP
 1    1    2    187.2     0.0     0.0     0.0
 2    2    3  14294.9     0.0     0.0     0.0
 3    3    4   8039.0     0.0     0.0     0.0
              MIGRATION PATH PROPERTIES ARRAY
*****


***** gwttuzsz.res
     1      2.8018E+01    2.6307E+01    2.9378E+01    2.5479E+01    1.7330E+03
  1.9684E+03    2.4106E+01
   5.4781E+02      4.8541E+03      4.8541E+03      2.1640E+03      2.1640E+03
2.2151E+03    2.2151E+03    2.2151E+03
   2.9545E+03      4.8821E+03      4.8804E+03      2.1933E+03      2.1894E+03
3.9481E+03    4.1835E+03    2.2392E+03
  3.5023E+03
***** C:\TESTING_3.2.3E\SCR273\FLAG1\TEST1\10K\V3.2.3\GWTTUZSZ.RES
     1      2.8018E+01    2.6307E+01    2.9378E+01    2.5479E+01    1.7330E+03
  1.9684E+03    2.4106E+01
   5.4781E+02      5.0860E+03      5.0794E+03      2.3381E+03      2.3349E+03
2.3794E+03    2.3758E+03    2.3743E+03
   3.1383E+03      5.1140E+03      5.1057E+03      2.3675E+03      2.3604E+03
4.1124E+03    4.3442E+03    2.3984E+03
  3.6861E+03
```

SCR273\flag14\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag14\test1\10k\v3.2.3e subdirectory shows no differences through the UZ release rates in the output files compared to the SCR273\flag1\test1\10k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The differences in the results begin after the SZ computation when the SAV layer is removed. The following information shows that the SAV layer was removed from nefiisz.inp and that the GWTT

was affected. Moreover, the SZ release rates with SAV removed began at 1,700 yr, whereas these releases began at 3,200 yr with the STFF layer present. It was possible to readily modified the data to generate v3.2.3 results that matched v3.2.3e results with the SAV layer removed (refer to the filecom2.out file in SCR273\flag14\test1\10k\v3.2.3e which compares results in this run with those in SCR273\flag14\test1\10k\v3.2.3_modified). The results are consistent, as expected.

SCR273\flag14\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag14\test1\100k\v3.2.3e subdirectory shows no differences through the UZ release rates in the output files compared to the SCR273\flag1\test1\100k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The differences in the results begin after the SZ computation when the SAV layer is removed. The following information shows that the SAV layer was removed from nefiisz.inp. Moreover, the SZ release rates with SAV removed began at 2,800 yr, whereas these releases began at 3,200 yr with the SAV layer present.(Note that for the 100-kyr simulations the SEISMO flag was not activated, because of reasons described previously.) It was possible to readily modified the data to generate v3.2.3 results that matched v3.2.3e results with the SAV layer removed (refer to the filecom2.out file in SCR273\flag14\test1\100k\v3.2.3e which compares results in this run with those in SCR273\flag14\test1\100k\v3.2.3_modified). The results are consistent, as expected.

```
***** nefiisz.inp
 2    2    3  14294.9     0.0     0.0     0.0
            MIGRATION PATH PROPERTIES ARRAY
***** C:\TESTING_3.2.3E\SCR273\FLAG1\TEST1\10K\V3.2.3\NEFIISZ.INP
 2    2    3  14294.9     0.0     0.0     0.0
 3    3    4   8039.0     0.0     0.0     0.0
            MIGRATION PATH PROPERTIES ARRAY
*****


***** gwttuzsz.res
      1      2.8018E+01     2.6307E+01     2.9378E+01     2.5479E+01     1.7330E+03
1.9684E+03    2.4106E+01
  5.4781E+02    2.3196E+02    2.2538E+02    1.7412E+02    1.7093E+02    1.6429E+02
1.6072E+02    1.5917E+02
  1.8380E+02    2.5997E+02    2.5169E+02    2.0350E+02    1.9641E+02    1.8973E+03
2.1291E+03    1.8327E+02
  7.3160E+02
***** C:\TESTING_3.2.3E\SCR273\FLAG1\TEST1\10K\V3.2.3\GWTTUZSZ.RES
      1      2.8018E+01     2.6307E+01     2.9378E+01     2.5479E+01     1.7330E+03
```

1.9684E+03 2.4106E+01
5.4781E+02 5.0860E+03 5.0794E+03 2.3381E+03 2.3349E+03 2.3794E+03
2.3758E+03 2.3743E+03
3.1383E+03 5.1140E+03 5.1057E+03 2.3675E+03 2.3604E+03 4.1124E+03
4.3442E+03 2.3984E+03
3.6861E+03
*****

SCR273\flag15\test1\10k - Expected Results: The filecomp.out file in the SCR273\flag15\test1\10k\v3.2.3e subdirectory shows no differences through the SZ release rates in the output files compared to the SCR273\flag1\test1\10k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The differences in the results begin after the computation of dose which uses the pumping rate in v3.2.3 and the streamtube flow rate in v3.2.3e for the dilution volume. See the file totdose.res for the dilution volume. The pumping rate is 1.0902e+07 m3/yr (sampled parameter) in v3.2.3. This value is replaced in the v3.2.3e simulation for flag15 with 3.7452e+05 m3/yr in v3.2.3e, which is the sum of the SZ streamtube flow rates (562+585+523+377 m3/yr/m) times the mixing zone thickness (182.9616 m). In the v3.2.3e runs, a smaller dilution volume is used and the doses are higher by this ratio (e.g., the dose at 10 kyr is 1.6624E-01 mrem/yr (v3.2.3e) compared to 5.7110E-03 mrem/yr (v3.2.3). Note that the ratio of this doses is the same ratio as the dilution volume ratio (29.1). Thus, the results are reasonable and expected. Also, an additional run was performed in the SCR273\flag15\test1\10k\v3.2.3_modified subdirectory in which the pumping volume was made very small that caused the next largest dilution volume to be used in the computations. These results exactly matched those in SCR273\flag15\test1\10k\v3.2.3e (see SCR273\flag15\test1\10k\v3.2.3e\filecom2.out).

SCR273\flag15\test1\100k - Expected Results: The filecomp.out file in the SCR273\flag15\test1\100k\v3.2.3e subdirectory shows no differences through the SZ release rates in the output files compared to the SCR273\flag1\test1\100k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The differences in the results begin after the computation of dose which uses the pumping rate in v3.2.3 and the streamtube flow rate in v3.2.3e for the dilution volume. See the file totdose.res for the dilution volume. The pumping rate is 1.0902e+07 m3/yr (sampled parameter) in v3.2.3. This value is replaced in the v3.2.3e simulation for flag15 with 3.7452e+05 m3/yr in v3.2.3e, which is the sum of the SZ streamtube flow rates (562+585+523+377 m3/yr/m) times the mixing zone thickness (182.9616 m). In the v3.2.3e runs, a smaller dilution volume is used and the doses are higher by this ratio (e.g., the dose at 100 kyr is 9.2359E+00 mrem/yr (v3.2.3e) compared to 3.1716E-01 mrem/yr (v3.2.3). Note that the ratio of this doses is the same ratio as the dilution volume ratio (29.1). Thus,

the results are reasonable and expected. Also, an additional run was performed in the SCR273\flag15\test1\100k\v3.2.3_modified subdirectory in which the pumping volume was made very small that caused the next largest dilution volume to be used in the computations. These results exactly matched those in SCR273\flag15\test1\100k\v3.2.3e (see SCR273\flag15\test1\100k\v3.2.3e\filecom2.out).

TESTING FOR SCR274

SCR274\test1\10k - Expected Results: See the description above of SCR273 for flag1\test1\10k. The results are in the v3.2.3 and v3.2.3e subdirectories of SCR273 for flag1\test1\10k and are consistent with the expected results.

SCR274\test1\100k - Expected Results: See the description above of SCR273 for flag1\test1\100k. The results are in the v3.2.3 and v3.2.3e subdirectories of SCR273 for flag1\test1\100k and are consistent with the expected results. The output below from the information printed to the screen during a TPA simulation (see tpa.inp) illustrates that the early peak releases are not being treated as no releases in v3.2.3e. Note that only Tc99 was analyzed in this test for illustrative purposes because it exhibits source depletion using SF dissolution rate model 1and has no ingrowth.

```
v3.2.3e-----------------------------------------------------------------------
        subarea  1 of  7        realization   1 of   1
      ---------------------------------------------------------------------
      xec: calling uzflow
      xec: calling nfenv
      xec: calling ebsfail
         ebsfail: time of WP failure =   20525.6  yr
      xec: failed WPs from INITIAL   event =    16 at time =     0.0 yr
      xec: failed WPs from CORROSION event =  1647 at time =  20525.6 yr
       *** failed WPs: all WPs failed ***
      xec: calling ebsrel
                Highest release rates from Sub Area        1
            Tc99   2.5854E+01 [Ci/yr/SA] at  2.216E+04 yr
      xec: calling uzft
         *** NEFTRAN is skipped for this UZ path since no layers have significant ground water
      travel time. ***
                Highest release rates from UZ
            Tc99   2.5854E+01 [Ci/yr/SA] at  2.216E+04 yr
      xec: calling szft
                Highest release rates from SZ
            Tc99   1.0061E+01 [Ci/yr/SA] at  5.375E+04 yr
```

```
v3.2.3 ----------------------------------------------------------------------
        subarea  1 of  7        realization   1 of   1
      ----------------------------------------------------------------------
      xec: calling uzflow
      xec: calling nfenv
      xec: calling ebsfail
         ebsfail: time of WP failure =   20525.6  yr
      xec: failed WPs from INITIAL   event =    16 at time =     0.0 yr
      xec: failed WPs from CORROSION event =  1647 at time =  20525.6 yr
       *** failed WPs: all WPs failed ***
      xec: calling ebsrel
                Highest release rates from Sub Area        1
             Tc99   2.5854E+01 [Ci/yr/SA] at  2.216E+04 yr
      xec: calling uzft
                     There is no UZ release
      xec: calling szft
                     There is no SZ release
```

TESTING FOR SCR275

SCR275\test1\10k - Expected Results: See the description above of SCR273 for flag1\test1\10k. The results are in the v3.2.3 and v3.2.3e subdirectories of SCR273 for flag1\test1\10k and are consistent with the expected results.

SCR275\test1\100k - Expected Results: See the description above of SCR273 for flag1\test1\100k. The results are in the v3.2.3 and v3.2.3e subdirectories of SCR273 for flag1\test1\100k and are consistent with the expected results.

SCR275\test2\10k and SCR275\test2\100k - Unexpected Results: The filecomp.out file in the SCR275\test2\10k\v3.2.3e and SCR275\test2\100k\v3.2.3e subdirectories shows many differences in the output files when compared to the results in the SCR275\test2\10k\v3.2.3_modified and SCR275\test2\100k\v3.2.3_modified subdirectories. The results from these runs are quite different because of what appears to be inconsistencies in the output from ashplume.exe. The results in the ASHPLUME output file (ashplume.out) are different for the two v3.2.3e and v3.2.3_modified runs even though the input files have the same input values. Note that this is first test in which the VOLCANO flag was activated and is the reason this difference has not been observed previously. Additionally, the SNLLHS.EXE output file, lhs.out, does not have a date and time; while both the v3.2.3 and v3.2.3e versions of the ASHPLUME.EXE output file have the time and date.

****

Source Code Correction Recommended: Because of the different results, the following three findings from these test results should be addressed: (1) it is unclear why both the v3.2.3 and v3.2.3e ASHPLUME output files (ashplume.out) have the time and date, (2) the time and date are not present in the SNLLHS output file (lhs.out), and (3) the ASHPLUME output files are different for the v3.2.3 and v3.2.3e simulations (it looks as though the v3.2.3e output is correct, but it is puzzling why the v3.2.3 results are different).
****

TESTING FOR SCR276

SCR276\test1\10k - Expected Results: See the description above of SCR273 for flag1\test1\10k. The results are in the v3.2.3 and v3.2.3e subdirectories of SCR273 for flag1\test1\10k and are consistent with the expected results (i.e., the constant parameters in cp.tpa are written to this v3.2.3e file in double precision, instead of single precision as in v3.2.3).

SCR276\test1\100k - Expected Results: See the description above of SCR273 for flag1\test1\100k. The results are in the v3.2.3 and v3.2.3e subdirectories of SCR273 for flag1\test1\100k and are consistent with the expected results (i.e., the constant parameters in cp.tpa are written to this v3.2.3e file in double precision, instead of single precision as in v3.2.3).

TESTING FOR SCR277

SCR277\test1\10k - Expected Results: See the description above of SCR273 for flag1\test1\10k. The results are in the v3.2.3 and v3.2.3e subdirectories of SCR273 for flag1\test1\10k and are consistent with the expected results.

SCR277\test1\100k - Expected Results: See the description above of SCR273 for flag1\test1\100k. The results are in the v3.2.3 and v3.2.3e subdirectories of SCR273 for flag1\test1\100k and are consistent with the expected results.

SCR277\test2\10k and SCR277\test2\100k - Expected Results: The filecomp.out files in the SCR277\test2\10k\v3.2.3e and SCR277\test2\100k\v3.2.3e subdirectories show many differences in the results compared to the SCR273\flag1\test1\10k\v3.2.3 and SCR273\flag1\test1\100k\v3.2.3 subdirectories, including the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The v3.2.3_modified subdirectories contains output from simulations that stopped execution because the TPA v3.2.3 code did not have the capability to accept a tpa.inp parametre names that wasn't previously defined in the tpanames.dbs file. The differences in the v3.2.3 and v3.2.3e results arise from the additional of new sampled parameters in the tpa.inp file, which causes a different set of output values from the LHS sampling. Most significant to this test

is that not only were the 10 new sampled parameters and two flags added to the sp.tpa, cp.tpa, spquery.tpa files, but also the 10 new parameters were added to the tpanames.dbs file was shown below:

new1parameter	1
new2parameter	2
new3parameter	3
new4parameter	4
new5parameter	5
new6parameter	6
new7parameter	7
new8parameter	8
new9parameter	9
new12parameter	10

Additionally, in the samplpar.hdr file, the new parameter names are not listed with a name or abbreviation (see below):

```
Input file tpa.inp as supplied with TPA Version 3.2.4b Code.
8-27-99
TPA 3.2.3.e PVM capable, Job started: Sat Nov 06 09:21:44 1999
Names for Sampled Parameters (Nonconstant)

Specified in "tpa.inp" - Values for Each Vector

 1
 2
 3
 4
 5
 6
 7
 8
 9
10
11 AAMAI@S   ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
12 MAPM@GM   MeanAveragePrecipitationMultiplierAtGlacialMaximum
13 MATI@GM   MeanAverageTemperatureIncreaseAtGlacialMaximum[degC]
14 FOC-R     FractionOfCondensateRemoved[1/yr]
```

It would be reasonable to write either a dummy abbreviation or a number with the parameter name in this file.

****

Note Concerning This Change: It was noted that certain tpa.inp parameter names were added to the tpanames.dbs file which were previously not included in this file because the values were not considered to be sampled parameters under any circumstances (e.g., the beginning four times of SEISMO intervals, the reflux model selected, and the parameters that determine time steps).

Suggested Source Code Change This appears to be a change in the philosophy regarding the information contained in this file. For the source code change, the information in the tpanames.dbs file should match the information in the samplpar.hdr, samplpar.abb, and sp.tpa files as described in the screen messages (tpa.out)

****

SCR277\test3\10k and SCR277\test3\100k - Expected Results: The filecomp.out files in the SCR277\test3\10k\v3.2.3e and SCR277\test3\100k\v3.2.3e subdirectories show many differences in the results compared to the SCR273\flag1\test1\10k\v3.2.3 and SCR273\flag1\test1\100k\v3.2.3 subdirectories, including the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The differences in the results arise from the additional of new sampled parameters in the tpa.inp file, which causes a different set of output values from the LHS sampling. Most significant to this test is that not only was the new sampled parameter added to the sp.tpa, cp.tpa, spquery.tpa files, but also the new parameter was added to the tpanames.dbs file was shown below:

BeginningOfSEISMOWPFailureInterval3[yr]	SeisInt3
BeginningOfSEISMOWPFailureInterval4[yr]	SeisInt4
FOCTR	FOCTR1

(note that parameter name matched an abbreviation in tpanames.dbs and that the abbreviation was changed appropriately)

SCR277\test4\10k and SCR277\test4\100k - Expected Results: The filecomp.out files in the SCR277\test4\10k\v3.2.3e and SCR277\test4\100k\v3.2.3e subdirectories show many differences in the results compared to the SCR273\flag1\test1\10k\v3.2.3 and SCR273\flag1\test1\100k\v3.2.3 subdirectories, including the expected differences noted in the test plan for the cp.tpa file (single vs. double precision), the time, date and header of the run, and differences described and explained earlier in this report. The differences in the results arise from the additional of two new sampled parameters in the tpa.inp file, which causes a different set of output values from the LHS sampling. Most significant to this test is that not only were the two new sampled parameter added to the sp.tpa,

cp.tpa, spquery.tpa files, but also the new parameter was added to the tpanames.dbs file was shown below:

BeginningOfSEISMOWPFailureInterval3[yr]	SeisInt3
BeginningOfSEISMOWPFailureInterval4[yr]	SeisInt4
AbCdEfGhIjKlMnOpQrStUvWxYz	ACEGIKMO
AaCcEeGgIiKkMmOoQqSsUuWwYy	ACEGIKM1

(note that the upper case letters were the same in the two parameter names and that the abbreviation was changed appropriately)

****

Notes Concerning This Testing: Several observations were recorded during the SCR 273-277 testing which may need to be addressed at some time. These observations include:

- the sp.tpa, samplpar.res, cp.tpa, and lhs.out do not contain the values used when Importance Analysis flags are activated.

- the *gs*.* are written even though the ground surface flag (VOLCANO) is not activated. This approach is inconsistent because, the *gs*.tpa files are only written when the ground surface flag (VOLCANO) is activated.

- the ASHPLUME output file name could be changed to something different and more explanatory than junk.out.

- the logbeta and iuniform distributions are not supported in SNLLHS.

- should the Importance Analysis flags be the first information in tpa.inp?

- why are there no other *.cum files? (e.g., ebsfilt.cum, nefiisz.cum, ashplume.cum, etc.)
****

11/19/99 - 11/23/99 Follow-up the version 3.2.3e testing

Prepared a test plan to follow-up the version 3.2.3e testing. The following test plan was assembled and sent to R. Janetzke for his review and approval:

Follow-up Testing to

TPA Version 3.3 Test Plans: PA-SCR-273 to 277

Task Description: Perform follow-up testing on issues identified in testing conducted for SCRs 273 to 277 as documented in the test report submitted to R. Janetzke on 11/19/99.

Reason for Tests: The following two tests will be performed as a follow-up to SCR 273 to 277 testing: (1) Some modifications were made to version 3.2.3e to ensure the *chldmf.dat* file was not overwritten by *failt.f* when the UUL was removed in the importance analysis (Test 2) and (2) SEISMO contains a modified methodology, which is a part of the importance analysis, to compute the WP stiffness instead of using a sampled parameter in tpa.inp; the correct implementation of this methodology will be tested (Test 3); this test was not performed in the initial testing for SCRs 273 to 277, because it was not clear that this modification had been implemented. Note the *.cum files (APPEND option files) were not generated in the PC runs, but were written during UNIX runs; the TPA code will be modified for version 4.0 to address this issue and no testing will be performed in this test plan. Other issues identified in the SCR 273 to 277 testing do not require additional testing.

Analyst: Robert Rice **Date:** 11/21/99

Controlled Version: Version 3.2.3 Released July 15,1999
Modified Version: Version 3.2.3n Received from R. Janetzke on a CD 11/19/99

Tests:

Test 1. Run Versions 3.2.3 and 3.2.3n with their accompanying tpa.inp files for 10,000 and 100,000 yr with all append files ON, and ImportanceAnalysisFlag(yes=1,no=0) = 0 in Version 3.2.3n.

Purpose: Because Versions 3.2.3 and 3.2.3n should have the same results using their accompanying tpa.inp files, this test verifies the modifications introduced in Version 3.2.3e do not change the output with the importance analysis OFF.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file filecomp.bat)
- tpa.inp
- all *.res files
- all *.tpa files
- all append files (*.ech, *.rlt, and *.cum)

Pass/Fail Criteria:

The results in all output files should be the same (within the differences of single versus double precision in the cp.tpa file), except for the time and date of the run and small differences in the release rates that are attributable to modifications to the interpolator in releaset.f of v3.2.3n which allows for a variable time steps. See the filecomp.out file for the differences between these two runs.

Documentation of Testing:

This test is stored in the followup/test1 directory with 10k and 100k subdirectories; both of these subdirectories have two subdirectories (v3.2.3 and v3.2.3n). All testing output files are archived on a CD.

Test 2. Repeat the test for SCR273\flag6\test1\10k and SCR273\flag6\test1\100k, which involves running Versions 3.2.3 and 3.2.3n with their accompanying tpa.inp files for 10,000 and 100,000 yr with all append files ON, and ImportanceAnalysisFlag(yes=1,no=0) = 1 (ON) and UpperUnsaturatedLayerPresenceFlag(yes=1,no=0) = 0 (Barrier NOT Present) in Version 3.2.3n. Also, a run of the Version 3.2.3 code will be conducted by setting the tpa.inp file parameters to the values described above (i.e., rock density = 1.0e-27, rock specific heat = 0.1, rock thermal conductivity = 1000.0, drift wall emissivity = 0.4, ground surface elevation = 1072.0, Fmult = 0.1, Fow = 1.0, subarea wet fraction = 1.0, and chloride concentration = 0.0) and these results should match the Version 3.2.3n output.

Purpose: This test verifies that (1) the TPA code output is reasonable considering the UUL is removed and (2) the TPA values as described above are changed in Version 3.2.3n. In the third run with Version 3.2.3 (change tpa.inp parameter values), the test verifies that the only changes made are those associated with the tpa.inp parameters listed above. Additionally, this test verifies that zero values for the chloride concentration are found in the chlrdmf.dat file.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file filecomp.bat)
- tpa.inp
- all *.res files
- all *.tpa files
- all append files (*.ech, *.rlt, and *.cum)
- ebsfail.inp
- ebsrel.inp
- chlrdmf.dat

Pass/Fail Criteria:

The results from Versions 3.2.3 and 3.2.3n (with the UUL flag = 0) should be different and most likely will show earlier and larger releases from the EBS, UZ, and SZ and larger groundwater doses, because the UUL has been removed. The values for the parameters described above should be in the ebsfail.inp, ebsrel.inp, and chlrdmf.dat files. For the second run of Version 3.2.3 (using the above values for the input parameters), the output files should be consistent with the Version 3.2.3n results. Specifically, because the chloride concentrations will be the same, WP failure time from corrosion should be consistent in v3.2.3 and

v.3.2.3n. See the filecomp.out file for the differences between these runs.

Documentation of Testing:

This test is stored in the followup/test2 directory with 10k and 100k subdirectories; both of these subdirectories have two subdirectories (v3.2.3n and v3.2.3_modified). The second subdirectory (v3.2.3_modified) contains output for the Version 3.2.3 run with modified tpa.inp parameters (see the previous section). The Version 3.2.3 results (not modified tpa.inp values) are the same files as those stored in the v3.2.3 subdirectory in followup/test1/10k and followup/test1/100k. All testing output files are archived on a CD.

Test 3. This test will verify the implementation of the method to compute the WP stiffness in v3.2.3n, instead of the v3.2.3 method which uses a value specified in the tpa.inp file. The SEISMO module contains a methodology, which is a part of the importance analysis, to compute the WP stiffness instead of using a sampled parameter in tpa.inp. The correct implementation of this methodology will be tested. This test was not performed in the initial testing for SCRs 273 to 277, because it was not clear that this modification had been implemented. To accomplish this testing, runs of versions 3.2.3 and 3.2.3n with their accompanying tpa.inp files will be conducted for 10,000 and 100,000 yr with all append files ON, and ImportanceAnalysisFlag(yes=1,no=0) = 0 in Version 3.2.3n. The only change to the v3.2.3 tpa.inp file will be specifying a constant value for the WP stiffness that is consistent with the value that should be computed in v3.2.3n. The WP stiffness will be computed using the following equations.

```
 WPWall = OuterWPThickness + AInnerWPThickness
 Rave = WPDiameter - WPWall/2.0d0
 Package_Stiffness = 48.d0 * Package_Modulus * 3.14159d0 *
&                    Rave**3 * WPWall /  WPLength**3
```

with the following values (these values are specified in tpa.inp):

OuterWPThickness = 0.1 m
AInnerWPThickness = 0.02 m
WPDiameter = 1.802 m
Package_Modulus = 2.07 x 10^{11} Pa
WPLength = 5.682 m

Thus, using these values, Package_Stiffness = 1.2146 x 10^{10} Pa-m. This value will be specified in the v3.2.3 tpa.inp file for the WP stiffness.

Purpose: This test verifies the correct implementation of the above equations which are used to compute the WP stiffness.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file filecomp.bat)
- tpa.inp
- all *.res files
- all *.tpa files
- all append files (*.ech, *.rlt, and *.cum)

Pass/Fail Criteria:

The results in all output files should be the same (within the differences of single versus double precision in the cp.tpa file), except for the time and date of the run. See the filecomp.out file for the differences between these two runs.

Documentation of Testing:

This test is stored in the followup/test3 directory with 10k and 100k subdirectories; both of these subdirectories have two subdirectories (v3.2.3n and v3.2.3_modified). The second subdirectory (v3.2.3_modified) contains output for the Version 3.2.3 run with modified tpa.inp parameters for WP stiffness (see the previous section). The Version 3.2.3 results (not modified tpa.inp values) are the same files as those stored in the v3.2.3 subdirectory in followup/test1/10k and followup/test1/100k. All testing output files are archived on a CD.

Approved by: **Date:**

Follow-up testing for SCRs 273 to 277 was performed and the results summarized below. This write-up will be extracted and used for the test report.

Note: In the follow-up test results provided in this report, the v3.2.3 and v3.2.3n output is different not only because of the reasons identified in the tet plan (i.e., differences of single versus double precision in the cp.tpa file and the time and date of the run) but also because of changes introduced in the versions from 3.2.3e to 3.2.3n. Specifically, the releaset.f values are somewhat different because of a modification in the interpolation algorithm that allowed for variable time steps. Also, determination of the SEISMO magnitude of events was changed from the method in v3.2.3 and v3.2.3e to the method in v3.2.3n. Consequently, comparison of the results as described in the follow-up test plan may need to be altered slightly. Any differences will be highlighted in the following discussion of results.

follow_up\test1\10k - Expected Results: This test is establishes a baseline between the version 3.2.3 and 3.2.3n results for 10,000 yr and is a follow-up to SCR273\flag1\test1\10k. The filecomp.out file in follow_up\test1\10k\v3.2.3n shows reasonable results and no unexpected differences in the output files

when compared to the results in the follow_up\test1\10k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision); the time, date and header of the run; and the differences in the release rates from releaset.f and the magnitude of the seismic events, which were expected as described at the beginning of this test report.

follow_up\test1\100k - Expected Results: This test is establishes a baseline between the version 3.2.3 and 3.2.3n results for 100,000 yr and is a follow-up to SCR273\flag1\test1\100k. The filecomp.out file in follow_up\test1\100k\v3.2.3n shows reasonable results and no unexpected differences in the output files when compared to the results in the follow_up\test1\100k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision); the time, date and header of the run; and the differences in the release rates from releaset.f and the magnitude of the seismic events, which were expected as described at the beginning of this test report.

follow_up\test2\10k - Expected Results: This test is a follow-up to SCR273\flag6\test1\10k. The filecomp.out file in follow_up\test2\10k\v3.2.3n shows reasonable results and no unexpected differences in the output files when compared to the results in the follow_up\test2\10k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision); the time, date and header of the run; and the differences in the release rates from releaset.f and the magnitude of the seismic events, which were expected as described at the beginning of this test report. Specifically, this test verifies that the chloride concentration is zeroed out in the chlrdmf.dat file for v3.2.3n when the UUL is removed.

follow_up\test2\100k - Expected Results: This test is a follow-up to SCR273\flag6\test1\100k. The filecomp.out file in follow_up\test2\100k\v3.2.3n shows reasonable results and no unexpected differences in the output files when compared to the results in the follow_up\test2\100k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision); the time, date and header of the run; and the differences in the release rates from releaset.f and the magnitude of the seismic events, which were expected as described at the beginning of this test report. Specifically, this test verifies that the chloride concentration is zeroed out in the chlrdmf.dat file for v3.2.3n when the UUL is removed.

follow_up\test3\10k and follow_up\test3\100k - Expected Results: This test is a follow-up to the SCR273\flag1\test1\10k and SCR273\flag1\test1\100k testing which identified a difference in the implementation of the WP stiffness (i.e., a tpa.inp parameter in v3.2.3 and a computed value in v3.2.3n). The filecomp.out file in follow_up\test3\10k\v3.2.3n shows reasonable results and no unexpected differences in the output files when compared to the results in the follow_up\test3\10k\v3.2.3 subdirectory, except for the expected differences noted in the test plan for the cp.tpa file (single vs. double precision); the time, date and header of the run; and the differences in the release rates from releaset.f and the magnitude of the seismic events, which were expected as described at the beginning of this test report. Because of the change in the methodology used to determine the magnitude of the seismic event and that there were no seismic events in both v3.2.3 and v3.2.3n output, it was not possible to directly match outputs. However, a hand calculation using an equation in the v3.2.3n seismo.f and the values specified in tpa.inp that were used to compute the WP stiffness in v3.2.3n was consistent with the constant value for the WP stiffness specified in v3.2.3 tpa.inp. The hand calculation and source code in v3.2.3n seismo.f are shown below:

```
 WPWall = OuterWPThickness + AInnerWPThickness
 Rave = WPDiameter - WPWall/2.0d0
 Package_Stiffness = 48.d0 * Package_Modulus * 3.14159d0 *
&                    Rave**3 * WPWall /  WPLength**3
```

with the following values (these values are specified in tpa.inp):

```
OuterWPThickness = 0.1 m
AInnerWPThickness = 0.02 m
WPDiameter = 1.802 m
Package_Modulus = 2.07 x 10^11 Pa
WPLength = 5.682 m
```

Using these values, Package_Stiffness = 1.2146 x 10^{10} Pa-m. A value of 1.21 x 10^{10} Pa-m was specified in v3.2.3 tpa.inp.

1/10/00 - 1/12/00

Modified the TPA Version 3.3a source code to allow the user to select the water contact mode (i.e., either bathtub or flowthrough) for each of the eight WP failure modes (initial, faulting, volcanic, seismic intervals 1 to 4, and corrosion). Modifications were made to add the following text with 8 flags to the tpa.inp file:

```
iflag
WaterContactMode_Initial(0=BathTub,1=FlowThrough)
0
**
iflag
WaterContactMode_Faulting(0=BathTub,1=FlowThrough)
1
**
iflag
WaterContactMode_Volcanic(0=BathTub,1=FlowThrough)
1
**
iflag
WaterContactMode_SeismicInterval1(0=BathTub,1=FlowThrough)
0
**
iflag
WaterContactMode_SeismicInterval2(0=BathTub,1=FlowThrough)
0
**
iflag
WaterContactMode_SeismicInterval3(0=BathTub,1=FlowThrough)
0
**
```

```
iflag
WaterContactMode_SeismicInterval4(0=BathTub,1=FlowThrough)
0
**
iflag
WaterContactMode_Corrosion(0=BathTub,1=FlowThrough)
0
```

(Note that the default water contact modes were set as the flowthrough model for faulting and volcano and to bathtub for the initial, 4 seismic, and corrosion WP failure modes.)

The following flag was removed from tpa.inp because it was no longer needed:

```
iflag
FlowModelFlag(0=BathTub,1=FlowThrough)
0
```

The ebsrel.f source code was modified to write the above eight new flags to the releaset.f input file, ebsrel.inp. However, the template file for ebsrel.inp, ebsrel.def, also needed modifications as shown below:

```
**********************************************************************
```

(old line)

```
2335., 1.0, 0                          ! xcon: # of WP; sawetfrac: wetted
subarea; bathflow: flow model
```

(new line)

```
2335., 1.0                             ! xcon: # of WP; sawetfrac: wetted
subarea

**********************************************************************
```

(old lines)

```
\Fuel leaching model paramters
5.e-1                            ! wetfrac(1): ht. fraction of wet SF in
initially def. WPs
5.e-1                            ! wetfrac(2): ht. fraction of wet SF in
faulting failure WPs
5.e-1                            ! wetfrac(3): ht. fraction of wet SF in
volcanic failure WPs
5.e-1                            ! wetfrac(4): ht. fraction of wet SF in
seismt1 failure WPs
```

```
5.e-1                          ! wetfrac(5): ht. fraction of wet SF in
seismt2 failure WPs
5.e-1                          ! wetfrac(6): ht. fraction of wet SF in
seismt3 failure WPs
5.e-1                          ! wetfrac(7): ht. fraction of wet SF in
seismt4 failure WPs
5.e-1                          ! wetfrac(8): ht. fraction of wet SF in
corrosion failure WPs
```

(new lines)

```
\Fuel leaching model paramters and water contact mode (bathtub=0,
flowthru=1)
5.e-1          0        ! wetfrac(1),iwatcont(1): init def ht fract of
wet SF and water contact
5.e-1          1        ! wetfrac(2),iwatcont(2): fau fail ht fract of
wet SF and water contact
5.e-1          1        ! wetfrac(3),iwatcont(3): vol fail ht fract of
wet SF and water contact
5.e-1         0        ! wetfrac(4),iwatcont(4): seim1 fail ht fract of
wet SF and water contact
5.e-1         0        ! wetfrac(5),iwatcont(5): seim2 fail ht fract of
wet SF and water contact
5.e-1         0        ! wetfrac(6),iwatcont(6): seim3 fail ht fract of
wet SF and water contact
5.e-1         0        ! wetfrac(7),iwatcont(7): seim4 fail ht fract of
wet SF and water contact
5.e-1          0        ! wetfrac(8),iwatcont(8): cor fail ht fract of
wet SF and water contact
```

****

Using the modified ebsrel.f, tpa.inp, and ebsrel.def files, the TPA code was compiled using LF90 and a simulation performed. This TPA simulation stopped during execution of releaset.f, because the bathtub/flowthrough value was removed from the ebsrel.def (and hence the ebsrel.inp files). However, this testing showed that values for the eight flags specified in tpa.inp were correctly written to the ebsrel.inp file; and the ebsrel.inp template, ebsrel.def, was modified correctly. The following lines from ebsrel.inp show the correct implementation of these modifications:

(old ebsrel.inp)

```
   2.78000E+02     8.08114E-01   0 ! xcon: # of WP; sawetfrac: wetted
subarea; bathflow: flow model

. . .
```

```
\Fuel leaching model paramters
 1.99136E-01                    ! wetfrac(1): ht. fraction of wet SF in
initially def. WPs
 7.59571E-01                    ! wetfrac(2): ht. fraction of wet SF in
faulting failure WPs
 1.63517E-01                    ! wetfrac(3): ht. fraction of wet SF in
volcanic failure WPs
 9.49294E-01                    ! wetfrac(4): ht. fraction of wet SF in
seismt1 failure WPs
 4.53967E-01                    ! wetfrac(5): ht. fraction of wet SF in
seismt2 failure WPs
 1.64902E-01                    ! wetfrac(6): ht. fraction of wet SF in
seismt3 failure WPs
 7.60013E-01                    ! wetfrac(7): ht. fraction of wet SF in
seismt4 failure WPs
 8.08787E-01                    ! wetfrac(8): ht. fraction of wet SF in
corrosion failure WPs
```

(new ebsrel.inp)

```
   1.66300E+03    8.08114E-01     ! xcon: # of WP; sawetfrac: wetted

. . .

\Fuel leaching model paramters and water contact mode (bathtub=0,
flowthru=1)
 1.70100E-01   0        ! wetfrac(1),iwatcont(1): init def ht fract of
wet SF and water contact
 7.59571E-01   1        ! wetfrac(2),iwatcont(2): fau fail ht fract of
wet SF and water contact
 1.63517E-01   1        ! wetfrac(3),iwatcont(3): vol fail ht fract of
wet SF and water contact
 6.98734E-01   0        ! wetfrac(4),iwatcont(4): seim1 fail ht fract of
wet SF and water contact
 2.88837E-01   0        ! wetfrac(5),iwatcont(5): seim2 fail ht fract of
wet SF and water contact
 3.79248E-01   0        ! wetfrac(6),iwatcont(6): seim3 fail ht fract of
wet SF and water contact
 9.16183E-01   0        ! wetfrac(7),iwatcont(7): seim4 fail ht fract of
wet SF and water contact
 7.34452E-01   0        ! wetfrac(8),iwatcont(8): cor fail ht fract of
wet SF and water contact
```

The remaining work will be performed by R. Codell and will involve modifying releaset.f to account for different modes of water contact by failure type.

1/17/00 - 1/22/00

The following work was performed to allow for temporal variability in the Fow and Fmult factors, instead of using a sampled value specified in tpa.inp for each of these parameters. The time history for Fow and Fmult will be stored in a data file (wpflow.def) and the ebsrel.f module will utilize values in this file to write Fow and Fmult to ebsflo.dat. The ebsflo.dat file is an input file for releaset.f. A WP flow multiplication factor will be implemented similar to the chloride multiplication factor. Also, modifications will be made for the Importance Analysis. The following information provides an explanation of the source code and data file modifications.

The primary TPA input file, tpa.inp, was modified to remove the Fow and Fmult factors and to add the WP flow multiplication factor. The file comparison between the original and modified file is presented below (note that the correlations with Fow and Fmult were removed).

```
Comparing files tpa.inp and TPA.INP.ORIGINAL
***** tpa.inp
**
** rwr 1/17/00 modified to allow for temporal variability
**             in FowFactor and FmultFactor as specified
**             in the new data file, wpflow.dat, and added
**             the waste package flow multiplication factor
** lognormal
** FowFactor
** 0.01, 3.0
**
** lognormal
** FmultFactor
** 0.01, 0.2
**
***** TPA.INP.ORIGINAL
**
lognormal
FowFactor
0.01, 3.0
**
lognormal
FmultFactor
0.01, 0.2
**
*****

***** tpa.inp
uniform
WastePackageFlowMultiplicationFactor
0.0, 2.0
**
uniform
SubAreaWetFraction
```

```
***** TPA.INP.ORIGINAL
uniform
SubAreaWetFraction
*****

***** tpa.inp
**
** rwr 1/17/00 modified to allow for temporla variability
**             in Fmult and Fow
** correlateinputs
** FowFactor
** ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
** -0.224
**
** correlateinputs
** FowFactor
** MatrixPermeability_TSw_[m2]
** 0.13
**
** correlateinputs
** FowFactor
** SubAreaWetFraction
** -0.366
**
***** TPA.INP.ORIGINAL
**
correlateinputs
FowFactor
ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
-0.224
**
*****

***** tpa.inp
correlateinputs
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Pu
0.964
**
***** TPA.INP.ORIGINAL
correlateinputs
FowFactor
MatrixPermeability_TSw_[m2]
0.13
**
*****

***** tpa.inp
correlateinputs
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_U
0.346
```

```
**
***** TPA.INP.ORIGINAL
correlateinputs
FowFactor
SubAreaWetFraction
-0.366
**
*****

***** tpa.inp
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Np
0.837
**
***** TPA.INP.ORIGINAL
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Pu
0.964
**
*****

***** tpa.inp
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Th
0.112
**
***** TPA.INP.ORIGINAL
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_U
0.346
**
*****

***** tpa.inp
correlateinputs
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_U
0.489
**
***** TPA.INP.ORIGINAL
correlateinputs
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Np
0.837
**
*****

***** tpa.inp
correlateinputs
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_Np
0.881
```

```
**
***** TPA.INP.ORIGINAL
correlateinputs
AlluviumMatrixRD_SAV_Am
AlluviumMatrixRD_SAV_Th
0.112
**
*****

***** tpa.inp
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_Th
0.109
**
***** TPA.INP.ORIGINAL
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_U
0.489
**
*****

***** tpa.inp
correlateinputs
AlluviumMatrixRD_SAV_Np
AlluviumMatrixRD_SAV_Th
0.260
**
***** TPA.INP.ORIGINAL
correlateinputs
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_Np
0.881
**
*****

***** tpa.inp
correlateinputs
AlluviumMatrixRD_SAV_Np
AlluviumMatrixRD_SAV_U
0.610
**
***** TPA.INP.ORIGINAL
correlateinputs
AlluviumMatrixRD_SAV_Pu
AlluviumMatrixRD_SAV_Th
0.109
**
*****

***** tpa.inp
correlateinputs
AlluviumMatrixRD_SAV_Th
```

```
***** TPA.INP.ORIGINAL
correlateinputs
AlluviumMatrixRD_SAV_Np
AlluviumMatrixRD_SAV_Th
0.260
**
correlateinputs
AlluviumMatrixRD_SAV_Np
AlluviumMatrixRD_SAV_U
0.610
**
correlateinputs
AlluviumMatrixRD_SAV_Th
*****
```

To accommodate the new sampled parameter for the WP flow multiplication factor and the removal of Fow and Fmult from the tpa.inp file, the tpanames.dbs file was modified as shown in the following comparison file.

```
Comparing files tpanames.dbs and TPANAMES.DBS.ORIGINAL
***** tpanames.dbs
FractureToughness[MPa-m**0.5]                                    FracTgh
SubAreaWetFraction                                               SbArWt%
***** TPANAMES.DBS.ORIGINAL
FractureToughness[MPa-m**0.5]                                    FracTgh
FowFactor                                                        Fow*
FmultFactor                                                      Fmult*
SubAreaWetFraction                                               SbArWt%
*****

***** tpanames.dbs
WastePackageFlowMultiplicationFactor                             WPFlowMF
***** TPANAMES.DBS.ORIGINAL
*****
```

The template file, ebsrel.def, for the releaset.f input file, ebsrel.inp, was also modified by removing the Fow and Fmult variables. The comparison file is provided below.

```
Comparing files ebsrel.def and EBSREL.DEF.ORIGINAL
***** ebsrel.def
'ebsflo.dat'                    ! hydfil: flow parameters file
|
***** EBSREL.DEF.ORIGINAL
'ebsflo.dat'                    ! hydfil: flow parameters file
1.0, 0.9                       ! fmult; fow: fraction of flow into the
wp
|
*****
```

Because the template file, ebsrel.def, for the releaset.f input file, ebsrel.inp, was modified, the TPA module ebsrel.f which writes ebsrel.inp from ebsrel.def also needed to be modified. The ebsrel.f module also writes the ebsflo.dat file which contains the time history of Fow and Fmult and the flow rate of water towards the WP (before diversions modeled by Fow and Fmult) that is modified by the WP flow multiplication factor. The comparison file showing these modifications is provided below.

```
Comparing files ebsrel.f and EBSREL.F.ORIGINAL
***** ebsrel.f
      common / ebsrel10 / iebsnefdat
cc rwr 1/12/00 modified to allow temporal variability
cc             in Fow and Fmult
cc       common / ebsrel11 / ifmult, ifow
      common / ebsrel11 / iwpflow

      common / ebsrel13 / iiappend_flag
***** EBSREL.F.ORIGINAL
      common / ebsrel10 / iebsnefdat
      common / ebsrel11 / ifmult, ifow
      common / ebsrel13 / iiappend_flag
*****

***** ebsrel.f

cc rwr 1/12/00 modified to allow temporal variability
cc             in Fow and Fmult
      dimension flowtimdef(100000)
      dimension fmultdef(100000)
      dimension fowdef(100000)
      dimension fmultnew(maxntime)
      dimension fownew(maxntime)

cc
***** EBSREL.F.ORIGINAL

cc
*****

***** ebsrel.f
        irelfracout = igetunitnumber('ebsrel  ')

cc rwr 1/17/00 modified to allow for temporal variability
cc             in Fow and Fmult
        call clearchar(80,command)
        command = 'cp ' // dpath // 'data/wpflow.def .'
        istatus=zportsh(command)
***** EBSREL.F.ORIGINAL
        irelfracout = igetunitnumber('ebsrel  ')

        iebspacnuc = igetunitnumber('ebsrel  ')
        ifirsttime = 1
```

```
        call clearchar( 60, name )
        name = 'InvertBypass(0=ebsfilt,1=bypass-ebsfilt)'
        iinvflg = ispquery( name )
        invflg = ivaluesp(iinvflg)
cc
cc >>>***   EBSFILT unit number section.   ***<<<
cc
      if (invflg .eq. 0) then
        iebsfilttmp = igetunitnumber('ebsrel  ')
        iebsfiltinp = igetunitnumber('ebsrel  ')
      end if

c       Copy .def files for later modification.
c       These files stay open through all realizations.

        call clearchar(80,command)
        command = 'cp ' // dpath // 'data/ebsrel.def .'
        istatus=zportsh(command)
*****

***** ebsrel.f
        endif
cc rwr 1/17/00 note that wpflow.def is the template data
cc             file from the data subdirectory and wpflow.dat
cc             contains fmult and fow values interpolated from
cc             wpflow.def to TPA time steps (these values, or
cc             the values set in the Importance Analysis, are written
cc             to ebsflo.dat
        iwpflowdat1 = igetunitnumber('ebsrel  ')
        iwpflowdat2 = igetunitnumber('ebsrel  ')
        open(unit=iwpflowdat1,file='wpflow.def',status='old')
        open(unit=iwpflowdat2,file='wpflow.dat',status='unknown')
        read(iwpflowdat1,'(a80)',err=50) aline
        write(iwpflowdat2,'(a80)') aline
        read(iwpflowdat1,'(a80)',err=50) aline
        write(iwpflowdat2,'(a80)') aline
        icount = 0
        do while (.true.)
          icount = icount + 1
          read(iwpflowdat1,*,err=50,end=60)
     &       flowtimdef(icount),fmultdef(icount),fowdef(icount)
          if (icount .ge. 100000) then
            print *, ' ***>>> Error in ebsrel <<<*** '
            print *, ' the number of times in wpflow.dat'
            print *, ' exceeds the maximum (100000)'
            stop
          endif
        enddo
 50     continue
        print *, ' ***>>> Error in ebsrel <<<*** '
        print *, ' can not read from wpflow.def'
        stop
```

```
 60     continue
        close(iwpflowdat1)
        icount = icount - 1
        call maplist(icount, flowtimdef(1), fmultdef(1),
     &    ntim, tim(1), fmultnew(1))
        call maplist(icount, flowtimdef(1), fowdef(1),
     &    ntim, tim(1), fownew(1))
        do i = 1,ntim
          write(iwpflowdat2,'(3(1pe14.5))') tim(i),
     &      fmultnew(i), fownew(i)
        enddo
        close(iwpflowdat2)

        iebspacnuc = igetunitnumber('ebsrel  ')
        ifirsttime = 1

        call clearchar( 60, name )
        name = 'InvertBypass(0=ebsfilt,1=bypass-ebsfilt)'
        iinvflg = ispquery( name )
        invflg = ivaluesp(iinvflg)

cc
cc >>>***   EBSFILT unit number section.   ***<<<
cc
***** EBSREL.F.ORIGINAL
        endif
cc
cc >>>***   EBSFILT data copy section.   ***<<<
cc
*****

***** ebsrel.f
      if (invflg .eq. 0) then
        iebsfilttmp = igetunitnumber('ebsrel  ')
        iebsfiltinp = igetunitnumber('ebsrel  ')
      end if

c       Copy .def files for later modification.
c       These files stay open through all realizations.

***** EBSREL.F.ORIGINAL
      if (invflg .eq. 0) then
cc ebsfilt.f standalone code (which writes ebsnef2.dat).

*****

***** ebsrel.f
        call clearchar(80,command)
        command = 'cp ' // dpath // 'data/ebsrel.def .'
        istatus=zportsh(command)
***** EBSREL.F.ORIGINAL
        call clearchar(80,command)
```

```
        command = 'cp ' // dpath // 'data/ebsfilt.def .'
        istatus=zportsh(command)
*****

***** ebsrel.f
        endif
cc
cc >>>***   EBSFILT data copy section.   ***<<<
cc
***** EBSREL.F.ORIGINAL
        endif
      end if

c       Open .def files for later modification.
c       These files stay open through all realizations.

        open(unit=iebsreltmp, file='ebsrel.def', status='old' )

cc
cc >>>***   EBSFILT open .def file section.   ***<<<
cc
*****

***** ebsrel.f
      if (invflg .eq. 0) then
cc ebsfilt.f standalone code (which writes ebsnef2.dat).

        call clearchar(80,command)
        command = 'cp ' // dpath // 'data/ebsfilt.def .'
        istatus=zportsh(command)
***** EBSREL.F.ORIGINAL
      if (invflg .eq. 0) then
        open(unit=iebsfilttmp, file='ebsfilt.def', status='old' )
      end if

c       Copy over other files such as executable programs.

        call clearchar(80, command)
        command = 'cp ' // path // 'codes/releaset.e .'
        istatus=zportsh(command)
*****

***** ebsrel.f
        endif
      end if

c       Open .def files for later modification.
c       These files stay open through all realizations.

        open(unit=iebsreltmp, file='ebsrel.def', status='old' )

cc
```

```
cc >>>***   EBSFILT open .def file section.   ***<<<
cc
***** EBSREL.F.ORIGINAL
        endif
cc
cc >>>***   EBSFILT copy executable section.   ***<<<
cc
*****

***** ebsrel.f
      if (invflg .eq. 0) then
        open(unit=iebsfilttmp, file='ebsfilt.def', status='old' )
      end if

c       Copy over other files such as executable programs.

        call clearchar(80, command)
        command = 'cp ' // path // 'codes/releaset.e .'
        istatus=zportsh(command)
***** EBSREL.F.ORIGINAL
      if (invflg .eq. 0) then
cc ebsfilt.f standalone code (which writes ebsnef2.dat).
        call clearchar(80, command)
        command = 'cp ' // path // 'codes/ebsfilt.e .'
        istatus=zportsh(command)
*****

***** ebsrel.f
        endif
cc
cc >>>***   EBSFILT copy executable section.   ***<<<
cc
      if (invflg .eq. 0) then
cc ebsfilt.f standalone code (which writes ebsnef2.dat).
        call clearchar(80, command)
        command = 'cp ' // path // 'codes/ebsfilt.e .'
        istatus=zportsh(command)
        if( istatus .ne. 0 ) then
          print *, ' ***>>> Error in ebsrel <<<*** '
          print *, ' istatus .ne. 0 '
          print *, ' istatus = sh( ', command, ' )'
          print *, ' istatus = ', istatus
          stop
        endif
      end if
***** EBSREL.F.ORIGINAL
        endif
      end if
*****

***** ebsrel.f
```

```
cc rwr 1/17/00 modified to allow temporal variability
cc             in Fow and Fmult
cc         call clearchar( 60, name )
cc         name = 'FmultFactor'
cc         ifmult = ispquery( name )
cc
cc         call clearchar( 60, name )
cc         name = 'FowFactor'
cc         ifow = ispquery( name )
        call clearchar( 60, name )
        name = 'WastePackageFlowMultiplicationFactor'
        iwpflow = ispquery( name )

***** EBSREL.F.ORIGINAL

        call clearchar( 60, name )
        name = 'FmultFactor'
        ifmult = ispquery( name )

*****

***** ebsrel.f
        call clearchar( 60, name )
        name = 'SubAreaWetFraction'
        i_sawetfrac = ispquery( name )

***** EBSREL.F.ORIGINAL
        call clearchar( 60, name )
        name = 'FowFactor'
        ifow = ispquery( name )

*****

***** ebsrel.f
        call clearchar( 60, name )
        name = 'WastePackagePayload[MTU]'
        i_wp_payload = ispquery( name )

***** EBSREL.F.ORIGINAL
        call clearchar( 60, name )
        name = 'SubAreaWetFraction'
        i_sawetfrac = ispquery( name )

*****

***** ebsrel.f
        call clearchar( 60, name )
        name = 'DefectiveFractionOfWPs/cell'
        i_deffrac = ispquery( name )

***** EBSREL.F.ORIGINAL
        call clearchar( 60, name )
```

```
        name = 'WastePackagePayload[MTU]'
        i_wp_payload = ispquery( name )

*****

***** ebsrel.f
        call clearchar( 60, name )
        name = 'OutputMode(0=None,1=All,2=UserDefined)'
        iiappend_flag  =  ispquery( name )

***** EBSREL.F.ORIGINAL
        call clearchar( 60, name )
        name = 'DefectiveFractionOfWPs/cell'
        i_deffrac = ispquery( name )

*****

***** ebsrel.f
        call clearchar( 60, name )
        name = 'UserDefinedLowerRealizationAppended'
        iiappend_lower  =  ispquery( name )

***** EBSREL.F.ORIGINAL
        call clearchar( 60, name )
        name = 'OutputMode(0=None,1=All,2=UserDefined)'
        iiappend_flag  =  ispquery( name )

*****

***** ebsrel.f
        call clearchar( 60, name )
        name = 'UserDefinedUpperRealizationAppended'
        iiappend_upper  =  ispquery( name )

***** EBSREL.F.ORIGINAL
        call clearchar( 60, name )
        name = 'UserDefinedLowerRealizationAppended'
        iiappend_lower  =  ispquery( name )

*****

***** ebsrel.f
        call clearchar( 60, name )
        name = 'SelectAppendFiles'
***** EBSREL.F.ORIGINAL
        call clearchar( 60, name )
        name = 'UserDefinedUpperRealizationAppended'
        iiappend_upper  =  ispquery( name )

        call clearchar( 60, name )
        name = 'SelectAppendFiles'
*****
```

```
***** ebsrel.f

cc rwr 1/17/00 modified to allow temporal variability
cc             in Fow and Fmult
cc      read(iebsreltmp, 100 ) aline
cc       fow = valuesp( ifow )
cc       fow = aiafilter( 'FowFactor', fow )
cc
cc       fmult = valuesp( ifmult )
cc       fmult = aiafilter( 'FmultFactor', fmult )
cc
cc       write( aline(1:30), fmt='(2(1pe14.5,1x))' ) fmult, fow

CC   oldLINE 19
***** EBSREL.F.ORIGINAL

      read(iebsreltmp, 100 ) aline
      fow = valuesp( ifow )
      fow = aiafilter( 'FowFactor', fow )

      fmult = valuesp( ifmult )
      fmult = aiafilter( 'FmultFactor', fmult )

      write( aline(1:30), fmt='(2(1pe14.5,1x))' ) fmult, fow
CC   oldLINE 19
*****

***** ebsrel.f
CC      LINE 23
cc       write(iebsrelinp, 100 ) aline

***** EBSREL.F.ORIGINAL
CC      LINE 23
      write(iebsrelinp, 100 ) aline

*****

***** ebsrel.f
c-----------------------------------------------------------------------

cc rwr 1/17/00 modified to allow for temporal variability
cc             in Fow and Fmult
      wpflow = valuesp( iwpflow )
      wpflow =
     &  aiafilter( 'WastePackageFlowMultiplicationFactor', wpflow )

C==>      liquid flow rate
***** EBSREL.F.ORIGINAL
c-----------------------------------------------------------------------

C==>      liquid flow rate
*****
```

```
***** ebsrel.f
 836      format( i15, '            ! number of rows of data to follow')

cc rwr 1/17/00 modified to allow for temporal variability
cc             in Fow and Fmult
cc           write( iebsflodat, 837 ) tim(1), qm3peryrperwpinsahitwp(1)
cc   837       format( 2e15.4, '         ! =time(yr) and drip rate/wp
(m^3/yr)')
cc           do it = 2, ntim
cc                                write(  iebsflodat,  838  )  tim(it),
qm3peryrperwpinsahitwp(it)
cc  838        format( 2e15.4 )
cc           enddo
        iwpflowdat3 = igetunitnumber('ebsrel  ')
        open(unit=iwpflowdat3,file='wpflow.dat',status='old')
        read(iwpflowdat3,'(a80)') aline
        read(iwpflowdat3,'(a80)') aline
        do icount = 1,ntim
          read(iwpflowdat3,*)
     &       ajunktime,fmultnew(icount),fownew(icount)
        enddo
        close(iwpflowdat3)

        write( iebsflodat, 837 ) tim(1),
     &     qm3peryrperwpinsahitwp(1) * wpflow, fmultnew(1), fownew(1)
 837     format(4(1pe14.5),'       ! t(yr),drip/wp(m^3/yr),fmult,fow')
         do it = 2, ntim
           write( iebsflodat, 838 ) tim(it),
     &       qm3peryrperwpinsahitwp(it) * wpflow,
     &       fmultnew(it) , fownew(it)
 838       format( 4(1pe14.5) )
         enddo
         close( unit=iebsflodat )

***** EBSREL.F.ORIGINAL
 836      format( i15, '            ! number of rows of data to follow')
          write( iebsflodat, 837 ) tim(1), qm3peryrperwpinsahitwp(1)
 837      format( 2e15.4, '       ! time(yr) and drip rate/wp (m^3/yr)')
          do it = 2, ntim
           write( iebsflodat, 838 ) tim(it), qm3peryrperwpinsahitwp(it)
 838        format( 2e15.4 )
          enddo
          close( unit=iebsflodat )

*****
```

Note that the changes listed previously in ebsrel.f will modify the format for ebsflo.dat. The "old" and "new" formats for ebsflo.dat are listed below.

(old format)

```
            1.0                  ! flowfactr: flow factor
            201               ! number of rows of data to follow
     0.0000E+00     0.0000E+00       ! time(yr) and drip rate/wp (m^3/yr)
     0.2310E+01     0.6257E+00

. . .

     0.9543E+04     0.3560E+00
     0.9769E+04     0.3562E+00
     0.1000E+05     0.3562E+00
```

(new format)

```
            1.0                  ! flowfactr: flow factor
            201               ! number of rows of data to follow
    0.00000E+00    0.00000E+00    4.99874E-02    5.53805E-02          !
t(yr),drip/wp(m^3/yr),fmult,fow
   2.31016E+00   1.35555E-01   4.99874E-02   5.53805E-02

. . .

   9.54325E+03   7.71246E-02   4.99874E-02   5.53805E-02
   9.76898E+03   7.71548E-02   4.99874E-02   5.53805E-02
   1.00000E+04   7.71548E-02   4.99874E-02   5.53805E-02
```

A template file containing data for the time history of Fow and Fmult was created and resides in the /data subdirectory. The name of this file is wpflow.def and its format is provided below.

```
Time history of the factors for flow diversion (Fmult) and flow
contacting waste packages (Fow) used in releaset (rwr 1/17/00)
      time (yr)        Fmult          Fow
      0.0000        4.99874E-02   5.53805E-02
    250.0000        4.99874E-02   5.53805E-02
    500.0000        4.99874E-02   5.53805E-02

. . .

  99500.0000        4.99874E-02   5.53805E-02
  99750.0000        4.99874E-02   5.53805E-02
 100000.0000        4.99874E-02   5.53805E-02
```

(note that this data is currently a placeholder or "stub" with mean values for Fow and Fmult and will most likely be replaced later)

The above template file for Fow and Fmult, wpflow.def, is read by ebsrel.f. This time history is interpolated to TPA times using the maplist utility and then these values are written to wpflow.dat.

A portion of the wpflow.dat file is provided below.

```
Time history of the factors for flow diversion (Fmult) and flow
contacting waste
      time (yr)        Fmult          Fow

   0.00000E+00   4.99874E-02   5.53805E-02
   2.31016E+00   4.99874E-02   5.53805E-02

. . .

   9.54325E+03   4.99874E-02   5.53805E-02
   9.76898E+03   4.99874E-02   5.53805E-02
   1.00000E+04   4.99874E-02   5.53805E-02
```

(note that the times in wpflow.def were interpolated to TPA times for constant values of Fow and Fmult)

To accommodate Importance Analysis, the values for Fow and Fmult should be reset to 0.1 and 1.0 in the ia.f module. Changes made in ia.f to accomplish these modifications are given below.

```
Comparing files ia.f and IA.F.ORIGINAL
***** ia.f
cc rwr 1/17/00 modified to allow for temporal variaibility
      aiacompctrlvalue(39) = 1.0d+00

      ciacompname( 1) = 'Cladding'
***** IA.F.ORIGINAL

      ciacompname( 1) = 'Cladding'
*****

***** ia.f

cc rwr 1/17/00 modified to allow for temporal variability
cc             in Fmult and Fow
      common / ia / ikeyia

      double precision aiafilter
***** IA.F.ORIGINAL

      double precision aiafilter
*****

***** ia.f
```

```
cc rwr 1/17/00 modified to allow for temporal variability
cc             in Fow and Fmult
      integer zportsh
      external igetunitnumber
      external zportsh
      character*80 command
      character*100 aline

cc  Start here.
***** IA.F.ORIGINAL

cc  Start here.
*****

***** ia.f
          end if
cc rwr 1/17/00 modified to allow for temporal variaibility
cc             in Fow and Fmult
cc       else if (param_name .eq. 'FmultFactor') then
cc           if (iacompctrlflag(25) .eq. 1) then
cc              aiafilter = aiacompctrlvalue(36)
cc           else
cc              aiafilter = sample_value
cc           end if
cc       else if (param_name .eq. 'FowFactor') then
cc           if (iacompctrlflag(25) .eq. 1) then
cc              aiafilter = aiacompctrlvalue(37)
cc           else
cc              aiafilter = sample_value
cc           end if
      else if (param_name .eq.
     &  'WastePackageFlowMultiplicationFactor') then
          if (iacompctrlflag(25) .eq. 1) then
             aiafilter = aiacompctrlvalue(39)
cc rwr 1/17/00 make sure the following is only performed once
             if (ikeyia .ne. 543262) then
               iunitwpflow1 = igetunitnumber('ebsrel  ')
               iunitwpflow2 = igetunitnumber('ebsrel  ')
cc rwr 1/17/00 replace the values in wpflow.dat with
cc            the Fow and Fmult values specified in this
cc            subroutine (use wpflow.old as a template)
               call clearchar( 80, command)
               command = 'cp wpflow.dat wpflow.old'
               istatus=zportsh(command)
               if (istatus .ne. 0) then
                 print *, ' ***>>> Error in ia <<<*** '
                 print *, ' istatus .ne. 0 '
                 print *, ' istatus = sh( ',command, ' )'
                 print *, 'istatus = ', istatus
                 stop
               endif
               call clearchar( 80, command)
```

```
                 command = 'rm wpflow.dat '
                 istatus=zportsh(command)
                 if (istatus .ne. 0) then
                   print *, ' ***>>> Error in ia <<<*** '
                   print *, ' istatus .ne. 0 '
                   print *, ' istatus = sh( ',command, ' )'
                   print *, 'istatus = ', istatus
                   stop
                 endif
                 open(unit=iunitwpflow1,file='wpflow.old',status='old')
                 open(unit=iunitwpflow2,file='wpflow.dat',status='new')
                 read(iunitwpflow1,'(a80)',err=400,end=500) aline
                 write(iunitwpflow2,'(a80)') aline
                 read(iunitwpflow1,'(a80)',err=400,end=500) aline
                 write(iunitwpflow2,'(a80)') aline
                 do while (.true.)
                   read(iunitwpflow1,*,err=400,end=500) val1,val2,val3
                   write(iunitwpflow2,'(3(1pe14.5,2x))' ) val1,
     &               aiacompctrlvalue(36), aiacompctrlvalue(37)
                 enddo
400              continue
                 print *, ' ***>>> Error in ia <<<*** '
                 print *, ' trouble reading from the wpflow.dat '
                 print *, ' file template (wpflow.old) '
                 stop
500              continue
                 close(iunitwpflow1)
                 close(iunitwpflow2)
                 call clearchar( 80, command)
                 command = 'rm wpflow.old '
                 istatus=zportsh(command)
                 if (istatus .ne. 0) then
                   print *, ' ***>>> Error in ia <<<*** '
                   print *, ' istatus .ne. 0 '
                   print *, ' istatus = sh( ',command, ' )'
                   print *, 'istatus = ', istatus
                   stop
                 endif
                 ikeyia = 543262
               endif
             else
***** IA.F.ORIGINAL
             end if
         else if (param_name .eq. 'FmultFactor') then
             if (iacompctrlflag(25) .eq. 1) then
                aiafilter = aiacompctrlvalue(36)
             else
*****

***** ia.f
             end if
```

```
      else if (param_name .eq. 'SubAreaWetFraction') then
          if (iacompctrlflag(25) .eq. 1) then
             aiafilter = aiacompctrlvalue(38)
          else
***** IA.F.ORIGINAL
          end if
      else if (param_name .eq. 'FowFactor') then
          if (iacompctrlflag(25) .eq. 1) then
             aiafilter = aiacompctrlvalue(37)
          else
*****

***** ia.f
          end if
cc
***** IA.F.ORIGINAL
          end if
      else if (param_name .eq. 'SubAreaWetFraction') then
          if (iacompctrlflag(25) .eq. 1) then
             aiafilter = aiacompctrlvalue(38)
          else
             aiafilter = sample_value
          end if
cc
*****
```

Thus, the above changes will write the Fow and Fmult values specified either in wpflow.def or in the Importance Analysis specifications to wpflow.dat and then to ebsflo.dat for the TPA time steps. Also, the WP flow multiplication factor will be multiplied by the flow rates from NFENV in ebsflo.dat.

Moreover, the Fow and Fmult factors are also utilized to write infiltration flow rates after diversion to the infilper.res. Consequently, the exec.f source code was modified to read Fow and Fmult from wpflow.dat and were then multiplied by the infiltration rates prior to being written to infilper.res. The comparison file for the exec.f modifications are listed below.

```
Comparing files exec.f and EXEC.F.ORIGINAL
***** exec.f

cc rwr 1/17/00 modified to allow for temporal variability
cc             in Fow and Fmult
      dimension fmult(maxntime)
      dimension fow(maxntime)

      character*1600 columnheader1
***** EXEC.F.ORIGINAL

      character*1600 columnheader1
*****
```

```
***** exec.f

cc rwr 1/17/00 modified to allow for temporal variability
cc             in Fow and Fmult
cc         call clearchar( 60, name )
cc         name = 'FmultFactor'
cc         ifmult = ispquery( name )
cc         fmult = valuesp( ifmult )
cc         fmult = aiafilter( 'FmultFactor', fmult )
cc
cc         call clearchar( 60, name )
cc         name = 'FowFactor'
cc         ifow = ispquery( name )
cc         fow = valuesp( ifow )
cc         fow = aiafilter( 'FowFactor', fow )
        call clearchar( 60, name )
        name = 'WastePackageFlowMultiplicationFactor'
        iwpflow = ispquery( name )
        wpflow = valuesp( iwpflow )
        wpflow =
     &    aiafilter( 'WastePackageFlowMultiplicationFactor', wpflow )
        iunitwpflow = igetunitnumber('exec    ')
        open(unit=iunitwpflow,file='ebsflo.dat',status='old')
        read(iunitwpflow,'(a80)') aline
        read(iunitwpflow,'(a80)') aline
        do itime = 1, ntim
          read(iunitwpflow,*) ajunktime, ajunkflow,
     &      fmult(itime), fow(itime)
        enddo
        close(iunitwpflow)

***** EXEC.F.ORIGINAL

        call clearchar( 60, name )
        name = 'FmultFactor'
        ifmult = ispquery( name )
        fmult = valuesp( ifmult )
        fmult = aiafilter( 'FmultFactor', fmult )

        call clearchar( 60, name )
        name = 'FowFactor'
        ifow = ispquery( name )
        fow = valuesp( ifow )
        fow = aiafilter( 'FowFactor', fow )

*****

***** exec.f
     &                                percinfil(j,itime,2)
cc rwr 1/17/00 modified to allow for temporal variability
cc             in Fow and Fmult
cc          cumpercinfil(itime,3) = cumpercinfil(itime,3) +
```

```
cc      &                                   percinfil(j,itime,2) *
cc      &                                   fmult * fow
         cumpercinfil(itime,3) = cumpercinfil(itime,3) +
     &                                percinfil(j,itime,2) *
     &                                fmult(itime) * fow(itime) *
     &                                wpflow

          enddo
***** EXEC.F.ORIGINAL
     &                                percinfil(j,itime,2)
            cumpercinfil(itime,3) = cumpercinfil(itime,3) +
     &                                percinfil(j,itime,2) *
     &                                fmult * fow
          enddo
*****
```

Prior to a discussion of the testing results and as a final note related to the source code modifications discussed previously, these changes were made to meet the format required in modifications by R. Codell to releaset.f. However, minor modifications to the releaset.f source code were made to remove Fow and Fmult from common blocks and real*8 declarations and the read statement in releaset.f for Fow and Fmult in ebsrel.inp was commented out. The comparison file for these minor modifications follow.

```
Comparing files releaset7.for and RELEASET7.FOR.ORIGINAL
***** releaset7.for
c
cc rwr 1/21/00 remove fmult and fow
cc          real*8 fmult,fow,gscmrl, oxgnovpr, phvalue, qin,
        real*8 gscmrl, oxgnovpr, phvalue, qin,
     &       r0z, flowfactr
***** RELEASET7.FOR.ORIGINAL
c
        real*8 fmult,fow,gscmrl, oxgnovpr, phvalue, qin,
     &       r0z, flowfactr
*****

***** releaset7.for
        common /ccoro1/ cftime, tcaqu, icfcon
cc rwr 1/21/00 remove fmult and fow
cc          common /cgeom / cvol, xcon, sawetfrac, fmult,fow,mtot

        common /cgeom / cvol, xcon, sawetfrac, mtot
        common /cnucl1/ elem(maxele), namall(maxnuc, maxmem)
***** RELEASET7.FOR.ORIGINAL
        common /ccoro1/ cftime, tcaqu, icfcon
        common /cgeom / cvol, xcon, sawetfrac, fmult,fow,mtot
        common /cnucl1/ elem(maxele), namall(maxnuc, maxmem)
*****

***** releaset7.for
```

```
C*** Start of declarations inserted by SPAG
cc rwr 1/21/00 remove fmult and fow
cc         real*8 amassc, cftime, ctemp, cvol, floref, flowfactr,
cc      &       fueden, fmult,fow, rpor, simtimex,
        real*8 amassc, cftime, ctemp, cvol, floref, flowfactr,
     &       fueden, rpor, simtimex,
     &       tcaqu, tflo
***** RELEASET7.FOR.ORIGINAL
C*** Start of declarations inserted by SPAG
        real*8 amassc, cftime, ctemp, cvol, floref, flowfactr,
     &       fueden, fmult,fow, rpor, simtimex,
     &       tcaqu, tflo
*****

***** releaset7.for
        common /ccoro1/ cftime, tcaqu, icfcon
cc rwr 1/21/00 remove fmult and fow
cc         common /cgeom / cvol, xcon, sawetfrac,fmult,fow,mtot
        common /cgeom / cvol, xcon, sawetfrac,mtot
        common /cnume1/ simtimex, imax, jmax
***** RELEASET7.FOR.ORIGINAL
        common /ccoro1/ cftime, tcaqu, icfcon
        common /cgeom / cvol, xcon, sawetfrac,fmult,fow,mtot
        common /cnume1/ simtimex, imax, jmax
*****

***** releaset7.for
        real*8 xfrac
cc rwr 1/21/00 remove fmult and fow
cc         real*8 floref, flowfactr, fueden, fmult,fow,
        real*8 floref, flowfactr, fueden,
     &       oxgnovpr, phvalue, r0z, radu, radsg, rpor
***** RELEASET7.FOR.ORIGINAL
        real*8 xfrac
        real*8 floref, flowfactr, fueden, fmult,fow,
     &       oxgnovpr, phvalue, r0z, radu, radsg, rpor
*****

***** releaset7.for
        common /ccoro1/ cftime, tcaqu, icfcon
cc rwr 1/21/00 remove fow and fmult
cc         common /cgeom / cvol, xcon,sawetfrac,fmult,fow, mtot
        common /cgeom / cvol, xcon,sawetfrac, mtot
        common /cnume1/ simtimex, imax, jmax
***** RELEASET7.FOR.ORIGINAL
        common /ccoro1/ cftime, tcaqu, icfcon
        common /cgeom / cvol, xcon,sawetfrac,fmult,fow, mtot
        common /cnume1/ simtimex, imax, jmax
*****

***** releaset7.for
        read (4, *) hydfil
```

```
cc rwr 1/21/00 remove fmult and fow
cc        read (4, *) fmult,fow

***** RELEASET7.FOR.ORIGINAL
        read (4, *) hydfil
        read (4, *) fmult,fow

*****
```

The following examples of TPA output and intermediate files document the first-level testing conducted to verify the correct implementation of the changes described previously (note that, because changes to ebsrel.f and ebsrel.def that allow the user to specify either the bathtub or flowthrough model for each failure type were not made in releaset.f, to allow the releaset.f code to run, the ebsrel.def file in /data was modified to specify 0 [bathtub] on the first line of data; releaset.f will be modified in the future to include this capability and remove the need for this artificial fix).

(wpflow.def)

```
Time history of the factors for flow diversion (Fmult) and flow
contacting waste packages (Fow) used in releaset (rwr 1/17/00)
      time (yr)        Fmult          Fow
      0.0000         4.99874E-02   5.53805E-02
    250.0000         4.99874E-02   5.53805E-02
    500.0000         4.99874E-02   5.53805E-02
    750.0000         4.99874E-02   5.53805E-02
```

(wpflow.dat)

```
Time history of the factors for flow diversion (Fmult) and flow
contacting waste
      time (yr)        Fmult          Fow

   0.00000E+00   4.99874E-02   5.53805E-02
   2.31016E+00   4.99874E-02   5.53805E-02
   4.67440E+00   4.99874E-02   5.53805E-02
   7.09399E+00   4.99874E-02   5.53805E-02
   9.57023E+00   4.99874E-02   5.53805E-02
```

(ebsflo.dat)

```
            1.0                ! flowfactr: flow factor
            201             ! number of rows of data to follow
    0.00000E+00    0.00000E+00    4.99874E-02    5.53805E-02          !
t(yr),drip/wp(m^3/yr),fmult,fow
```

```
   2.31016E+00   1.35555E-01   4.99874E-02   5.53805E-02
   4.67440E+00   9.51107E-02   4.99874E-02   5.53805E-02
   7.09399E+00   8.48853E-02   4.99874E-02   5.53805E-02
```

(ebsrel.def)

```
\Flow parameters
'ebsflo.dat'                        ! hydfil: flow parameters file
|
```

(ebsrel.inp)

```
\Flow parameters

'ebsflo.dat'                        ! hydfil: flow parameters file

|
```

The following portions of TPA output and intermediate files illustrate the correct implementation of the Importance Analysis.

(wpflow.dat)

```
Time history of the factors for flow diversion (Fmult) and flow
contacting waste packages (Fow) used in releaset (rwr 1/17/00)
      time (yr)        Fmult          Fow
      0.0000         4.99874E-02   5.53805E-02
    250.0000         4.99874E-02   5.53805E-02
    500.0000         4.99874E-02   5.53805E-02
    750.0000         4.99874E-02   5.53805E-02
```

(wpflow.dat)

```
Time history of the factors for flow diversion (Fmult) and flow
contacting waste
      time (yr)        Fmult          Fow

   0.00000E+00      1.00000E-01      1.00000E+00
   2.31016E+00      1.00000E-01      1.00000E+00
   4.67440E+00      1.00000E-01      1.00000E+00
   7.09399E+00      1.00000E-01      1.00000E+00
   9.57023E+00      1.00000E-01      1.00000E+00
```

(ebsflo.dat)

```
            1.0                  ! flowfactr: flow factor
            201               ! number of rows of data to follow
    0.00000E+00    6.87655E-02    1.00000E-01    1.00000E+00          !
t(yr),drip/wp(m^3/yr),fmult,fow
   2.31016E+00   6.87655E-02   1.00000E-01   1.00000E+00
   4.67440E+00   6.87655E-02   1.00000E-01   1.00000E+00
   7.09399E+00   6.87655E-02   1.00000E-01   1.00000E+00
   9.57023E+00   6.87655E-02   1.00000E-01   1.00000E+00
```

In addition to the verification testing, additional hand calculations were performed (not shown) to verify that the WP flow multiplication factor was corrected implemented in ebsrel.f as evident in ebsflo.dat and that this factor together with the temporally variable Fow and Fmult were correctly implemented in exec.f to compute values in infilper.res.

Additional testing of these modifications should be conducted once the bathtub/through option specification in releaset.f is complete.

TESTING TPA VERSION 4.0 CODE

Three SCRs were identified in the following table for testing by R. Rice (SCRs 304, 293, and 289). The testing for these three SCRs is described in the following pages. See the \testing_4.0 subdirectory on the CD accompanying the test results (submitted to R. Janetzke on 3/24/00) for the source code, executables, data, and output files. The test plans, the test results, and the scientific notebook are available in the \testing_4.0\testplan subdirectory.

The TPA Version 4.0beta code was received from R. Janetzke on a CD dated 2/18/00. Installation tests were conducted in the \testing_4.0\install_test subdirectory on an NT PC and the results compared to the results included on the CD. The output of the installation test was entirely consistent with the output files included on the CD (except for the expected differences in the time and date of the run).

The results from the TPA Version 4.0beta code were compared to the results from the TPA Version 3.3 code, which was available from R. Janetzke on a CD dated 11/29/99. The TPA Version 3.3 code files are located in the \tpa33 subdirectory.

The following pages provide the test plans and results of testing conducted for SCRs 304, 293, and 289.

TPA 4.0 Development Task List

Change #	Effort Level	Description	Implementer	Module	Work Outline	Area of Change	Tester	Status	SCR #	Rationale
0	M	Different corrosion rate for welds	Pensado/ Mohanty	failt.f	Weld corrosion built into overall corrosion calculation	code	Brossia	testing	294	Potential early failure mechanism
				ebsfail.f	Convert 6 hardwired values to input parameters.	code				
1	H	Flexibility in defining the exposure pathways	Muller	gentoo.f	Incorporate stand-alone GENII into TPA	code	LaPlante	testing	301	Capability to address concern of stakeholders
			LaPlante							
2	H	Stochastic biosphere and receptor group	Muller	gentoo.f	Incorporate stand-alone GENII into TPA, incorporate parameter for pluvial transition.	code	Weldy	testing		Capability to address concern of stakeholders
			Smith/ Janetzke/ LaPlante/ Mohanty							
4	H	Include drip shield	Pensado/ Mohanty	ebsrel.f, failt.f	New factor DRIP failure time given by CLST KTI.	code	Codell	testing	294	EDA-II Design
				tpa.inp	Add 2 new parameters.	data				
			Codell	releaset.f	Pre-exponential term.	code	Mohanty	testing		
19	L	Time-dependent mass loading (resuspension ash)	Weldy/ Esh	dcags.f	modify distribution (make time-dependent)	code	Smith	testing	292	Reduce excess conservatism
6	M	Alluvium length variation,	Menchaca/ Janetzke	szft.f	Modify hardwired minimum Tuff length	code	Menchaca	testing	300	Remove feature inconsistent with stochastic PA
			Winterle	strmtube.dat		data		testing		
		Clarify diffusion parameter	McCartin	szft.f	Add penetration distance and fractures per meter parameters.	code	Esh	testing	290	
11	L	# packages entrained in conduit and expelled to surface.	Janetzke	volcano.f	remove geometric consideration in volcano.f. Add/modify # packages distribution	code	Weldy	testing	293	Address possible non-conservatism
12	L	Number of magma induced mechanical failures remaining in drift.	Janetzke	volcano.f	Accommodate new sampled parameter.	code	Rice	testing		Improved information.

TPA 4.0 Development Task List

Change #	Effort Level	Description	Implementer	Module	Work Outline	Area of Change	Tester	Status	SCR #	Rationale
				tpa.inp	Add new sampled parameter.	data				
27	M	Temporal variability of flow rate.	Rice/ Esh	ebsrel.f	FMULT, FOW	code	Mohanty	testing	303	Improve dynamic features of code
				ebsrel.def						
			Codell	releaset.f		code				
30	H	WP Temperature	Mohanty	nfenv.f	Modify existing model based on EDA-II design	code	McCartin	testing	304	EDA-II Design
43	M	Repository layout	Janetzke	exec.f	Reflect EDA-II design	code	Rice	testing		EDA-II Design
40	M	SEISMO generate seismic events in a repeatable manner	Muller/ Janetzke	seismo.f	system -level code change	code	Janetzke	testing	298	improve interpretation.
42	M	Enable logbeta and iuniform sampled parameter distributions	Codell	snllhs.f	Add logbeta and iuniform distributions to snllhs.f.	code	Janetzke	testing	299	With these additional features the original internal Monte Carlo sampling scheme can be fully replaced with the LHS method.
8	M	Failure type dependent water contact model	Rice	ebsrel.f	Bathtub or flowthru based on failure type.	code	Pensado	testing	296	Remove potential code inconsistency
				ebsrel.def	Add new controls for failure types	data				
				tpa.inp	Add 8 flags to map failure type to model	data				
			Codell	releaset.f	Accommodate new ebsrel.inp file.	code	Mohanty	testing		
32	L	Radiolysis effects via H2O2.	Pensado/ Mohanty	failt.f ebsfail.f	New range of values for models 1 and 2 parameters.	code	Codell	testing	294	Improved infromation.
38		Variable times steps for reflux models 2 & 3.	Esh	nfenv.f	Use larger time steps after 10k years	code	Mayer	testing	305	Improve code execution.
35	L	Update mean infiltration.	Stohoff	uzflow.f	Move some of the precipitation and temperature modelling to a preprocessor .	code	Fedor	testing	291	Incorporate new theory and data, and reduce TPA run times.

TPA 4.0 Development Task List

Change #	Effort Level	Description	Implementer	Module	Work Outline	Area of Change	Tester	Status	SCR #	Rationale
45	I	Use data files for invent.f information	Rice	invent.f	Move bwr & pwr time histories and percentages to a data file.	code	Menchaca	testing	295	Improve flexibility of code.
Bug Fix		Modify qlhitsa to handle starting point outside and ending point inside quadrilateral	Janetzke	subarea.f		code	Rice	testing	289	
Bug Fix		The equation for 'average radius' in seismo was mistyped.	McCartin/ Janetzke	seismo.f	As a minimum rerun the importance analysis run that revealed the inconsistency.	Code	Pensado	testing	302	

****

SCR-304: Repository Layout

3/6/00 through 3/10/00

The test plan for SCR-304 is listed below:

TPA Test Plan SCR-304

Tester: Rob Rice

Test name: Repository Layout

Anticipated start date: March 6, 2000

Anticipated completion date: March 10, 2000

Amount of your time available to perform this test: 32 hours

Percent of testing time to be spent in process level testing and system level testing (e.g. 50/50):
90% system-level and 10% process-level testing will be performed. The TPA code reads information from the *tpa.inp* file and also uses the data in *repdes.dat* to compute the number of WPs in each drift. These values are written to the screen and to *drifts.dat*. Thus, the major effort in this testing, which will be sufficient to evaluate the correct application of this change, will be at the system level.

Output files to be checked: screen print and *drifts.dat*

Input files to be checked for proper data transfer to the program: *tpa.inp* and *repdes.dat*

Disposition of documentation (storage medium, physical location, and access method):
All tests will be archived on a CD-ROM and described in a scientific notebook that will be submitted to the TPA code custodian, Ron Janetzke, upon completion of the testing. On the CD-ROM, the \testing_4.0\ subdirectory will contain all testing output files.

Functional Test Descriptions:

Test 1: Using the repository area and 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 drifts, and the number of WPs in each drift, in addition to the correct assignment of WPs to each subarea, which are available in the screen print and *drifts.dat*.. Plots 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. These results are archived in the \testing_4.0\basecase subdirectory. Plots and EXCEL spreadsheets are archived in the \testing_4.0\data_plots subdirectory.

Test 2: Hand calculations similar to those in Test 1 will be performed using modified (tester-supplied) data for 1 subarea at 0 degrees using a 0 degree angle for the drifts. Because of the simplified geometry, the correct implementation of the changes in the TPA code will be evident by inspection of the results or by straight-forward calculations. These results are archived in the \testing_4.0\tester subdirectory.

Test 3: Hand calculations similar to those in Test 1 will be performed using modified (tester-supplied) data for 2 subareas at 0 degrees using a 0 degree angle for the drifts. Because of the simplified geometry, the correct implementation of the changes in the TPA code will be evident by inspection of the results or by straight-forward calculations. These results are archived in the \testing_4.0\tester2 subdirectory.

Test 4: Hand calculations similar to those in Test 1 will be performed using modified (tester-supplied) data for

1 subarea at -45 degrees using a -45 degree angle for the drifts. Because of the simplified geometry, the correct implementation of the changes in the TPA code will be evident by inspection of the results or by straight-forward calculations. These results are archived in the \testing_4.0\tester3 subdirectory.

Test 5: Hand calculations similar to those in Test 1 will be performed using modified (tester-supplied) data for 1 subarea at -45 degrees using a 0 degree angle for the drifts. Because of the simplified geometry, the correct implementation of the changes in the TPA code will be evident by inspection of the results or by straight-forward calculations. These results are archived in the \testing_4.0\tester4 subdirectory.

- Hand calculations: Hand calculations verify whether the computations are correct for determining the number of WPs in each subarea and each drift using an EXCEL spreadsheet or by inspection.

- Process-level: Process-level values written to the *drifts.dat* file in READER will be documented in the Tests 1 through 5 results and these values for the orientation, length, and number of WPs in each drift will be checked using the hand calculations described previously.

- System-level: Tests 1 through 5, as described above, will be performed using the TPA Version 4.0beta code. System-level results in the screen print and *wpsfail.res* file will be examined and analyzed using hand calculations to verify the WPs were correctly assigned to each subarea.

Reasonableness Test Description: Based on Tests 1 through 5 described above using TPA Version 4.0beta data and tester-supplied data, the reasonableness of the WP calculations will be verified and will be evident in the results for Tests 1 through 5.

Final Checklist (completed during testing):

- Did the modification substantially change the results? No. Because one subarea was added and the coordinates of the original seven subareas were modified slightly, there are a different number of WPs in the repository (6,920 compared to 6,427 in v3.3). This difference is attributable to the increased spent fuel emplaced in the repository (68,030 MTUs compared to about 63,000 MTUs in v3.3). These results are available in the *tpa.out* files in the \testing_4.0bkk\basecase and \tpa33\basecase subdirectories.

- Were TPA 3.3 and TPA 4.0beta compared using corresponding mean values in *tpa.inp*? Yes. A comparison in the EBS releases (*cumrel.res*) shows that the results are consistent for the mean value parameters for versions 3.3 and 4.0. These are differences can be attributed to changes introduced into version 4.0 (e.g., different number of WPs for each subarea. These results are archived in the \testing_4.0bkk\basecase_meanvalue and \tpa33\basecase_meanvalue subdirectories.

- Which nuclides were monitored to determine reasonableness of results in term of dose? The radionuclides with the highest dose rates in version 3.3 (i.e., I-129 and Cl-36) were monitored for purposes of evaluating the reasonableness of the results in terms of dose. This two radionuclides also appear in the version 4.0 results together with Tc-99. Again, the differences in the version 3.3 and 4.0 doses were reasonable. These results are also archived in the \testing_4.0bkk\basecase_meanvalue and \tpa33\basecase_meanvalue subdirectories.

Discussion of test results for SCR-304:

Test 1 Results:

The TPA Version 4.0beta code was run in the \testing_4.0\basecase subdirectory using the basecase *tpa.inp* file, except the append option was activated to generate the intermediate data transfer files (i.e., the **.rlt*, **.ech*, and **.cum* files) which are useful for process-level testing.

The following information provides the 8 subarea coordinates in the *tpa.inp* file:

```
subarea
8
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
547474.7,4077282.6
547887.3,4077238.1
547897.79,4076045.46
547655.97,4076123.07
547474.7,4077282.6
edaii 6-c
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
```

The TPA code uses these coordinates and the repository outline coordinates (including the emplacement block coordinates) in *repdes.dat* to compute the drift beginning and ending points and the number of WPs in each drift, which are available in the *drifts.dat* file. A listing of these files from the \testing_4.0\basecase subdirectory is given below:

Listing of *repdes.dat*:

```
TITLE:  test file for rep design.
**
** angle - radians
**
-.304d0
**
** rep outline vertices.
**
13
547645.27,4079656.06
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
547474.7,4077282.6
547370.95,4077922.04
547514.88,4079310.61
547645.27,4079656.06
**
** emplacement blocks
**
2
547504.18,   4079276.1, 548155.70,   4075962.6
547504.18,   4079276.1, 547732.82,   4081208.1
```

Listing of *drifts.dat*:

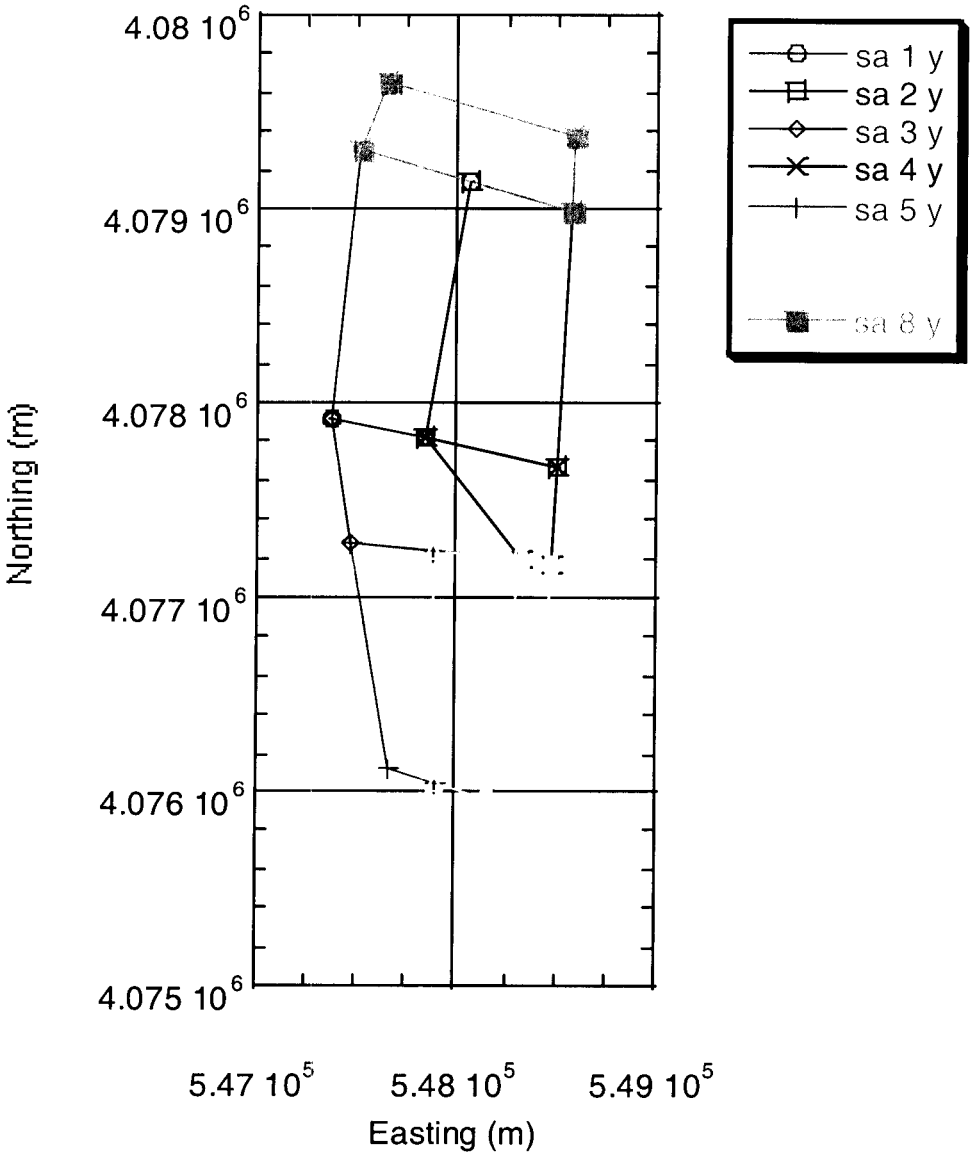
```
TITLE:
**
**
Emplacement Block
        1
**  Drift Endpoints
**   x1          y1          x2          y2        numWP
 5.48565342E+05 4.07890074E+06 5.47506817E+05 4.07923283E+06   180
 5.48561199E+05 4.07881715E+06 5.47498295E+05 4.07915061E+06   181
 5.48557056E+05 4.07873356E+06 5.47489773E+05 4.07906839E+06   182
 5.48552913E+05 4.07864996E+06 5.47481251E+05 4.07898617E+06   182
 5.48548770E+05 4.07856637E+06 5.47472728E+05 4.07890395E+06   183
```

```
 5.48544628E+05 4.07848278E+06 5.47464206E+05 4.07882173E+06  184
 5.48540485E+05 4.07839918E+06 5.47455684E+05 4.07873951E+06  185
 5.48536342E+05 4.07831559E+06 5.47447162E+05 4.07865729E+06  185
 5.48532199E+05 4.07823200E+06 5.47438639E+05 4.07857507E+06  186
 5.48528056E+05 4.07814841E+06 5.47430117E+05 4.07849286E+06  187
 5.48523913E+05 4.07806481E+06 5.47421595E+05 4.07841064E+06  188
 5.48519770E+05 4.07798122E+06 5.47413072E+05 4.07832842E+06  188
 5.48515627E+05 4.07789763E+06 5.47404550E+05 4.07824620E+06  189
 5.48511484E+05 4.07781403E+06 5.47396028E+05 4.07816398E+06  190
 5.48507341E+05 4.07773044E+06 5.47387506E+05 4.07808176E+06  191
 5.48503198E+05 4.07764685E+06 5.47378983E+05 4.07799954E+06  191
 5.48499054E+05 4.07756326E+06 5.47371783E+05 4.07791691E+06  192
 5.48494910E+05 4.07747966E+06 5.47386295E+05 4.07782746E+06  189
 5.48490766E+05 4.07739607E+06 5.47400808E+05 4.07773802E+06  186
 5.48486622E+05 4.07731248E+06 5.47415321E+05 4.07764857E+06  182
 5.48482478E+05 4.07722889E+06 5.47429833E+05 4.07755913E+06  179
 5.48478334E+05 4.07714529E+06 5.47444346E+05 4.07746968E+06  176
 5.48474191E+05 4.07706170E+06 5.47458859E+05 4.07738023E+06  173
 5.48470047E+05 4.07697811E+06 5.47473371E+05 4.07729079E+06  170
 5.48465904E+05 4.07689451E+06 5.47487378E+05 4.07720150E+06  167
 5.48461761E+05 4.07681092E+06 5.47501334E+05 4.07711223E+06  163
 5.48457618E+05 4.07672733E+06 5.47515290E+05 4.07702296E+06  160
 5.48443392E+05 4.07664690E+06 5.47529245E+05 4.07693369E+06  156
 5.48411859E+05 4.07657190E+06 5.47543201E+05 4.07684442E+06  148
 5.48380326E+05 4.07649690E+06 5.47557157E+05 4.07675515E+06  140
 5.48348794E+05 4.07642190E+06 5.47571113E+05 4.07666588E+06  132
 5.48317261E+05 4.07634690E+06 5.47585068E+05 4.07657661E+06  124
 5.48285728E+05 4.07627190E+06 5.47599024E+05 4.07648734E+06  117
 5.48254195E+05 4.07619690E+06 5.47612980E+05 4.07639806E+06  109
 5.48222663E+05 4.07612190E+06 5.47626936E+05 4.07630879E+06  101
 5.48191130E+05 4.07604690E+06 5.47640891E+05 4.07621952E+06   93
 5.48159597E+05 4.07597190E+06 5.47654847E+05 4.07613025E+06   86
**
Emplacement Block
      2
** Drift Endpoints
**  x1          y1          x2          y2        numWP
 5.48569485E+05 4.07898433E+06 5.47516426E+05 4.07931470E+06  179
 5.48573630E+05 4.07906793E+06 5.47545076E+05 4.07939061E+06  175
 5.48577774E+05 4.07915152E+06 5.47573726E+05 4.07946651E+06  171
 5.48581918E+05 4.07923511E+06 5.47602376E+05 4.07954242E+06  167
 5.48586063E+05 4.07931870E+06 5.47631026E+05 4.07961832E+06  163
```

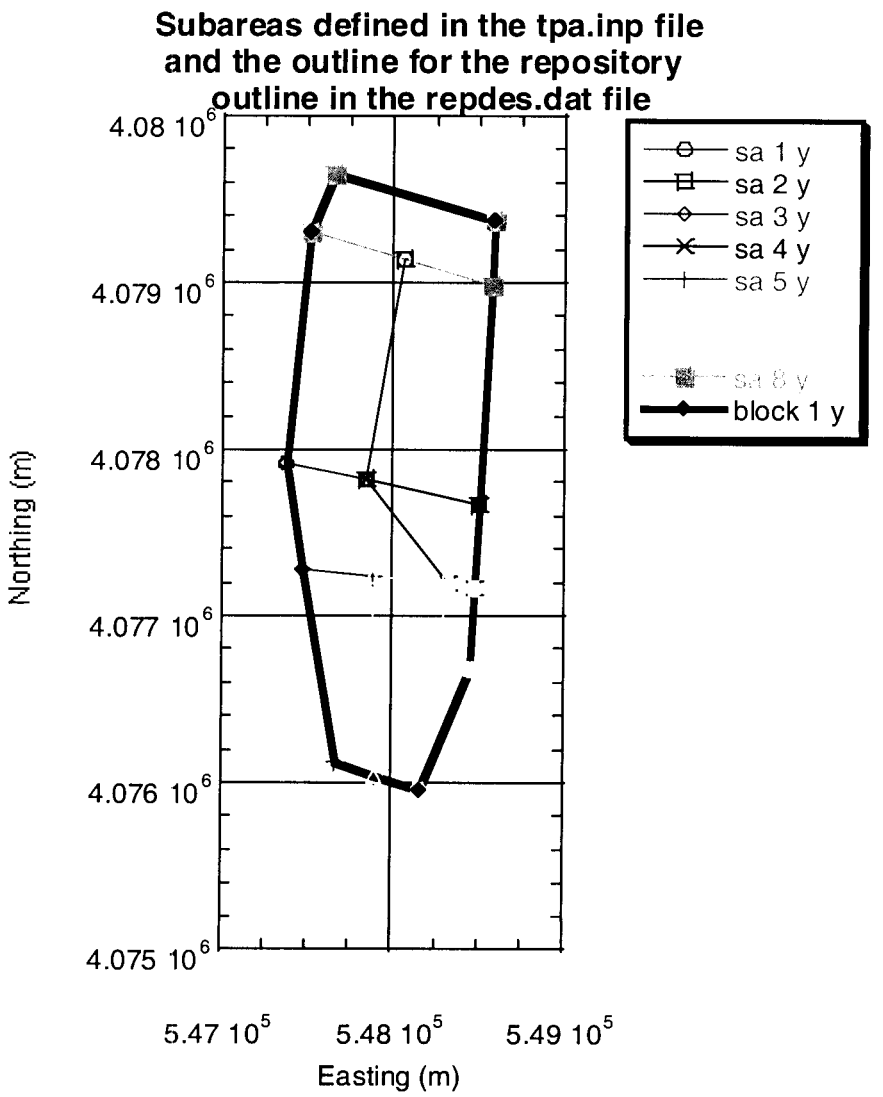
To verify that the subarea coordinates in the *tpa.inp* file are consistent with the coordinates for both the repository outline in *repdes.dat* and the drift end points in *drifts.dat*, several plots using these coordinates were generated. These plots are present below. The plots were created using Kaleidagraph and are available in the \testing_4.0\data_plots subdirectory.

(file: tpa_inp_coord.qpc)

Subareas Defined in the tpa.inp file

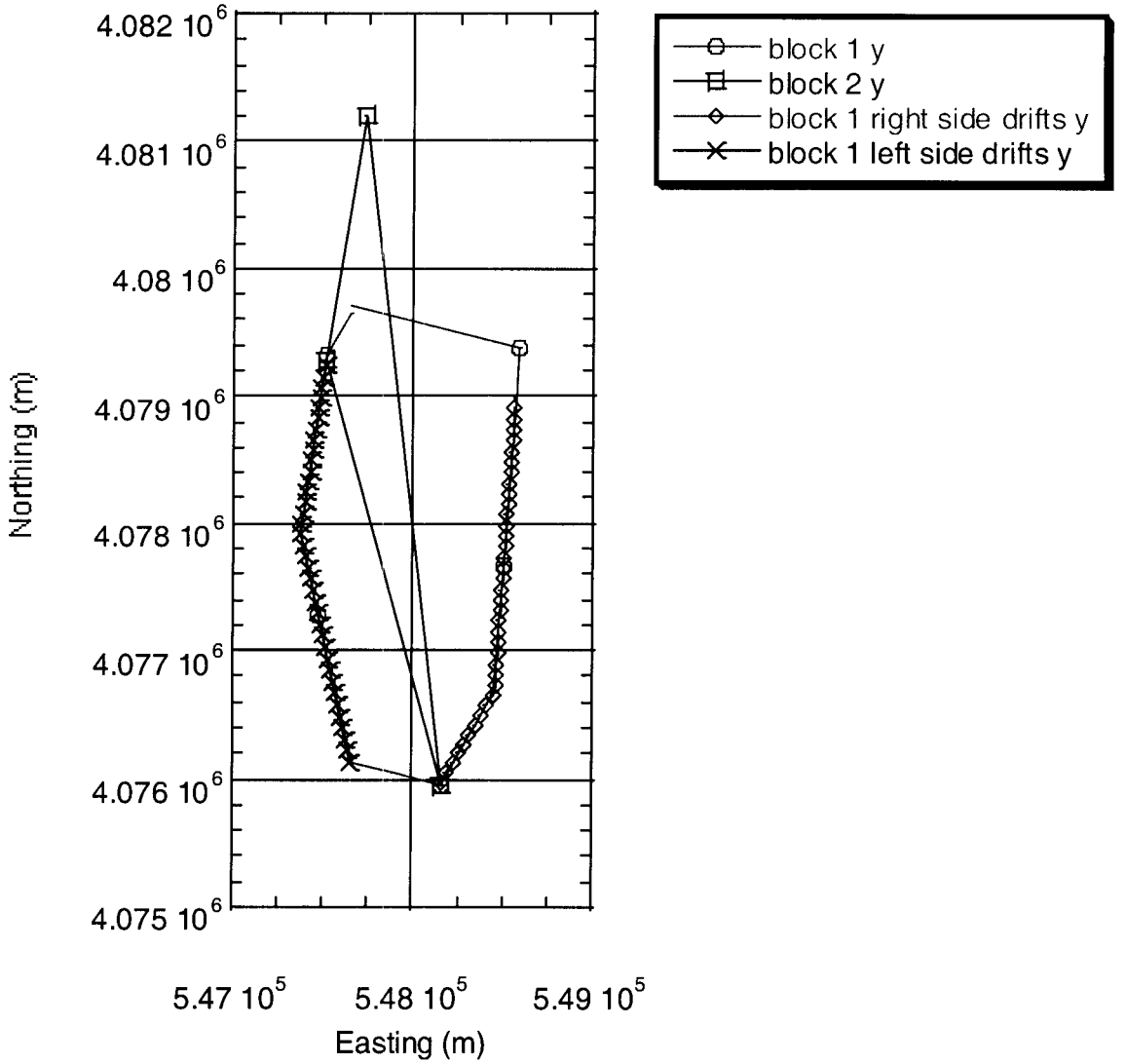


(file: block1.qpc)



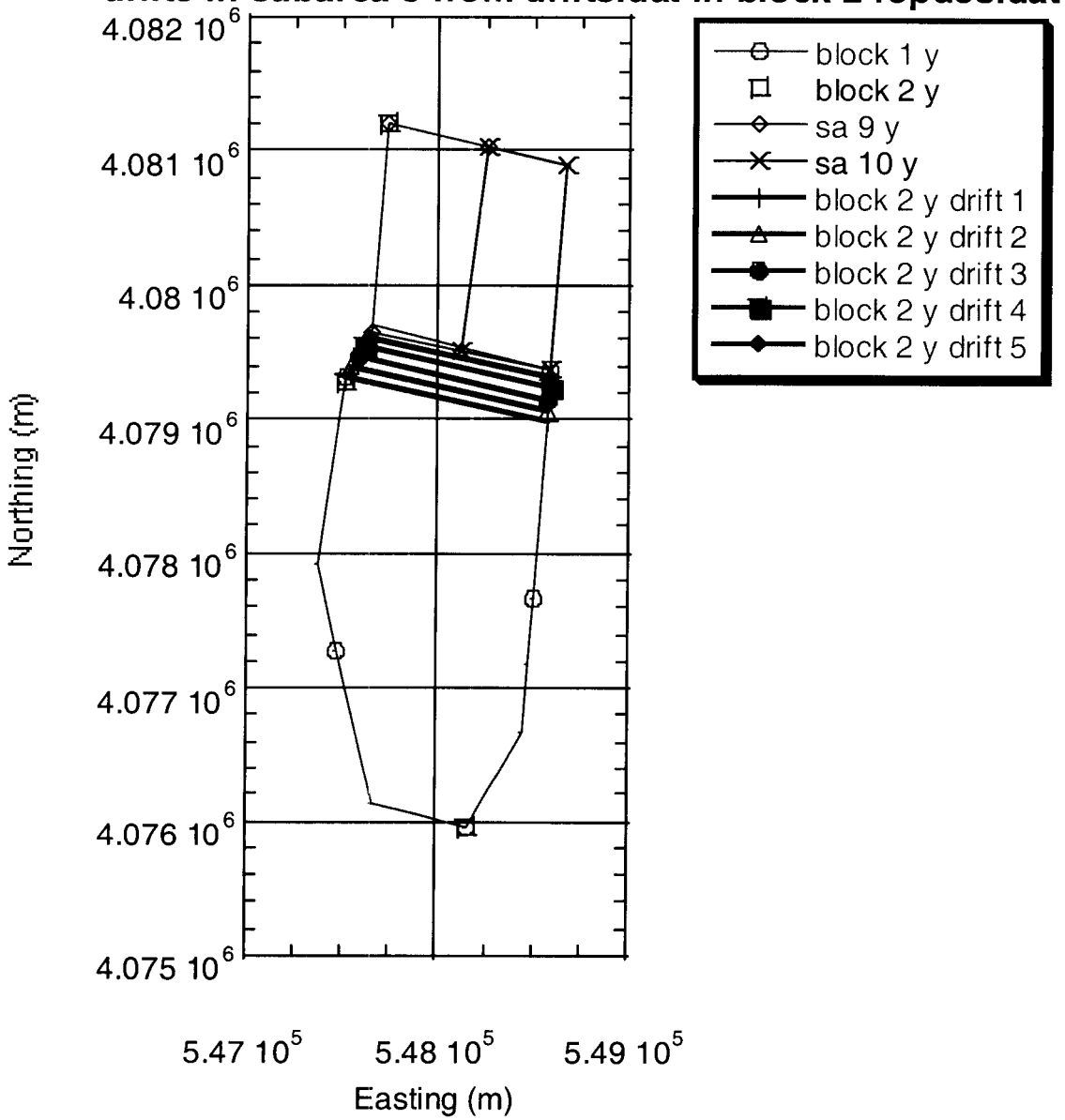
(file: block1_drifts.qpc)

Emplacement block 1 and 2 coordinates from repdes.dat and coordinates of the left and right side of the drift from drifts.dat



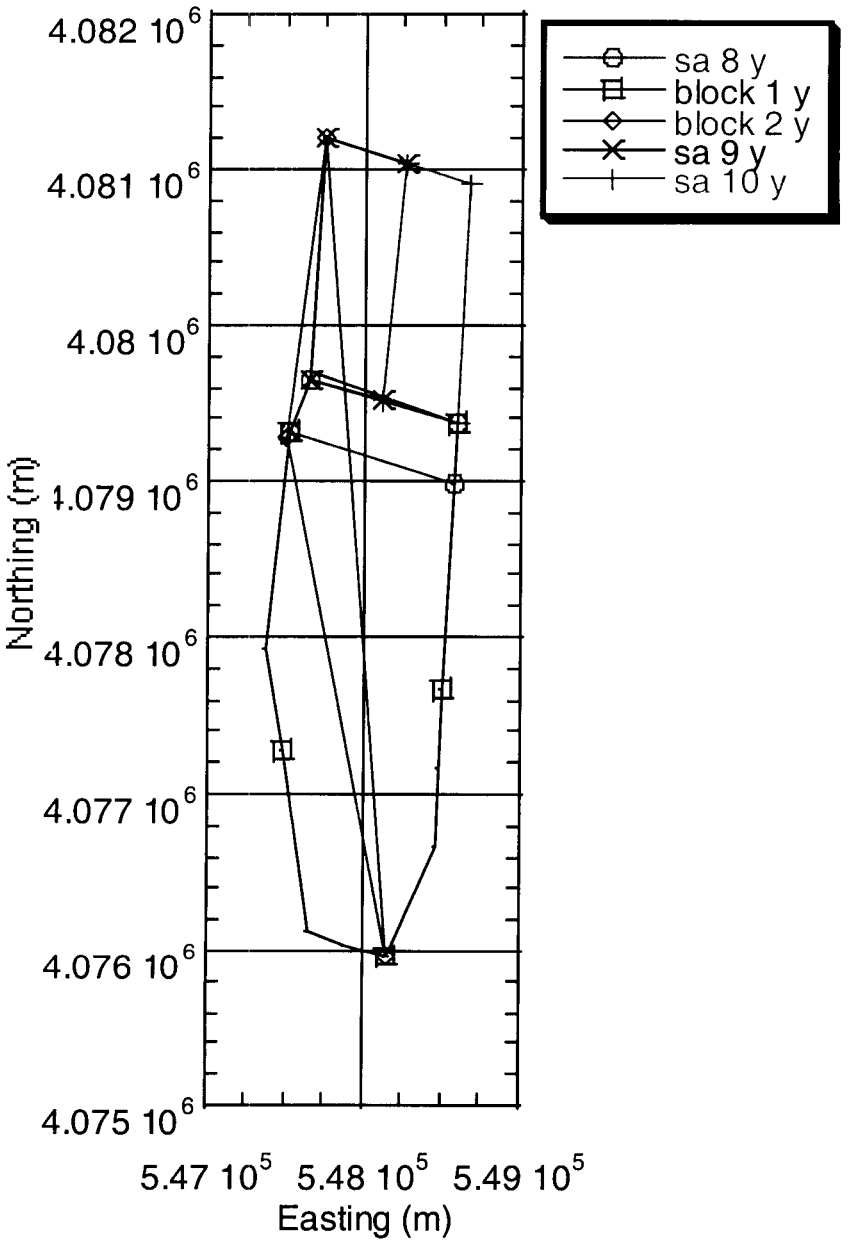
(file: block2_drifts.qpc)

Repository outline from repdes.dat (subareas 1 to 8) , subareas 9 and 10 (not used) from tpa.inp, and the five drifts in subarea 8 from drifts.dat in block 2 repdes.dat



(file: sa8910_blk12.qpc)

Repository outline for blocks 1 and 2 from repdes.dat and subareas 8,9, and 10 from tpa.inp



The titles for each of these graphs describe the plotted coordinates. The coordinates for the

subareas from *tpa.inp* are consistent with the coordinates for the repository outline in *repdes.dat* and the drift end points in *drifts.dat*. Additionally, emplacement block 1 and 2 coordinates are at the upper left hand corner of subarea 1 and subarea 8, respectively. (note that the coordinates plotted in the lower right part of subarea 7 are only place holders and are not used in calculations)

To verify the number of WPs in each drift (*drifts.dat*) is consistent with the total number of WPs in the repository, the number of WPs in *drifts.dat* was summed (6970) and compared to the sum of the number of WPs listed for each subarea in the screen print (6921). These results are consistent, even though there is a difference of 1 WP, with the difference being attributed to rounding. Moreover, the fraction of the total repository area occupied by one subarea (which was used in TPA Version 3.3 to determine the number of WPs in each subarea) roughly corresponds to the number of WPs computed using the drift coordinates (see below and \testing_4.0\data_plots\tpaout.xls) and the number of WPs based on fraction of the total area correspond (see below). This verifies that reasonableness of the assignment of WPs to each subarea.

Subarea #	Area [m^2]	Waste [MTU]	Number of WP	fract of area	fract of total wps	#WPs based on fract area
1	723591.3	13605.4	1394	0.20867448	0.19997131	1454.67
2	784763	15049.9	1542	0.226315616	0.221202123	1577.646
3	390372	7827.5	802	0.112578294	0.115048056	784.7833
4	207581.3	3904	400	0.059863793	0.057380577	417.3105
5	378972.8	7573.8	776	0.10929091	0.111318319	761.8669
6	424872.5	8452.2	866	0.122527797	0.124228949	854.1413
7	163938.3	3279.4	336	0.04727771	0.048199684	329.5729
8	393468.9	8344.8	855	0.1134714	0.122650983	791.0091
t o t a l area	**3467560**	**total wps 6971**				

To verify that the angle (-0.304 radians) and the drift and WP spacing (81 m and 6.1392 m, respectively, as specified in the tpa.inp file) computed in READER and written to the *drifts.dat* file were correctly used to determine the drift endpoints and the number of WPs in each drift, EXCEL spreadsheet analysis was performed. The file *data.xls* in the \testing_4.0\data_plots subdirectory contains the analysis. This analysis verifies that the WPs spacing was 6.1392 m, the drift spacing was 81 m and the drift angle was -0.304 radians.

Furthermore, the total MTUs emplacement in the repository (specified in tha *tpa.inp* file as 68,030 MTUs using 9.76 MTU/WP) was consistent with the repository MTUs in tpa.out (see the \testing_4.0\basecase subdirectory).

Thus, from the Test 1 results, the modifications are correctly implemented and are reasonable.

Test 2 through Test 5 Results:

Test 2 through Test 5 utilize tester-supplied data to check the correct implementation of determining drift locations, number of WPs in each drift, and the assignment of WPs to subareas. In these tests, data were modified, including the subarea coordinates in *tpa.inp* and the repository outline, drift angle, and emplacement block coordinates in *repdes.dat*. For each of the four tests, the

following data and output files will be provided: *tpa.inp* subarea coordinates, *repdes.dat*, *drifts.dat*, and the screen print from *tpa.out* showing the number of WPs in each subarea. The following list summarizes the tests and location of the input\output files from these tests.

Test	Test Description	Location of Test Files
Test 2	1 horizontal subarea and horizontal drifts	\testing_4.0\tester
Test 3	2 horizontal subareas and horizontal drifts	\testing_4.0\tester2
Test 4	1 subarea and drifts at -45 degrees	\testing_4.0\tester3
Test 5	1 subarea at -45 degrees and horizontal drifts	\testing_4.0\tester4

Test 2

(file: *tpa.inp*)

```
subarea
1
•
  0.0        0.0
  0.0      2000.0
2000.0      2000.0
2000.0        0.0
  0.0        0.0
```

(file: *repdes.dat*)

```
TITLE:  test file for rep design.
**
** angle - radians
**
0.0d0
**
** rep outline vertices.
**
5
0.0, 0.0
0.0, 2000.0
2000.0, 2000.0
2000.0, 0.0
0.0, 0.0
**
** emplacement blocks
**
2
0.0, 1000.0, 2000.0, 0.0
0.0, 1000.0, 0.0, 4000.0
```

(file: *drifts.dat*)

```
TITLE:
**
**
Emplacement Block
        1
** Drift Endpoints
** x1          y1          x2          y2        numWP
 1.21430643E-16 9.59500000E+02 2.00000000E+03 9.59500000E+02   325
 1.21430643E-16 8.78500000E+02 2.00000000E+03 8.78500000E+02   325
 1.21430643E-16 7.97500000E+02 2.00000000E+03 7.97500000E+02   325
 1.21430643E-16 7.16500000E+02 2.00000000E+03 7.16500000E+02   325
 1.21430643E-16 6.35500000E+02 2.00000000E+03 6.35500000E+02   325
 1.21430643E-16 5.54500000E+02 2.00000000E+03 5.54500000E+02   325
 1.21430643E-16 4.73500000E+02 2.00000000E+03 4.73500000E+02   325
 1.21430643E-16 3.92500000E+02 2.00000000E+03 3.92500000E+02   325
 1.21430643E-16 3.11500000E+02 2.00000000E+03 3.11500000E+02   325
 1.21430643E-16 2.30500000E+02 2.00000000E+03 2.30500000E+02   325
 1.21430643E-16 1.49500000E+02 2.00000000E+03 1.49500000E+02   325
 1.21430643E-16 6.85000000E+01 2.00000000E+03 6.85000000E+01   325
**
Emplacement Block
        2
** Drift Endpoints
** x1          y1          x2          y2        numWP
 1.21430643E-16 1.04050000E+03 2.00000000E+03 1.04050000E+03   325
 1.21430643E-16 1.12150000E+03 2.00000000E+03 1.12150000E+03   325
 1.21430643E-16 1.20250000E+03 2.00000000E+03 1.20250000E+03   325
 1.21430643E-16 1.28350000E+03 2.00000000E+03 1.28350000E+03   325
 1.21430643E-16 1.36450000E+03 2.00000000E+03 1.36450000E+03   325
 1.21430643E-16 1.44550000E+03 2.00000000E+03 1.44550000E+03   325
 1.21430643E-16 1.52650000E+03 2.00000000E+03 1.52650000E+03   325
 1.21430643E-16 1.60750000E+03 2.00000000E+03 1.60750000E+03   325
 1.21430643E-16 1.68850000E+03 2.00000000E+03 1.68850000E+03   325
 1.21430643E-16 1.76950000E+03 2.00000000E+03 1.76950000E+03   145
```

(file: *tpa.out*)

```
Subarea   Area      Waste   Number of WP
  #     [m^2]      [MTU]
  1   4000000.0   68027.2       6970
```

Test 3

(file: *tpa.inp*)

```
subarea
2
*
   0.0          0.0
   0.0        2000.0
 1000.0       2000.0
 1000.0          0.0
```

```
   0.0          0.0
*
 1000.0         0.0
 1000.0       2000.0
 2000.0       2000.0
 2000.0         0.0
 1000.0         0.0
```

(file: *repdes.dat*)

```
TITLE:  test file for rep design.
**
** angle - radians
**
0.0d0
**
** rep outline vertices.
**
5
0.0, 0.0
0.0, 2000.0
2000.0, 2000.0
2000.0, 0.0
0.0, 0.0
**
** emplacement blocks
**
2
0.0, 1000.0, 2000.0, 0.0
0.0, 1000.0, 0.0, 4000.0
```

(file: *drifts.dat*)

```
TITLE:
**
**
Emplacement Block
        1
**  Drift Endpoints
**   x1          y1          x2          y2        numWP
 1.21430643E-16 9.59500000E+02 2.00000000E+03 9.59500000E+02   325
 1.21430643E-16 8.78500000E+02 2.00000000E+03 8.78500000E+02   325
 1.21430643E-16 7.97500000E+02 2.00000000E+03 7.97500000E+02   325
 1.21430643E-16 7.16500000E+02 2.00000000E+03 7.16500000E+02   325
 1.21430643E-16 6.35500000E+02 2.00000000E+03 6.35500000E+02   325
 1.21430643E-16 5.54500000E+02 2.00000000E+03 5.54500000E+02   325
 1.21430643E-16 4.73500000E+02 2.00000000E+03 4.73500000E+02   325
 1.21430643E-16 3.92500000E+02 2.00000000E+03 3.92500000E+02   325
 1.21430643E-16 3.11500000E+02 2.00000000E+03 3.11500000E+02   325
 1.21430643E-16 2.30500000E+02 2.00000000E+03 2.30500000E+02   325
 1.21430643E-16 1.49500000E+02 2.00000000E+03 1.49500000E+02   325
 1.21430643E-16 6.85000000E+01 2.00000000E+03 6.85000000E+01   325
**
Emplacement Block
        2
```

```
** Drift Endpoints
** x1          y1          x2          y2          numWP
 1.21430643E-16 1.04050000E+03 2.00000000E+03 1.04050000E+03   325
 1.21430643E-16 1.12150000E+03 2.00000000E+03 1.12150000E+03   325
 1.21430643E-16 1.20250000E+03 2.00000000E+03 1.20250000E+03   325
 1.21430643E-16 1.28350000E+03 2.00000000E+03 1.28350000E+03   325
 1.21430643E-16 1.36450000E+03 2.00000000E+03 1.36450000E+03   325
 1.21430643E-16 1.44550000E+03 2.00000000E+03 1.44550000E+03   325
 1.21430643E-16 1.52650000E+03 2.00000000E+03 1.52650000E+03   325
 1.21430643E-16 1.60750000E+03 2.00000000E+03 1.60750000E+03   325
 1.21430643E-16 1.68850000E+03 2.00000000E+03 1.68850000E+03   325
 1.21430643E-16 1.76950000E+03 2.00000000E+03 1.76950000E+03   145
```

(file: *tpa.out*)

```
Subarea   Area      Waste   Number of WP
  #     [m^2]     [MTU]
  1   2000000.0   34013.6       3485
  2   2000000.0   34013.6       3485
```

Test 4

(file: *tpa.inp*)

```
subarea
1
*
   0.0          0.0
 1414.2         1414.2
   0.0         2828.4
-1414.2         1414.2
   0.0          0.0
```

(file: *repdes.dat*)

```
TITLE:  test file for rep design.
**
** angle - radians
**
-.7853982d0
**0.0d0
**
** rep outline vertices.
**
5
0.0, 0.0
-1414.2, 1414.2
0.0, 2828.427
1414.2, 1414.2
0.0, 0.0
**
** emplacement blocks
```

```
**
2
-1414.2, 1414.2, -2828.4, 2828.4
-1414.2, 1414.2, -5656.8, 5656.8
```

(file: *drifts.dat*)

```
TITLE:
**
**
Emplacement Block
        1
** Drift Endpoints
** x1          y1          x2          y2          numWP
-1.38556245E+03 1.44283810E+03 2.86377729E+01 2.86377729E+01  325
-1.32828735E+03 1.50011429E+03 8.59134222E+01 8.59134222E+01  325
-1.27101224E+03 1.55739049E+03 1.43189071E+02 1.43189071E+02  325
-1.21373714E+03 1.61466669E+03 2.00464721E+02 2.00464721E+02  325
-1.15646204E+03 1.67194288E+03 2.57740370E+02 2.57740370E+02  325
-1.09918694E+03 1.72921908E+03 3.15016019E+02 3.15016019E+02  325
-1.04191183E+03 1.78649527E+03 3.72291669E+02 3.72291669E+02  325
-9.84636731E+02 1.84377147E+03 4.29567318E+02 4.29567318E+02  325
-9.27361629E+02 1.90104767E+03 4.86842967E+02 4.86842967E+02  325
-8.70086526E+02 1.95832386E+03 5.44118616E+02 5.44118616E+02  325
-8.12811423E+02 2.01560006E+03 6.01394266E+02 6.01394266E+02  325
-7.55536321E+02 2.07287625E+03 6.58669915E+02 6.58669915E+02  325
-6.98261218E+02 2.13015245E+03 7.15945564E+02 7.15945564E+02  325
-6.40986116E+02 2.18742865E+03 7.73221213E+02 7.73221213E+02  325
-5.83711013E+02 2.24470484E+03 8.30496863E+02 8.30496863E+02  325
-5.26435911E+02 2.30198104E+03 8.87772512E+02 8.87772512E+02  325
-4.69160808E+02 2.35925723E+03 9.45048161E+02 9.45048161E+02  325
-4.11885706E+02 2.41653343E+03 1.00232381E+03 1.00232381E+03  325
-3.54610603E+02 2.47380963E+03 1.05959946E+03 1.05959946E+03  325
-2.97335501E+02 2.53108582E+03 1.11687511E+03 1.11687511E+03  325
-2.40060398E+02 2.58836202E+03 1.17415076E+03 1.17415076E+03  325
-1.82785296E+02 2.64563821E+03 1.23142641E+03 1.23142641E+03  145
```

(file: *tpa.out*)

```
Subarea   Area      Waste   Number of WP
  #     [m^2]      [MTU]
  1   3999923.3   68027.2       6970
```

<u>Test 5</u>

(file: *tpa.inp*)

```
subarea
1
*
  0.0          0.0
 1414.2        1414.2
```

```
   0.0        2828.4
-1414.2        1414.2
   0.0          0.0
```

(file: *repdes.dat*)

```
TITLE:  test file for rep design.
**
** angle - radians
**
**-.7853982d0
0.0d0
**
** rep outline vertices.
**
5
0.0, 0.0
-1414.2, 1414.2
0.0, 2828.427
1414.2, 1414.2
0.0, 0.0
**
** emplacement blocks
**
2
-1414.2, 1414.2, -2828.4, 2828.4
-1414.2, 1414.2, -5656.8, 5656.8
```

(file: *drifts.dat*)

```
TITLE:
**
**
Emplacement Block
        1
**  Drift Endpoints
**   x1            y1            x2            y2         numWP
-1.37370077E+03 1.45470000E+03 1.37370077E+03 1.45470000E+03   447
-1.29270232E+03 1.53570000E+03 1.29270232E+03 1.53570000E+03   421
-1.21170387E+03 1.61670000E+03 1.21170387E+03 1.61670000E+03   394
-1.13070541E+03 1.69770000E+03 1.13070541E+03 1.69770000E+03   368
-1.04970696E+03 1.77870000E+03 1.04970696E+03 1.77870000E+03   341
-9.68708505E+02 1.85970000E+03 9.68708505E+02 1.85970000E+03   315
-8.87710052E+02 1.94070000E+03 8.87710052E+02 1.94070000E+03   289
-8.06711598E+02 2.02170000E+03 8.06711598E+02 2.02170000E+03   262
-7.25713145E+02 2.10270000E+03 7.25713145E+02 2.10270000E+03   236
-6.44714691E+02 2.18370000E+03 6.44714691E+02 2.18370000E+03   210
-5.63716237E+02 2.26470000E+03 5.63716237E+02 2.26470000E+03   183
-4.82717784E+02 2.34570000E+03 4.82717784E+02 2.34570000E+03   157
-4.01719330E+02 2.42670000E+03 4.01719330E+02 2.42670000E+03   130
-3.20720877E+02 2.50770000E+03 3.20720877E+02 2.50770000E+03   104
-2.39722423E+02 2.58870000E+03 2.39722423E+02 2.58870000E+03    78
-1.58723970E+02 2.66970000E+03 1.58723970E+02 2.66970000E+03    51
-7.77255161E+01 2.75070000E+03 7.77255161E+01 2.75070000E+03    25
**
```

```
Emplacement Block
      2
** Drift Endpoints
** x1          y1          x2          y2          numWP
-1.37370077E+03 1.45470000E+03 1.37370077E+03 1.45470000E+03  447
-1.29270232E+03 1.53570000E+03 1.29270232E+03 1.53570000E+03  421
-1.21170387E+03 1.61670000E+03 1.21170387E+03 1.61670000E+03  394
-1.13070541E+03 1.69770000E+03 1.13070541E+03 1.69770000E+03  368
-1.04970696E+03 1.77870000E+03 1.04970696E+03 1.77870000E+03  341
-9.68708505E+02 1.85970000E+03 9.68708505E+02 1.85970000E+03  315
-8.87710052E+02 1.94070000E+03 8.87710052E+02 1.94070000E+03  289
-8.06711598E+02 2.02170000E+03 8.06711598E+02 2.02170000E+03  262
-7.25713145E+02 2.10270000E+03 7.25713145E+02 2.10270000E+03  122
```

(file: *tpa.out*)

```
Subarea  Area      Waste   Number of WP
  #    [m^2]     [MTU]
  1  3999923.3   68027.2       6970
```

Note that from this testing, all of the results are reasonable and correct for the number of WPs in each drift and the allocation of WPs to subareas (Test 3). These results are consistent for the different angles (0 and -45 degrees) in *repdes.dat*. Also note the expected symmetry in the number of WPs in each drift (*drifts.dat*) for Test 5 for horizontal drifts and a subarea at -45 degrees.

In summary, the results from Test 1 through Test 5 suggest that the modifications for the repository layout in SCR-304 were implemented correctly in the TPA Version 4.0 code. Thus, the code **PASSES** the tests outlined in the TSCR-304 test plan.

****

SCR-293: Number of magma induced mechanical failures remaining in drift

3/13/00 through 3/15/00

The test plan for SCR-293 is listed below:

TPA Test Plan SCR-293

Tester: Rob Rice

Test name: Number of magma induced mechanical failures remaining in drift

Anticipated start date: March 13, 2000

Anticipated completion date: March 15, 2000

Amount of your time available to perform this test: 24 hours

Percent of testing time to be spent in process level testing and system level testing (e.g. 50/50):
50% system-level and 50% process-level testing will be performed. The TPA code reads information

from the *tpa.inp* file, which is sampled and written to *sp.tpa*, and uses these values to determine the number of WPs ejected and the number of WPs failed from magma within the drift during an igneous event. These values are written to the screen and to *wpsfail.res.* However, the fraction of WPs failed by an igneous event is also contained in the *volcano.rlt* file and the number of WPs failed from igneous activity are contained in the *ebsrel.ech* file and the *ebsrel.inp* file. Thus, in this testing, which will be sufficient to evaluate the correct application of this change, both system level and process level testing will be performed.

Output files to be checked: screen print, *sp.tpa*, *wpsfail.res*, *ebsrel.ech*, and *volcano.rlt*

Input files to be checked for proper data transfer to the program: *tpa.inp*

Disposition of documentation (storage medium, physical location, and access method):
All tests will be archived on a CD-ROM and described in a scientific notebook that will be submitted to the TPA code custodian, Ron Janetzke, upon completion of the testing. On the CD-ROM, the \testing_4.0\volcano subdirectory will contain all testing output files.

<u>Functional Test</u> Descriptions:

Test 1: The values specified in *tpa.inp* that are sampled and written to *sp.tpa* for the number of WPs failed by the dike and ejected from the volcano will be checked against the values in the screen print, *wpsfail.res*, *ebsrel.ech*, and *ebsrel.inp* files, and the fraction of failed WPs in *volcano.rlt* file. The values examined should be consistent. These results are archived in the \testing_4.0\volcano\basecase subdirectory.

Test 2: Test 1 will be repeated, except for the activation of the direct release only flag in the *tpa.inp* file. These results for ground surface releases and doses in *tpa.out* and *dcags.rlt* should be the same as the Test 1 results. These results are archived in the \testing_4.0\volcano\directreleaseonly subdirectory.

- Hand calculations: Hand calculations for this testing are limited to verification that the total number of WPs failed in an igneous event is consistent with the sum of the WPs ejected and the WPs failed within the dike. These values can be checked in the screen print and the *sp.tpa*, *wpsfail.res*, and *ebsrel.ech* files. Also, the fraction of WPs failed in an igneous events will be checked to ensure the total number of failed WPs is correctly computed. These values are available in the *volcano.rlt* file.

- Process level: The process-level checks will be performed by examining the *ebsrel.inp, ebsrel.ech*, and *volcano.rlt* files as described in the "Hand calculations" section above.

- System level: The system-level checks will be performed by examining the screen print and the *sp.tpa* and *wpsfail.res* files as described in the "Hand calculations" section above.

Reasonableness Test Description: Based on the hand calculations and checks described above, the reasonableness of the determination of WPs ejected and failed within the dike will be verified and evident in the results for Tests 1 and 2.

Final Checklist (completed during testing):

- Did the modification substantially change the results? No. Because only the number of WPs ejected and failed within the dike are changed, but are within the range of WPs failures used in the

previous version of the TPA code, the ground surface doses from DCAGS did not change significantly with this modification (see the *tpa.out* files in the following sampled and mean value directories). These results are archived in the \testing_4.0bkk\volcano\basecase and \testing_4.0bkk\volcano_meanvalue subdirectories and the \tpa33\volcano and \tpa33\volcano_meanvalue subdirectories.

- Were TPA 3.3 and TPA 4.0beta compared using corresponding mean values in *tpa.inp*? Yes. The results for versions 3.3 and 4.0 were not significantly different. Refer to the previous question.

- Which nuclides were monitored to determine reasonableness of results in term of dose? The radionuclides with the highest dose rates in version 3.3 (i.e., I-129 and Cl-36) were monitored for purposes of evaluating the reasonableness of the results in terms of dose. This two radionuclides also appear in the version 4.0 results together with Tc-99. Again, the differences in the version 3.3 and 4.0 doses were reasonable. These results are also archived in the \testing_4.0bkk\basecase_meanvalue and \tpa33\basecase_meanvalue subdirectories.

Discussion of test results for SCR-293:

Test 1 Results: The following values were specified in the tpa.inp file for Test 1. For the files in Test1, refer to the \testing_4.0\volcano subdirectory.

(file: *tpa.inp*)

```
**
**        ***>>>  Disruptive Scenario flags  <<<***
**
iflag
VolcanismDisruptiveScenarioFlag(yes=1,no=0)
1
**
. . .

**
**
**        ***>>> VOLCANO <<<***
**
iconstant
VolcanoModel(1=Geometric,2=Distribution)
2
**

. . .

** For Distribution model only.
iconstant
SubareaOfVolcanicEvent[]
2
**
uniform
NumberOfWPsEntrainedByEjecta[]
1.0, 10.
**
uniform
```

```
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]
1.0, 150.0
**
```

All of the other *tpa.inp* file parameters were not changed.

Using the above parameters, the following error message from the TPA code was written to *tpa.out*.

```
exec: calling dcags
              Highest annual dose from GS
          Pu239  2.0785E+03 [mrem/yr] at  6.407E+03 yr
          Pu240  2.0336E+03 [mrem/yr] at  6.407E+03 yr
          Am243  1.2088E+02 [mrem/yr] at  6.407E+03 yr
          Pu242  1.6480E+01 [mrem/yr] at  6.407E+03 yr
          Np237  1.4925E+01 [mrem/yr] at  6.407E+03 yr
           U234  5.3939E+00 [mrem/yr] at  6.407E+03 yr
exec: end realizations
 ***>>> Error in igetunitnumber <<<***
   iopen .gt. maxunit
   iopen =        128
   maxunit =        127
   need to increase size of maxunit
```

As a result of this error message, Test 1 testing was stopped. To address this error, it was recommended that the number of file units in fu2.i (i.e., parameter (maxunit = 127)) should be increased from 127 to a larger value (e.g., 150).

Test 2 Results: For Test 2, the same parameters as shown in the *tpa.inp* file for Test 1 were used and additionally, the direct release only flag was activitated (see below).

(file: *tpa.inp*)

```
**
iflag
DirectReleaseOnlyFlag(yes=1,no=0)
1
**
```

With these parameters in the *tpa.inp* file, the following screen print was written to the *tpa.out* file.

```
-----------------------------------------------------------------------
   subarea  1 of  8        realization   1 of   1
-----------------------------------------------------------------------
exec: calling volcano
-----------------------------------------------------------------------
   subarea  2 of  8        realization   1 of   1
-----------------------------------------------------------------------
-----------------------------------------------------------------------
   subarea  3 of  8        realization   1 of   1
-----------------------------------------------------------------------
-----------------------------------------------------------------------
   subarea  4 of  8        realization   1 of   1
-----------------------------------------------------------------------
```

```
-----------------------------------------------------------------------
   subarea  5 of  8        realization   1 of   1
-----------------------------------------------------------------------
-----------------------------------------------------------------------
   subarea  6 of  8        realization   1 of   1
-----------------------------------------------------------------------
-----------------------------------------------------------------------
   subarea  7 of  8        realization   1 of   1
-----------------------------------------------------------------------
-----------------------------------------------------------------------
   subarea  8 of  8        realization   1 of   1
-----------------------------------------------------------------------
File specified STATUS= "OLD" doesn't exist (see "Input/Output" in the Lahey
 Fortran 90 Language Reference), FILE=ebsflo.dat, UNIT
```

The above error occurred because during the direct release calculations the *ebsflo.dat* file was not written, although the EXEC was expecting the file to exist.

The two problems (number of file units in Test 1 and no *ebsflo.dat* in Test 2) were communicated to the TPA code custodian, Ron Janetzke, who made the modifications and sent an email attachment with the modified files. Tests 1 and 2 were then conducted again using these files (see the \testing_4.0bkk [version k] subdirectory for these repeated tests - note that the second k was added to the subdirectory name because of a bug in the NT system which doesn't allow for 16 characters in the path designation [i.e., set TPA_DATA = c:\testing_4.0bk and set TPA_TEST = c:\testing_4.0bk both have 16 characters]).

Test 1 Results (repeated - see the \testing_4.0bkk\basecase subdirectory):

Using the same parameters shown above for the original Test 1, the following output files were generated. These files are intended to show the correct implementation of specifying the number of WPs in the dike and the subarea for the igneous activity, instead of using geometric considerations.

(file: *sp.tpa*) - shows the sampled values used in the calculations (note: ejected WPs range from 1 to 10 and dike failed WPs range from 1 to 150 - see previous Test 1)

. . .

NumberOfWPsEntrainedByEjecta[]
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]
WindSpeed[cm/s]
VolcanicEventDuration[s]
VolcanicEventPower[W]
AshMeanParticleLogDiameter[d_in_cm]
AirborneMassLoadAboveFreshAshBlanket[g/m3]

. . .

0.7844329E+01
0.6950236E+02
0.1026452E+04
0.3789644E+06
0.1729527E+12
0.3606378E+00
0.7010928E-02

Using the above values, the number of WPs ejected and failed within the dike should be 8 and 69, respectively, from subarea 2.

From the screen print in *tpa.out,* the number of WPs failed within each subarea are listed below.

```
-----------------------------------------------------------------------
   subarea   1 of   8          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling ebsfail
    *** No Corrosion WP Failure ***
exec: calling seismo
exec: calling volcano
exec: failed WPs from INITIAL   event =     11 at time =      0.0 yr
 *** failed WPs:          11  out of        1394 ***

. . .

-----------------------------------------------------------------------
   subarea   2 of   8          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling ebsfail
    *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =     12 at time =      0.0 yr
exec: failed WPs from VOLCANIC  event =     77 at time =   6407.3 yr (includes ejected WPs)
 *** failed WPs:          89  out of        1542 ***
 *** ejected WPs:          8

. . .

-----------------------------------------------------------------------
   subarea   3 of   8          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling ebsfail
    *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =      6 at time =      0.0 yr
 *** failed WPs:           6  out of         802 ***

. . .

-----------------------------------------------------------------------
   subarea   4 of   8          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling ebsfail
    *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =      3 at time =      0.0 yr
 *** failed WPs:           3  out of         400 ***

. . .
```

```
-----------------------------------------------------------------------
   subarea   5 of   8          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling ebsfail
    *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =      6 at time =      0.0 yr
 *** failed WPs:          6  out of         776 ***

. . .

-----------------------------------------------------------------------
   subarea   6 of   8          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling ebsfail
    *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =      7 at time =      0.0 yr
 *** failed WPs:          7  out of         866 ***

. . .

-----------------------------------------------------------------------
   subarea   7 of   8          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling ebsfail
    *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =      3 at time =      0.0 yr
 *** failed WPs:          3  out of         336 ***
. . .

-----------------------------------------------------------------------
   subarea   8 of   8          realization    1 of    1
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling nfenv
exec: calling ebsfail
    *** No Corrosion WP Failure ***
exec: failed WPs from INITIAL   event =      7 at time =      0.0 yr
 *** failed WPs:          7  out of         855 ***
```

Note that from the above results, only subarea 2 exhibited WP failure from VOLCANO with 77 total WPs (7 ejected and the remaining WPs within the dike). These results are expected given the sampled values in *sp.tpa* given above.

To verify the correct assignment of failed WPs from igneous activity, the *wpsfail.res* file is provided below (note that there are 77 WPs failing from igneous activity).

```
Input file tpa.inp as supplied with TPA Version 4.0beta Code.
Base case
TPA 4.0beta, Job started: Mon Mar 20 12:10:40 2000
Number of Failed WPs by Type of Disruptive Event
```

Including Time of Event - Values for Each Vector

vector	time	#corrode	#seismic	#fault	**#igact**
unitless	yr	unitless	unitless	unitless	unitless
1	6.4073E+03	0.0000E+00	0.0000E+00	0.0000E+00	**7.7000E+01**

To further verify the correct data transfer of failed WPs from igneous activity to the EBSREL module, the values in the *ebsrel.ech* are given below.

Input file tpa.inp as supplied with TPA Version 4.0beta Code.
Base case
TPA 4.0beta, Job started: Mon Mar 20 12:10:40 2000
Echo of EBSREL Input Values
with the output mode specified in "tpa.inp"

REALIZATION 1

SUBAREA 1

type of event	number wps failed	time of event
INITIAL	1.1000E+01	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	1.0000E+04
CORROSION	0.0000E+00	1.0000E+04
EXTRUSIVE	8.0000E+00	0.0000E+00

. . .

SUBAREA 2

type of event	number wps failed	time of event
INITIAL	1.2000E+01	0.0000E+00
FAULTING	0.0000E+00	0.0000E+00
VOLCANO	6.9000E+01	6.4073E+03
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	1.0000E+04
CORROSION	0.0000E+00	1.0000E+04
EXTRUSIVE	8.0000E+00	6.4073E+03

. . .

SUBAREA 3

type of event	number wps failed	time of event
INITIAL	6.0000E+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	1.0000E+04
CORROSION	0.0000E+00	1.0000E+04
EXTRUSIVE	8.0000E+00	0.0000E+00

. . .

SUBAREA 4

type of event	number wps failed	time of event
INITIAL	3.0000E+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	1.0000E+04
CORROSION	0.0000E+00	1.0000E+04
EXTRUSIVE	8.0000E+00	0.0000E+00

. . .

SUBAREA 5

type of event	number wps failed	time of event
INITIAL	6.0000E+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	1.0000E+04
CORROSION	0.0000E+00	1.0000E+04
EXTRUSIVE	8.0000E+00	0.0000E+00

. . .

SUBAREA 6

type of event	number wps failed	time of event
INITIAL	7.0000E+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	1.0000E+04
CORROSION	0.0000E+00	1.0000E+04
EXTRUSIVE	8.0000E+00	0.0000E+00

. . .

SUBAREA 7

type of event	number wps failed	time of event
INITIAL	3.0000E+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      1.0000E+04
  CORROSION        0.0000E+00       1.0000E+04
  EXTRUSIVE       8.0000E+00      0.0000E+00

. . .

SUBAREA   8

type of event    number wps failed    time of event
  INITIAL        7.0000E+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      1.0000E+04
  CORROSION        0.0000E+00       1.0000E+04
  EXTRUSIVE       8.0000E+00      0.0000E+00
```

Note in the above values from *ebsrel.ech*, the extrusive failures are reported as 8 WPs for each subarea and only subarea 2 show VOLCANO failures (69) at the time (6.4073E+03 yr) which corresponds to the time for the volcanic event (see the screen print from *tpa.out* above).

To verify that the correct fraction of WPs failed by the volcanic event is correctly transferred out of the VOLCANO module, the *volcano.rlt* is provided below.

```
Input file tpa.inp as supplied with TPA Version 4.0beta Code.
Base case
TPA 4.0beta, Job started: Mon Mar 20 12:10:40 2000
VOLCANO Results

with the output mode specified in "tpa.inp"


REALIZATION   1


ALL SUBAREAS

amtuejected =  7.6561E+01

subarea  volcanicamtufailed
   1      0.0000E+00
   2      6.7834E+02
   3      0.0000E+00
   4      0.0000E+00
   5      0.0000E+00
   6      0.0000E+00
   7      0.0000E+00
   8      0.0000E+00

Fraction of Waste Packages Failed by Volcanism
```

	time	subarea1	subarea2	subarea3	subarea4	subarea5
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00

. . .

179	5.9709E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
180	6.1130E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
181	6.2584E+03	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
182	6.4073E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
185	6.8750E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
186	7.0382E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
187	7.2053E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
188	7.3763E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
189	7.5513E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
190	7.7304E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
191	7.9137E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
192	8.1013E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
193	8.2933E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
194	8.4897E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
195	8.6908E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
196	8.8966E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
197	9.1072E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
198	9.3227E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
199	9.5433E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
200	9.7690E+03	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00
201	1.0000E+04	0.0000E+00	5.0160E-02	0.0000E+00	0.0000E+00	0.0000E+00

	time	subarea6	subarea7	subarea8
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	2.3102E+00	0.0000E+00	0.0000E+00	0.0000E+00

. . .

179	5.9709E+03	0.0000E+00	0.0000E+00	0.0000E+00
180	6.1130E+03	0.0000E+00	0.0000E+00	0.0000E+00
181	6.2584E+03	0.0000E+00	0.0000E+00	0.0000E+00
182	6.4073E+03	0.0000E+00	0.0000E+00	0.0000E+00
183	6.5596E+03	0.0000E+00	0.0000E+00	0.0000E+00
184	6.7154E+03	0.0000E+00	0.0000E+00	0.0000E+00
185	6.8750E+03	0.0000E+00	0.0000E+00	0.0000E+00
186	7.0382E+03	0.0000E+00	0.0000E+00	0.0000E+00
187	7.2053E+03	0.0000E+00	0.0000E+00	0.0000E+00
188	7.3763E+03	0.0000E+00	0.0000E+00	0.0000E+00
189	7.5513E+03	0.0000E+00	0.0000E+00	0.0000E+00
190	7.7304E+03	0.0000E+00	0.0000E+00	0.0000E+00
191	7.9137E+03	0.0000E+00	0.0000E+00	0.0000E+00
192	8.1013E+03	0.0000E+00	0.0000E+00	0.0000E+00
193	8.2933E+03	0.0000E+00	0.0000E+00	0.0000E+00
194	8.4897E+03	0.0000E+00	0.0000E+00	0.0000E+00
195	8.6908E+03	0.0000E+00	0.0000E+00	0.0000E+00
196	8.8966E+03	0.0000E+00	0.0000E+00	0.0000E+00
197	9.1072E+03	0.0000E+00	0.0000E+00	0.0000E+00
198	9.3227E+03	0.0000E+00	0.0000E+00	0.0000E+00
199	9.5433E+03	0.0000E+00	0.0000E+00	0.0000E+00
200	9.7690E+03	0.0000E+00	0.0000E+00	0.0000E+00
201	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00

Note that only subarea 2 shows WP failure from the igneous activity. Also note that amtuejected = 7.6561E+01, using 9.76 MTUs/WP, this corresponds to 7.8 (or 8) WPs. Additionally, amtuejected in subarea 2 = 6.7834E+02, and using 9.76 MTUs/WP, this corresponds to 69.5 (or 69) WPs. These values are consistent with the values reported above.

Moreover, the fraction of Wps failed by the igneous activity above (5.0160E-02) for subarea 2, which has 1542 WPs, corresponds to a total of 77 WPs (i.e., 69 + 8 by dike and ejected, respectively).

Thus, based on the above results for Test 1, using the \testing_4.0bkk files, the input data is correctly transferred within the TPA code and the modifications were implemented correctly.

Test 2 Results (repeated - see the \testing_4.0bkk\directreleaesonly subdirectory):

The above description of the *tpa.inp* file parameters for Test 2 in the \testing_4.0\directreleaseonly subdirectory was repeated in the \testing_4.0bkk\directreleaseonly subdirectory. The tpa.out files were compared to verify the results were consistent when all calculations (groundwater and ground surface in Test 1) are performed and when only direct release (ground surface in this test) calculations are performed.

(file: *tpa.out* from Test 1 [groundwater and ground surface])

```
exec: calling ashplumo
exec: calling ashrmovo
exec: calling dcags
            Highest annual dose from GS
        Pu239  5.6412E+02 [mrem/yr] at  7.730E+03 yr
        Pu240  4.9782E+02 [mrem/yr] at  7.730E+03 yr
        Am243  3.3735E+01 [mrem/yr] at  7.730E+03 yr
        Np237  8.2473E+00 [mrem/yr] at  7.730E+03 yr
         Tc99  7.6886E+00 [mrem/yr] at  7.730E+03 yr
         Nb94  6.5254E+00 [mrem/yr] at  7.730E+03 yr
exec: end realizations
```

(file: *tpa.out* from Test 2 [ground surface only]

```
exec: calling ashplumo
exec: calling ashrmovo
exec: calling dcags
            Highest annual dose from GS
        Pu239  5.6412E+02 [mrem/yr] at  7.730E+03 yr
        Pu240  4.9782E+02 [mrem/yr] at  7.730E+03 yr
        Am243  3.3735E+01 [mrem/yr] at  7.730E+03 yr
        Np237  8.2473E+00 [mrem/yr] at  7.730E+03 yr
         Tc99  7.6886E+00 [mrem/yr] at  7.730E+03 yr
         Nb94  6.5254E+00 [mrem/yr] at  7.730E+03 yr
exec: end realizations
```

Note that the above results for the ground surface doses are consistent, which indicate that the modifications tested in SCR-293 were correctly implemented. Thus, the TPA Version 4.0 code

PASSES the testing for SCR-293.

As an extra check on the TPA code results, the *ashout.res* values were checked for Tests 1 and 2. As a result of this comparison, it was discovered that when the direct release only flag was activiated, the time for the volcanic event was set equal to zero, instead of the actual time of the volcanic event (refer to the *ashout.res* files in the \testing_4.0bkk\volcano\basecase and \testing_4.0bkk\volcano\directreleaseonly subdirectories). The code custodian, Ron Janetzke, was contacted concerning this problem, modifications were accomplished to correct this problem in *exec.f*, and a new *exec.f* was tested in the \testing_4.0bkk2 subdirectory. The test results (which are actually the same tests as Tests 1 and 2) are archived in the \testing_4.0bkk2\volcano\basecase and \testing_4.0bkk2\volcano\directreleaseonly subdirectories and show the same files (and time for the volcanic event) in each file.

****

Testing Notes and Recommendations

Other testing was conducted to examine the robustness of the implemented changes that were not a part of the SCR-293 test plan. These tests examined acceptable ranges for the number of WPs ejected and failed within the dike. Through testing, it was discovered that when more WPs failures than the number of WPs in the subarea was specified, the TPA correctly provided an error message and code execution stopped. However, there was no similar check on specifying the number of failed or ejected WPs at less than zero or on specifying a non-existent subarea for the location of the volcanic event. It is recommended that simple error checks be introduced into the TPA code to check for ranges of failed WPs (i.e., greater than zero and less than the number of WPs in the subarea) and whether the subarea exists (i.e., if 8 subareas are specified in the *tpa.inp* file, the volcanic event can not occur in subarea 0 or 9).

Furthermore, it could be useful to easily allow certain users the capability to eject or fail all WPs in the repository by introducing a flag in the *tpa.inp* file, for example.

****

SCR-289: Modify qlhitsa to handle starting point outside and ending point inside quadrilateral

3/16/00 through 3/17/00

The test plan for SCR-289 is listed below:

TPA Test Plan SCR-289

Tester: Rob Rice

Test name: Modify qlhitsa to handle starting point outside and ending point inside quadrilateral

Anticipated start date: March 16, 2000

Anticipated completion date: March 17, 2000

Amount of your time available to perform this test: 16 hours

Percent of testing time to be spent in process level testing and system level testing (e.g. 50/50):
100% of the time will be spent developing a test driver program and the associated test to exercise the qlhitsa subroutine in the SUBAREA utility module. Thus, there is no process-level or system-level testing associated with this testing.

Output files to be checked: screen print from the test driver program

Input files to be checked for proper data transfer to the program: source code for the test driver program

Disposition of documentation (storage medium, physical location, and access method):
All tests will be archived on a CD-ROM and described in a scientific notebook that will be submitted to the TPA code custodian, Ron Janetzke, upon completion of the testing. On the CD-ROM, the \testing_4.0\ subdirectory will contain the test driver program (*test.f*) and the output from this driver (*test.out*). This test is associated with SCR-304 (line source instead of area source for the drift temperature calculation). Thus, the impact of this modification on the TPA results can examined in the SCR-304 testing results.

<u>Functional Test</u> Descriptions:

Test 1: The *subarea.f* file will be modified to call the qlhitsa subroutine and test six different sets of scenarios of interest for a line segment intersecting a quadriliateral. That is, line segment endpoints (1) both on the quadrilateral; (2) not intersecting the quadrilateral; (3) starting point outside and ending point inside the quadrilateral; (4) starting point inside and ending point outside the quadrilateral; (5) both points inside the quadrilateral; and (6) both points outside the quadrilateral. The \testing_4.0\ subdirectory contains the test driver program (*test.f*) and the output from this driver (*test.out*).

- **Hand calculations:** Hand calculations for this testing are limited to verification that the length of intersection of the line segment with the subarea is correctly computed. Because simplified geometry was used to specify the coordinates of the line segments and subarea in the six test sets, the correctness of the computations will be evident by inspection of the output from the *test.f* driver program in the *test.out* file that is available in the \testing_4.0\ subdirectory.

- **Process level:** N/A

- **System level:** N/A

Reasonableness Test Description: Based on the hand calculations described above, the correctness of the length of intersection of the line segment with the subarea will be evaluated.

Final Checklist (completed during testing):

- **Did the modification substantially change the results?** N/A (see SCR-304 test results)

- **Were TPA 3.3 and TPA 4.0beta compared using corresponding mean values in *tpa.inp*?** N/A (see SCR-304 test results)

- **Which nuclides were monitored to determine reasonableness of results in term of dose?** N/A (see SCR-304 test results)

Discussion of test results for SCR-289:

Test 1 Results: The listing for the test driver program (*test.f*) in the \testing_4.0 directory is provided below. Note that the test driver program echos the input data and also supplies the expected\correct output.

(file: *test.f* - driver program only)

```
program test_qlhitsa

implicit double precision (a-h,o-z)

INCLUDE 'maxnsuba.i'
INCLUDE 'subareaa.i'
INCLUDE 'subareab.i'
INCLUDE 'subareag.i'

dimension xyp1(2)
dimension xyp2(2)

nsastore = 7
ikey = 88923

xystore(1,1,1) = 0.0d0
xystore(2,1,1) = 0.0d0
xystore(1,2,1) = 1.0d1
xystore(2,2,1) = 0.0d0
xystore(1,3,1) = 1.0d1
xystore(2,3,1) = 1.0d1
xystore(1,4,1) = 0.0d0
xystore(2,4,1) = 1.0d1

isa = 1

xyp1(1) = 0.0d0
xyp1(2) = 5.0d0
xyp2(1) = 1.0d1
xyp2(2) = 5.0d0

call qlhitsa(xyp1,xyp2,isa,iflag,alengthinsa)

print *,' '
print *,' '
print *,'*************************'
print *,'TEST 1: BOTH POINTS ON SUABREA'
print *,'xyp1=',xyp1(1),xyp1(2)
print *,'xyp2=',xyp2(1),xyp2(2)
print *,' '
print *,'iflag=(1=hit,0=miss)',iflag
print *,'alengthinsa=',alengthinsa
print *,'(alengthinsa should be 10.0)'
print *,'*************************'
print *,' '
print *,' '

xyp1(1) = -0.1d0
xyp1(2) = 5.0d0
```

```
xyp2(1) = 9.9d0
xyp2(2) = 5.0d0

call qlhitsa(xyp1,xyp2,isa,iflag,alengthinsa)

print *,' '
print *,' '
print *,'*************************'
print *,'TEST 2: LEFT OUT AND RIGHT IN SUBAREA'
print *,'xyp1=',xyp1(1),xyp1(2)
print *,'xyp2=',xyp2(1),xyp2(2)
print *,' '
print *,'iflag=(1=hit,0=miss)',iflag
print *,'alengthinsa=',alengthinsa
print *,'(alengthinsa should be 9.9)'
print *,'*************************'
print *,' '
print *,' '

xyp1(1) = 0.1d0
xyp1(2) = 5.0d0
xyp2(1) = 1.1d1
xyp2(2) = 5.0d0

call qlhitsa(xyp1,xyp2,isa,iflag,alengthinsa)

print *,' '
print *,' '
print *,'*************************'
print *,'TEST 3: LEFT IN AND RIGHT OUT SUBAREA'
print *,'xyp1=',xyp1(1),xyp1(2)
print *,'xyp2=',xyp2(1),xyp2(2)
print *,' '
print *,'iflag=(1=hit,0=miss)',iflag
print *,'alengthinsa=',alengthinsa
print *,'(alengthinsa should be 9.9)'
print *,'*************************'
print *,' '
print *,' '

xyp1(1) = 0.1d0
xyp1(2) = 5.0d0
xyp2(1) = 9.9d0
xyp2(2) = 5.0d0

call qlhitsa(xyp1,xyp2,isa,iflag,alengthinsa)

print *,' '
print *,' '
print *,'*************************'
print *,'TEST 4: LEFT IN AND RIGHT IN SUBAREA'
print *,'xyp1=',xyp1(1),xyp1(2)
print *,'xyp2=',xyp2(1),xyp2(2)
print *,' '
print *,'iflag=(1=hit,0=miss)',iflag
print *,'alengthinsa=',alengthinsa
print *,'(alengthinsa should be 9.8)'
print *,'*************************'
print *,' '
```

```
      print *,' '

      xyp1(1) = -0.1d0
      xyp1(2) = 5.0d0
      xyp2(1) = 1.1d1
      xyp2(2) = 5.0d0

      call qlhitsa(xyp1,xyp2,isa,iflag,alengthinsa)

      print *,' '
      print *,' '
      print *,'*************************'
      print *,'TEST 5: LEFT OUT AND RIGHT OUT SUBAREA'
      print *,'xyp1=',xyp1(1),xyp1(2)
      print *,'xyp2=',xyp2(1),xyp2(2)
      print *,' '
      print *,'iflag=(1=hit,0=miss)',iflag
      print *,'alengthinsa=',alengthinsa
      print *,'(alengthinsa should be 10.0)'
      print *,'*************************'
      print *,' '
      print *,' '

      xyp1(1) = -0.1d0
      xyp1(2) = 5.0d1
      xyp2(1) = 1.1d1
      xyp2(2) = 5.0d1

      call qlhitsa(xyp1,xyp2,isa,iflag,alengthinsa)

      print *,' '
      print *,' '
      print *,'*************************'
      print *,'TEST 6: NO INTERSECTION WITH SUBAREA'
      print *,'xyp1=',xyp1(1),xyp1(2)
      print *,'xyp2=',xyp2(1),xyp2(2)
      print *,' '
      print *,'iflag=(1=hit,0=miss)',iflag
      print *,'alengthinsa=',alengthinsa
      print *,'(alengthinsa should be 0.0)'
      print *,'*************************'
      print *,' '
      print *,' '

      stop
      end
```

The *test.f* program was compiled to generate the *test.exe* file The output from this executable is available in \testing_4.0\test.out and is lsted below.

(file: *test.out*)

```
************************
TEST 1: BOTH POINTS ON SUABREA
xyp1=   0.00000000000000        5.00000000000000
xyp2=   10.0000000000000        5.00000000000000
```

```
iflag=(1=hit,0=miss)          1
alengthinsa=    10.0000000000000
(alengthinsa should be 10.0)
*************************

*************************
TEST 2: LEFT OUT AND RIGHT IN SUBAREA
xyp1=  -0.100000000000000        5.00000000000000
xyp2=    9.90000000000000        5.00000000000000

iflag=(1=hit,0=miss)          1
alengthinsa=    9.90000000000000
(alengthinsa should be 9.9)
*************************

*************************
TEST 3: LEFT IN AND RIGHT OUT SUBAREA
xyp1=   0.100000000000000        5.00000000000000
xyp2=    11.0000000000000        5.00000000000000

iflag=(1=hit,0=miss)          1
alengthinsa=    9.90000000000000
(alengthinsa should be 9.9)
*************************

*************************
TEST 4: LEFT IN AND RIGHT IN SUBAREA
xyp1=   0.100000000000000        5.00000000000000
xyp2=    9.90000000000000        5.00000000000000

iflag=(1=hit,0=miss)          1
alengthinsa=    9.80000000000000
(alengthinsa should be 9.8)
*************************

*************************
TEST 5: LEFT OUT AND RIGHT OUT SUBAREA
xyp1=  -0.100000000000000        5.00000000000000
xyp2=    11.0000000000000        5.00000000000000

iflag=(1=hit,0=miss)          1
alengthinsa=    10.0000000000000
(alengthinsa should be 10.0)
*************************

*************************
TEST 6: NO INTERSECTION WITH SUBAREA
xyp1=  -0.100000000000000        50.0000000000000
xyp2=    11.0000000000000        50.0000000000000

iflag=(1=hit,0=miss)          0
alengthinsa=    0.00000000000000
(alengthinsa should be 0.0)
*************************
```

Note that the expected and calculated output (i.e., alengthinsa) are the same for all tests. Thus, the testing results for SCR-289 reported above and archived in the \tesing_4.0 directory indicates the

TPA Version 4.0 code **PASSES** the test.

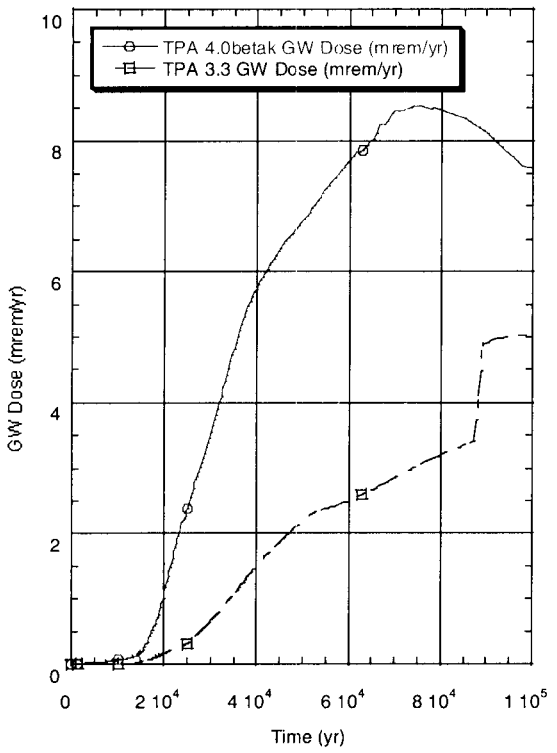
END OF TESTING FOR SCRS 304, 293, AND 289. AS PRESENTED ABOVE, THE TPA VERSION 4.0 CODE **PASSES** ALL OF THE TESTS DESCRIBED IN THE TEST PLANS FOR THESE SCRS.
****

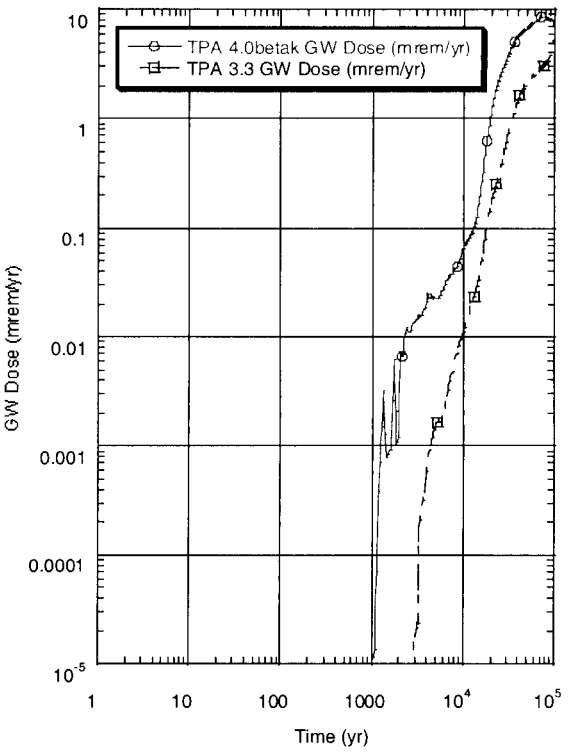
3/27/00

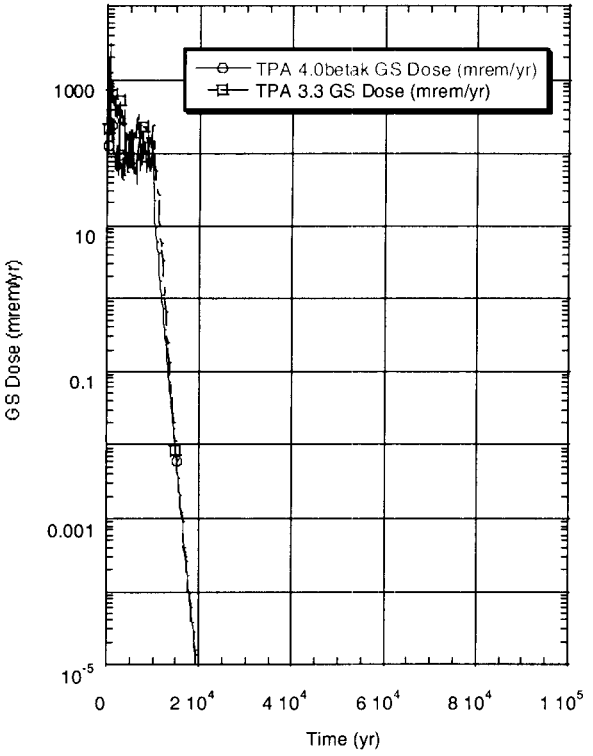
****

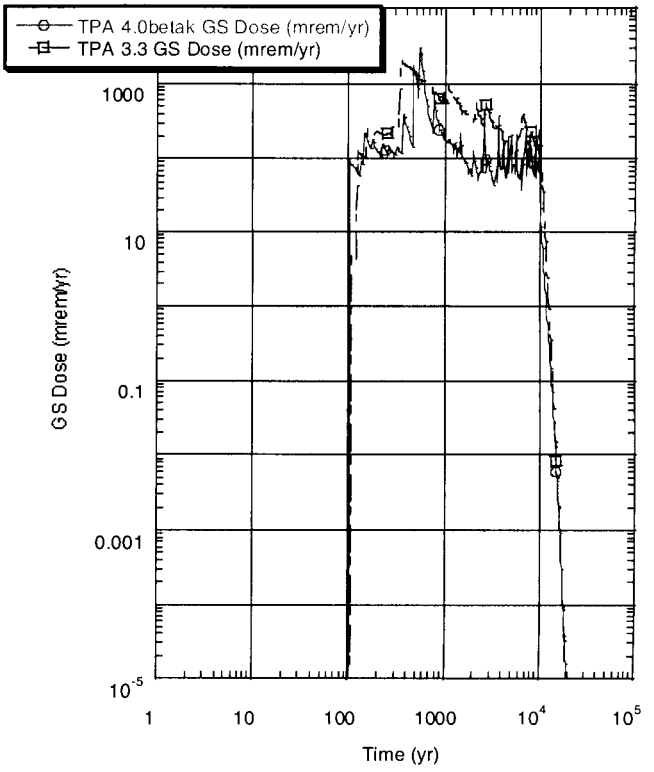
Other Testing Notes

500 vector runs using v3.3 and 4.0betak with volcano ON were completed and the results emailed to R. Jantezke and G. Wittmeyer. The plots are provided on the following pages.


TPA 4.0betak GW Dose (mrem/yr)
TPA 3.3 GW Dose (mrem/yr)
GW Dose (mrem/yr)
Time (yr)

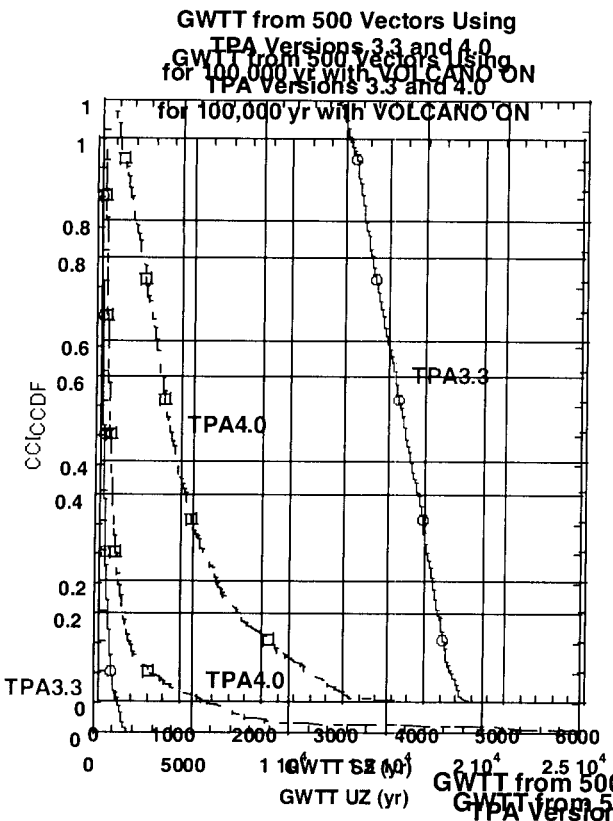

TPA 4.0betak GW Dose (mrem/yr)
TPA 3.3 GW Dose (mrem/yr)
GW Dose (mrem/yr)
Time (yr)

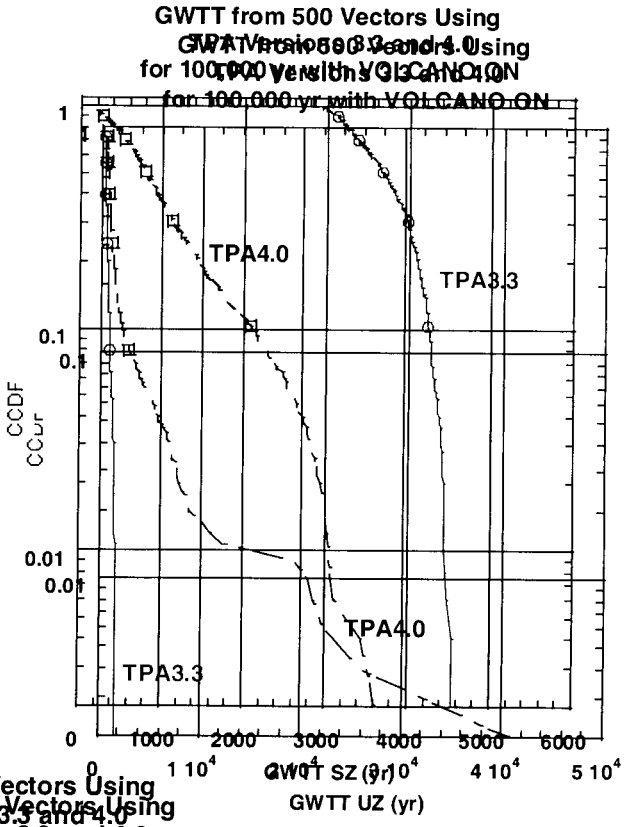

TPA 4.0betak GS Dose (mrem/yr)
TPA 3.3 GS Dose (mrem/yr)
GS Dose (mrem/yr)
Time (yr)

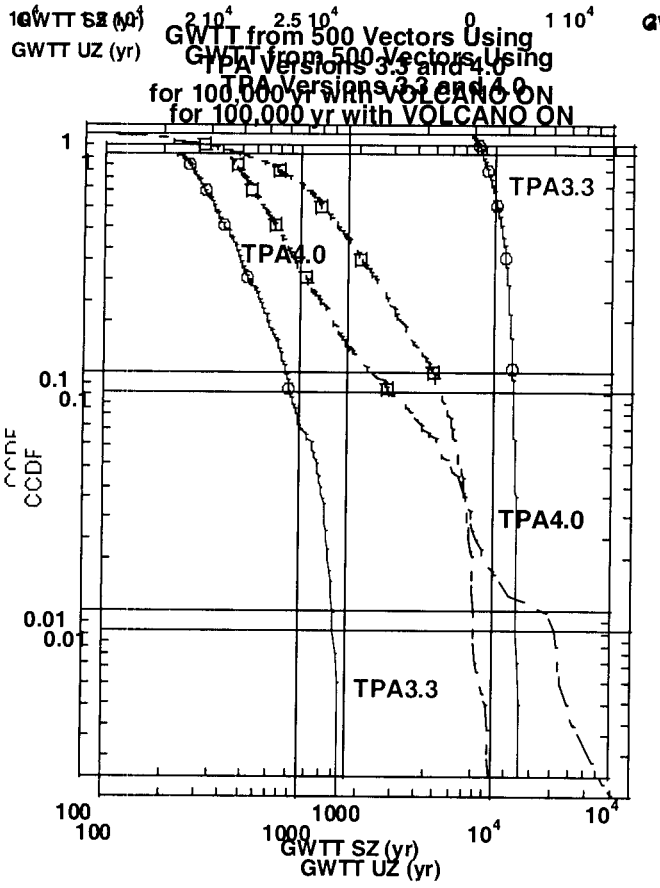

TPA 4.0betak GS Dose (mrem/yr)
TPA 3.3 GS Dose (mrem/yr)
GS Dose (mrem/yr)
Time (yr)

*
*
A

VE GWTT UZ (different axes)







AVE GWTT SZ (different axes)

Additionally, the *exec.f* file was modified to match the volcanic failures printed to the screen with the number of extrusive and intrusive WPs failures (as sampled in *tpa.inp*) - at least to match whenever possible (i.e., when there are sufficient WPs available). This file (modify.f) was emailed to R. Janetzke. A file comparison between the v4.0 betak *exec.f* and the modified *exec.f* (*modify.f*) that identifies the changes is provided below.

```
Comparing files EXEC.F and EXEC.F.ORIGINAL
***** EXEC.F
        if (numberoffailedwpsinsa .gt. 0) then
cc rwr 3/25/00
cc          if (isa .eq. 2) then
     call clearchar(60,name)
     name = 'NumberOfWPsEntrainedByEjecta[]'
     iwpentrained = ispquery( name )
     wpentrained = valuesp( iwpentrained )
     call clearchar(60,name)
     name = 'NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[]'
     iwpfailedindrift = ispquery( name )
     wpsfailedindrift = valuesp( iwpfailedindrift )
     voltotalwps = wpsfailedindrift + wpentrained
     nvoltotalwps = dint(voltotalwps)
     anumberoffailedwpsinsa = dble(numberoffailedwpsinsa)
       nwpsavailable = numberofwpsinsa -
    &    (nsafailed - numberoffailedwpsinsa)
      print *,'debug:nvoltotalwps=',nvoltotalwps
      print *,'debug:numberoffailedwpsinsa2=',numberoffailedwpsinsa2
      print *,'debug:anumberoffailedwpsinsa=',anumberoffailedwpsinsa
      print *,'debug:nwpsavailable=',nwpsavailable
       if (nwpsavailable .lt. nvoltotalwps) then
```

```
        print *,'debug: in loop 1'
       numberoffailedwpsinsa2 = nwpsavailable
        nsafailed = (nsafailed - numberoffailedwpsinsa) +
     &     numberoffailedwpsinsa2
        thispart2=dble(nwpsavailable)/dble(numberofwpsinsa)
        print *,'debug:thispart=',thispart
        print *,'debug:thispart=2',thispart2
         volcaniconly = volcaniconly - thispart + thispart2
         cumfailwp(i) = 1.0d0
        print *,'debug:volcaniconly=',volcaniconly
        print *,'debug:cumfailwp(i)=',cumfailwp(i)
        print *,'debug:numberoffailedwpsinsa2=',numberoffailedwpsinsa2
        print *,'debug:nsafailed=',nsafailed
             print '(a,i7,a,0pf9.1,a,a,/,a,a)',
     &          ' exec: failed WPs from VOLCANIC  event =',
     &            numberoffailedwpsinsa2,' at time =',tim(i),' yr',
     &          ' (includes ejected WPs)',
     & '(note:there are not enough intact WPs to match the sampled',
     & '     values in tpa.inp for intrusive and extrusive WP failures'
       else
        print *,'debug: in loop 2'
        numberoffailedwpsinsa2 = nvoltotalwps
        print *,'debug:numberoffailedwpsinsa2=',numberoffailedwpsinsa2
        nsafailed = (nsafailed - numberoffailedwpsinsa) +
     &     numberoffailedwpsinsa2
        print *,'debug:nsafailed=',nsafailed
         thispart2=dble((nwpsavailable-nvoltotalwps)/numberofwpsinsa)
        print *,'debug:thispart=',thispart
        print *,'debug:thispart=2',thispart2
         volcaniconly = volcaniconly + thispart2
         cumfailwp(i) = cumfailwp(i) + thispart2
        print *,'debug:volcaniconly=',volcaniconly
        print *,'debug:cumfailwp(i)=',cumfailwp(i)

             print '(a,i7,a,0pf9.1,a,a)',
***** EXEC.F.ORIGINAL
        if (numberoffailedwpsinsa .gt. 0) then
          if (isa .eq. 2) then
             print '(a,i7,a,0pf9.1,a,a)',
*****

***** EXEC.F
     &          ' exec: failed WPs from VOLCANIC  event =',
     &            numberoffailedwpsinsa2,' at time =',tim(i),' yr',
     &          ' (includes ejected WPs)'
        wpsfailedtime(4,icheck,1) =
     &     wpsfailedtime(4,icheck,1) -
     &     dble(numberoffailedwpsinsa) + dble(numberoffailedwpsinsa2)

       endif

cc rwr            else
cc rwr              print '(a,i7,a,0pf9.1,a)',
cc rwr     &          ' exec: failed WPs from VOLCANIC  event =',
cc rwr     &            numberoffailedwpsinsa,' at time =',tim(i),' yr'
cc rwr            end if
cc rwr          end if
      endif
```

```
        releasewpfailedtime(1,3) = numberoffailedwpsinsa2
        releasewpfailedtime(2,3) = tim(i)
***** EXEC.F.ORIGINAL
    &         ' exec: failed WPs from VOLCANIC  event =',
    &           numberoffailedwpsinsa,' at time =',tim(i),' yr',
    &         ' (includes ejected WPs)'
          else
            print '(a,i7,a,0pf9.1,a)',
    &         ' exec: failed WPs from VOLCANIC  event =',
    &           numberoffailedwpsinsa,' at time =',tim(i),' yr'
          end if
        end if

        releasewpfailedtime(1,3) = numberoffailedwpsinsa
        releasewpfailedtime(2,3) = tim(i)
*****
```

In additional testing of the repository layout changes (i.e., drift location and allowable amounts of waste that can be emplaced in the repository), the following observations are noted:

The v. 4.0betak *tpa.inp* parameters and data (*repdes.dat*) fill subareas 1 through 8 with about 68,030 MTUs of waste. When the user changes the WP or drift spacing, MTUs in repository, subarea coordinates, repository outline or angle, a number of situations may arise including,

- errors resulting from no WPs being assigned to a subarea

- once the repository subareas are filled with waste, the drifts (and MTUs) outside of the subareas is not used.

- the TPA code allows for a part of the subarea to filled with WPs, although the entire subarea area (i.e., based on the tpa.inp coordinates) is considered for TPA calculations

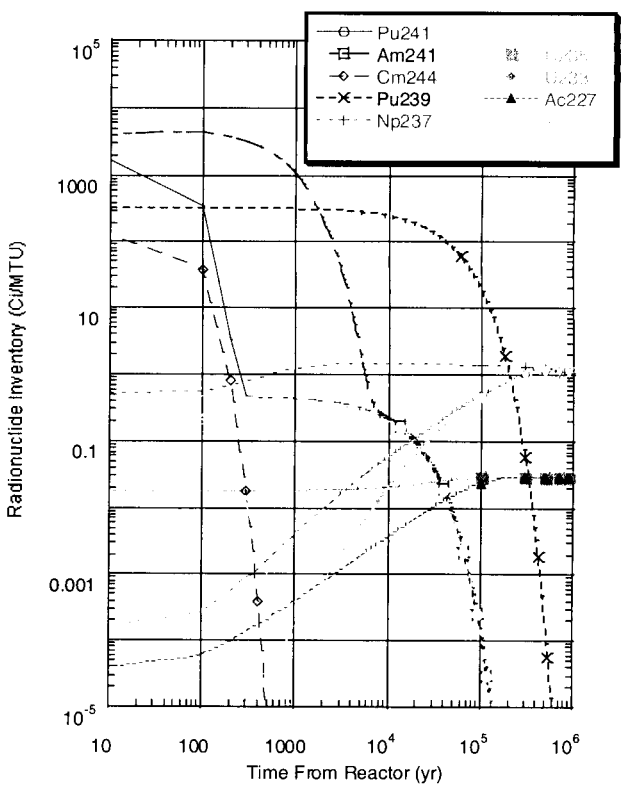
****

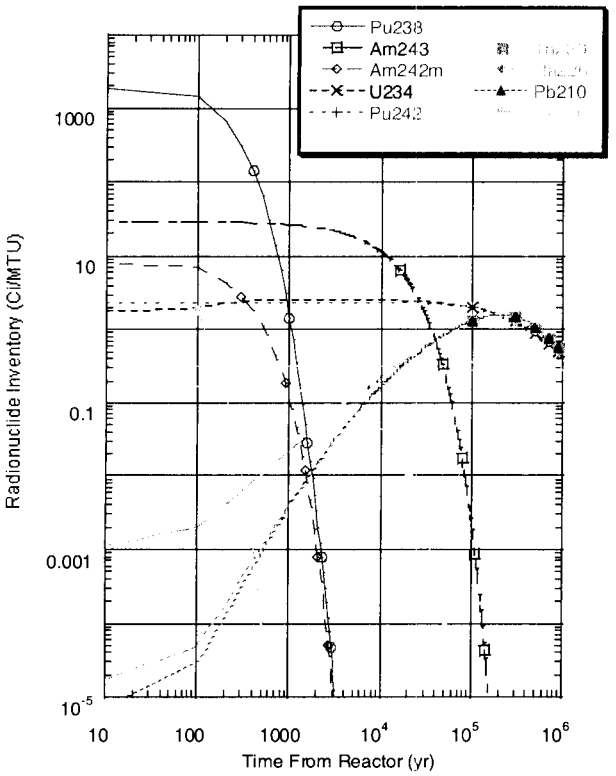
Also, wrote a short program to generate the WP inventory for each of the 43 TPA radionuclides and plotted the results. The program was included in the EBSREL module and the file comparison is shown below.

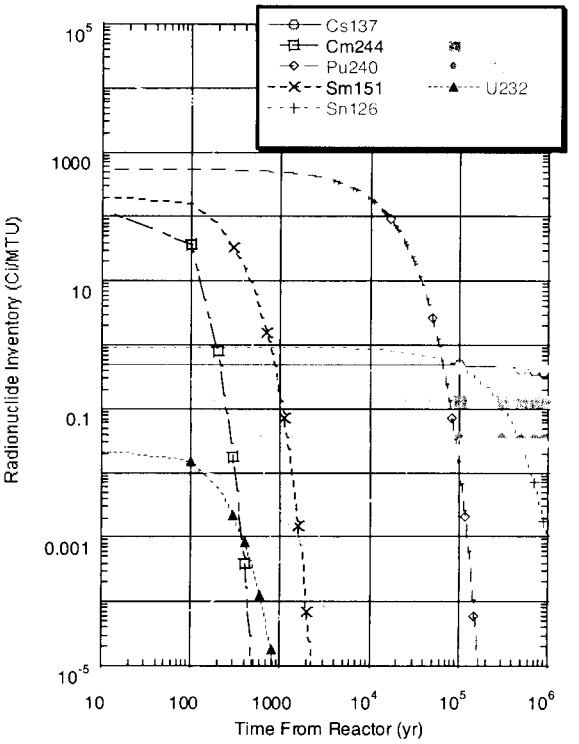
```
Comparing files ebsrel.f and EBSREL.F.ORIGINAL
***** ebsrel.f

cc rwr debug: find radionuclide inventory
    dimension cipermtustore(43)
    dimension amolepermtu(43)

    character*100 aline
***** EBSREL.F.ORIGINAL

    character*100 aline
```

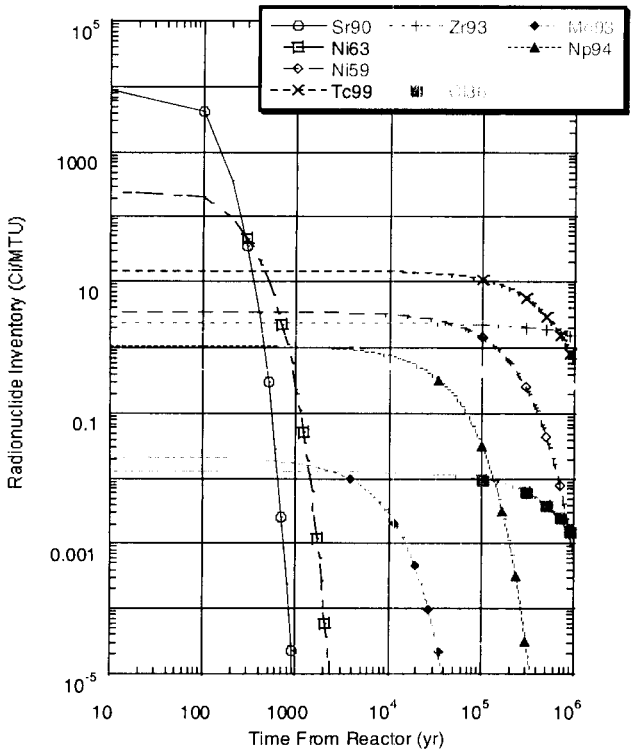
```
*****

***** ebsrel.f
      enddo
cc rwr debug      close(iebspacnuc)

cc rwr debug:find radionuclide inventory
        write(iebspacnuc,fmt='(a)')
     &   'time    inventory of 43 TPA nuclides (Ci/MTU)'
      time = 0.0d0
      do i = 1,10001
        call decay43mol(time,amolepermtu)
        do j = 1,43
          cipermtustore(j)=amolepermtu(j)*activityperiso(j)
        enddo
        write(iebspacnuc,fmt='(44(1pe15.4,3x))')time,
     &  (cipermtustore(k),k=1,43)
        time = time + 100.0d0
      enddo

      close(iebspacnuc)
      stop
c-----------------------------------------------------------------------
***** EBSREL.F.ORIGINAL
      enddo
      close(iebspacnuc)

cc rwr debug
cc      call test_inv
cc      stop

c-----------------------------------------------------------------------
*****
```

Plots of results were emailed to S. Mohanty. These plots will update the v.3.2 User's Guide figure 3-9. See these figures below.









3/29/00

Received the new initial inventory for all 43 radionuclides from S. Mohanty via email (see below). These values were used to replace the values in the last column of the *nuclides.dat* file. The new nuclides.dat file was emailed to R. Janetzke.

RADIONUCLIDE INVENTORIES

Previous fuel fractions used to calculated the NEW inventories

0.35	= BWR blend
0.65	= PWR blend

Isotope	NEW Version 3.2 Inventory Ci/MTIHM	Activity@10 y (Ci/MTU)
C-14	1.4425	13.3
Cl-36	0.011461	0.0117
Ni-59	2.44185	24.6
Ni-63	372.395	305
Se-79	0.45847	0.38
Sr-90	62549	53100
Zr-93	2.47465	18.5
Mo-93	0.0151	0.0101
Nb-94	0.847985	0.504
Tc-99	14.54	12.3
Pd-107	0.13127	0.105
Ag-108m	0.012613	0.012
Sn-121m	1.035585	0.797
Sn-126	0.885445	0.716
I-129	0.035708	0.0295
Cs-135	0.535605	0.351
Cs-137	91536	76400
Sm-151	428.075	318
Pb-210	5.67E-08	4.72E-08
Ra-226	4.11E-07	3.67E-07
Ac-227	7.51E-06	5.19E-06
Th-229	2.75E-07	1.39E-07
Th-230	0.000137	0.000129
Pa-231	2.69E-05	1.95E-05
U-232	0.039307	0.0248
U-233	3.44E-05	0.000024
U-234	1.1818	11.3
U-235	0.017087	0.0169
U-236	0.28093	0.24
Np-237	0.434255	0.287
Pu-238	3769	2110
U-238	0.31529	0.319
Pu-239	368.57	308
Pu-240	543.915	508
Pu-241	92174.5	74400
Am-241	2076.7	1640
Pu-242	2.09895	16
Am-242m	24.7785	74.9
Cm-243	25.528	15.3
Am-243	26.356	15.4
Cm-244	2675.1	1150

Cm-245	0.365635	0.125
Cm-246	0.076229	0.0256

The old and new *nuclides.dat* files are provided below.

(old *nuclides.dat* file)

```
TITLE: TPA4.0 nuclide data used for the invent.f module.
TITLE: (data extracted from invent.f - prepared by jmm)
** mas Se79 & Ag108m half-lives updated 3/17/00
**     idx = Nuclide index
**     NIS = namesisotopesave
**     NES = nameselemsave
** CPMTU@10 = cipermtuat10yr
**     --- = unitless
** Number of nuclides to be read follows:
43
**idx,   NIS,   NIS2,   NIS3, NES,   wmole, halflife,   epalim,  CPMTU@10
**---    ---,    ---,    ---, ---,  [g/mol],    [yr], [Ci/MTU],  [Ci/MTU]
  01    U238   U238    U238    U   238.0d0  4.468d9     0.10   3.15d-01
  02   Cm246  Cm246   CM246   Cm   246.0d0  4.731d3     0.10   1.76d-01
  03   Pu242  Pu242   PU242   Pu   242.0d0  3.869d5     0.10   2.37d+00
  04  Am242m Am242m  AM242M   Am   242.0d0  1.520d2     0.10   1.19d+01
  05   Pu238  Pu238   PU238   Pu   238.0d0  8.774d1     0.10   3.67d+03
  06    U234   U234    U234    U   234.0d0  2.445d5     0.10   1.25d+00
  07   Th230  Th230   TH230   Th   230.0d0  7.700d4     0.01   1.48d-04
  08   Ra226  Ra226   RA226   Ra   226.0d0  1.600d3     0.10   4.50d-07
  09   Pb210  Pb210   PB210   Pb   210.0d0  2.230d1     1.00   6.49d-08
  10   Cm243  Cm243   CM243   Cm   243.0d0  2.850d1     0.10   3.00d+01
  11   Am243  Am243   AM243   Am   243.0d0  7.380d3     0.10   2.89d+01
  12   Pu239  Pu239   PU239   Pu   239.0d0  2.406d4     0.10   3.36d+02
  13    U235   U235    U235    U   235.0d0  7.038d8     0.10   1.78d-02
  14   Pa231  Pa231   PA231   Pa   231.0d0  3.277d4     0.10   2.83d-05
  15   Ac227  Ac227   AC227   Ac   227.0d0  2.177d1     0.10   7.97d-06
  16   Cm245  Cm245   CM245   Cm   245.0d0  8.499d3     0.10   4.71d-01
  17   Pu241  Pu241   PU241   Pu   241.0d0  1.440d1  1000.00   9.26d+04
  18   Am241  Am241   AM241   Am   241.0d0  4.322d2     0.10   2.09d+03
  19   Np237  Np237   NP237   Np   237.0d0  2.140d6     0.10   3.99d-01
  20    U233   U233    U233    U   233.0d0  1.585d5     0.10   3.23d-05
  21   Th229  Th229   TH229   Th   229.0d0  7.339d3     0.10   3.95d-07
  22   Cm244  Cm244   CM244   Cm   244.0d0  1.811d1  1000.00   3.19d+03
  23   Pu240  Pu240   PU240   Pu   240.0d0  6.537d3     0.10   5.38d+02
  24    U236   U236    U236    U   236.0d0  2.341d7     0.10   2.96d-01
  25    U232   U232    U232    U   232.0d0  7.200d1     0.10   4.63d-02
  26   Sm151  Sm151   SM151   Sm   151.0d0  8.999d1     1.00   3.86d+02
  27   Cs137  Cs137   CS137   Cs   137.0d0  3.000d1     1.00   9.62d+04
  28   Cs135  Cs135   CS135   Cs   135.0d0  2.300d6     1.00   5.02d-01
  29    I129   I129    I129    I   129.0d0  1.570d7     0.10   3.73d-02
  30   Sn126  Sn126   SN126   Sn   126.0d0  1.000d5     1.00   9.16d-01
  31  Sn121m Sn121m  SN121M   Sn   121.0d0  4.997d1     1.00   1.05d+00
  32  Ag108m Ag108m  AG108M   Ag   108.0d0  4.180d2     1.00   1.36d-02
  33   Pd107  Pd107   PD107   Pd   107.0d0  6.496d6     1.00   1.40d-01
  34    Tc99   Tc99    TC99    Tc    99.0d0  2.130d5    10.00   1.51d+01
  35    Mo93   Mo93    MO93    Mo    93.0d0  3.498d3     1.00   2.10d-02
  36    Nb94   Nb94    NB94    Nb    94.0d0  2.030d4     1.00   1.06d+00
  37    Zr93   Zr93    ZR93    Zr    93.0d0  1.530d6     1.00   2.35d+00
```

```
 38    Sr90   Sr90    SR90    Sr    90.0d0  2.912d1     1.00  6.55d+04
 39    Se79   Se79    SE79    Se    79.0d0  1.100d6     1.00  4.82d-01
 40    Ni63   Ni63    NI63    Ni    63.0d0  9.200d1     1.00  5.07d+02
 41    Ni59   Ni59    NI59    Ni    59.0d0  8.000d4     1.00  3.46d+00
 42    Cl36   Cl36    CL36    Cl    36.0d0  3.010d5     1.00  1.27d-02
 43     C14   C14     C14     C     14.0d0  5.729d3     0.10  1.71d+00
```

(new *nuclides.dat* file)

```
TITLE: TPA4.0 nuclide data used for the invent.f module.
TITLE: (data extracted from invent.f - prepared by jmm)
** mas Se79 & Ag108m half-lives updated 3/17/00
** rwr added new initial inventories 3/28/00
**     idx = Nuclide index
**     NIS = namesisotopesave
**     NES = nameselemsave
** CPMTU@10 = cipermtuat10yr
**     --- = unitless
** Number of nuclides to be read follows:
43
**idx,    NIS,    NIS2,    NIS3, NES,    wmole, halflife,   epalim,  CPMTU@10
**---     ---,     ---,     ---, ---,  [g/mol],     [yr], [Ci/MTU],  [Ci/MTU]
  01    U238   U238    U238    U   238.0d0  4.468d9     0.10  3.15d-01
  02   Cm246  Cm246   CM246   Cm   246.0d0  4.731d3     0.10  7.62d-02
  03   Pu242  Pu242   PU242   Pu   242.0d0  3.869d5     0.10  2.10d+00
  04  Am242m Am242m  AM242M   Am   242.0d0  1.520d2     0.10  2.48d+01
  05   Pu238  Pu238   PU238   Pu   238.0d0  8.774d1     0.10  3.77d+03
  06    U234   U234    U234    U   234.0d0  2.445d5     0.10  1.18d+00
  07   Th230  Th230   TH230   Th   230.0d0  7.700d4     0.01  1.37d-04
  08   Ra226  Ra226   RA226   Ra   226.0d0  1.600d3     0.10  4.11d-07
  09   Pb210  Pb210   PB210   Pb   210.0d0  2.230d1     1.00  5.67d-08
  10   Cm243  Cm243   CM243   Cm   243.0d0  2.850d1     0.10  2.55d+01
  11   Am243  Am243   AM243   Am   243.0d0  7.380d3     0.10  2.64d+01
  12   Pu239  Pu239   PU239   Pu   239.0d0  2.406d4     0.10  3.69d+02
  13    U235   U235    U235    U   235.0d0  7.038d8     0.10  1.71d-02
  14   Pa231  Pa231   PA231   Pa   231.0d0  3.277d4     0.10  2.69d-05
  15   Ac227  Ac227   AC227   Ac   227.0d0  2.177d1     0.10  7.51d-06
  16   Cm245  Cm245   CM245   Cm   245.0d0  8.499d3     0.10  3.66d-01
  17   Pu241  Pu241   PU241   Pu   241.0d0  1.440d1  1000.00  9.22d+04
  18   Am241  Am241   AM241   Am   241.0d0  4.322d2     0.10  2.08d+03
  19   Np237  Np237   NP237   Np   237.0d0  2.140d6     0.10  4.34d-01
  20    U233   U233    U233    U   233.0d0  1.585d5     0.10  3.44d-05
  21   Th229  Th229   TH229   Th   229.0d0  7.339d3     0.10  2.75d-07
  22   Cm244  Cm244   CM244   Cm   244.0d0  1.811d1  1000.00  2.68d+03
  23   Pu240  Pu240   PU240   Pu   240.0d0  6.537d3     0.10  5.44d+02
  24    U236   U236    U236    U   236.0d0  2.341d7     0.10  2.81d-01
  25    U232   U232    U232    U   232.0d0  7.200d1     0.10  3.93d-02
  26   Sm151  Sm151   SM151   Sm   151.0d0  8.999d1     1.00  4.28d+02
  27   Cs137  Cs137   CS137   Cs   137.0d0  3.000d1     1.00  9.15d+04
  28   Cs135  Cs135   CS135   Cs   135.0d0  2.300d6     1.00  5.36d-01
  29    I129   I129    I129    I   129.0d0  1.570d7     0.10  3.57d-02
  30   Sn126  Sn126   SN126   Sn   126.0d0  1.000d5     1.00  8.85d-01
  31  Sn121m Sn121m  SN121M   Sn   121.0d0  4.997d1     1.00  1.04d+00
  32  Ag108m Ag108m  AG108M   Ag   108.0d0  4.180d2     1.00  1.26d-02
  33   Pd107  Pd107   PD107   Pd   107.0d0  6.496d6     1.00  1.31d-01
  34    Tc99   Tc99    TC99    Tc    99.0d0  2.130d5    10.00  1.45d+01
  35    Mo93   Mo93    MO93    Mo    93.0d0  3.498d3     1.00  1.51d-02
  36    Nb94   Nb94    NB94    Nb    94.0d0  2.030d4     1.00  8.48d-01
```

37	Zr93	Zr93	ZR93	Zr	93.0d0	1.530d6	1.00	2.47d+00
38	Sr90	Sr90	SR90	Sr	90.0d0	2.912d1	1.00	6.25d+04
39	Se79	Se79	SE79	Se	79.0d0	1.100d6	1.00	4.58d-01
40	Ni63	Ni63	NI63	Ni	63.0d0	9.200d1	1.00	3.72d+02
41	Ni59	Ni59	NI59	Ni	59.0d0	8.000d4	1.00	2.44d+00
42	Cl36	Cl36	CL36	Cl	36.0d0	3.010d5	1.00	1.15d-02
43	C14	C14	C14	C	14.0d0	5.729d3	0.10	1.44d+00

Using these files, the basecase *tpa.inp* file was used in two TPA runs. The changes in the screen print are given below. Note that there are small changes in the GW doses. These differences are attributable to the change in the *nuclides.dat* initial inventories.

(partial screen print using the old *nuclides.dat* file)

```
exec: calling dcagw
            Highest annual dose GW pathway
        I129   1.9839E-03 [mrem/yr]  at  1.000E+04 yr
        Ni59   6.6130E-05 [mrem/yr]  at  1.000E+04 yr
        Cl36   2.2136E-05 [mrem/yr]  at  8.691E+03 yr
        Tc99   9.3104E-10 [mrem/yr]  at  1.000E+04 yr
   The remaining        16  nuclide(s) have zero release
      At end of TPI, annual dose GW pathway
        I129   1.9839E-03 [mrem/yr]
        Ni59   6.6130E-05 [mrem/yr]
        Cl36   1.8147E-05 [mrem/yr]
        Tc99   9.3104E-10 [mrem/yr]
          sum  2.0681E-03 [mrem/yr]
   The remaining        16  nuclide(s) have zero release
exec: end realizations

exec:  Run Successfully Completed
```

(partial screen print using the new *nuclides.dat* file)

```
exec: calling dcagw
            Highest annual dose GW pathway
        I129   1.8988E-03 [mrem/yr]  at  1.000E+04 yr
        Ni59   4.6639E-05 [mrem/yr]  at  1.000E+04 yr
        Cl36   2.0045E-05 [mrem/yr]  at  8.691E+03 yr
        Tc99   8.9352E-10 [mrem/yr]  at  1.000E+04 yr
   The remaining        16  nuclide(s) have zero release
      At end of TPI, annual dose GW pathway
        I129   1.8988E-03 [mrem/yr]
        Ni59   4.6639E-05 [mrem/yr]
        Cl36   1.6433E-05 [mrem/yr]
        Tc99   8.9352E-10 [mrem/yr]
          sum  1.9619E-03 [mrem/yr]
   The remaining        16  nuclide(s) have zero release
exec: end realizations

exec:  Run Successfully Completed
```

Using the results from the program in EBSREL shown above which generates the time history of inventory for all 43 radionuclides, the TPA code was run and the inventories as a function of time were plotted in Kaleidagraph for all 43 radionuclides. The times at which inventories were computed were modified for plotting purposes as shown below in *ebsrel.f.*

(*ebsrel.f* modifications)

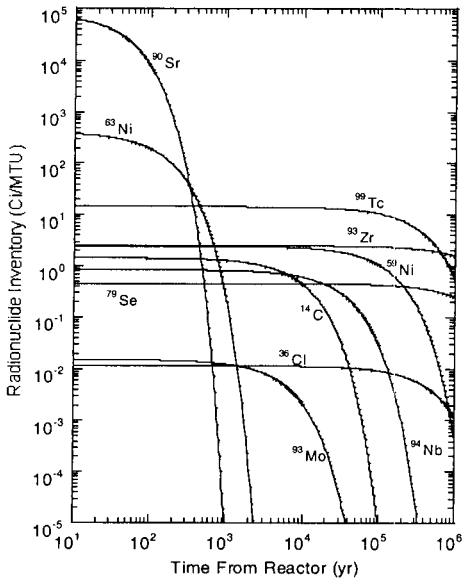
```
cc rwr debug: find radionuclide inventory
    dimension cipermtustore(43)
    dimension amolepermtu(43)
```

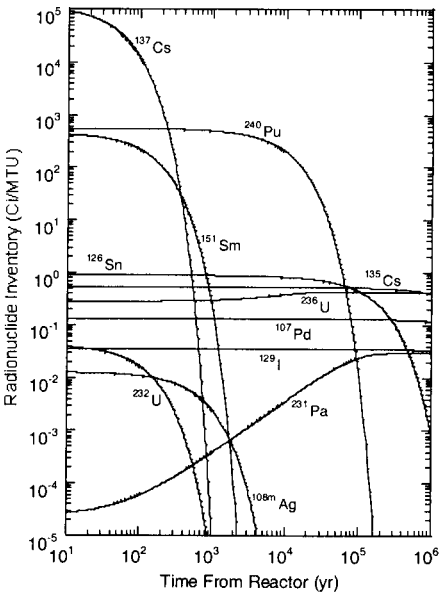
and

```
cc rwr debug     close(iebspacnuc)

cc rwr debug:find radionuclide inventory
          write(iebspacnuc,fmt='(a)')
   &   'time    inventory of 43 TPA nuclides (Ci/MTU)'
    time = 0.0d0
    do i = 1,501
          call decay43mol(time,amolepermtu)
          do j = 1,43
            cipermtustore(j)=amolepermtu(j)*activityperiso(j)
          enddo
          timeprint = time + 10.0d0
          write(iebspacnuc,fmt='(44(1pe15.4,3x))')timeprint,
   &  (cipermtustore(k),k=1,43)
          if (time .le. 100.0) then
            time = time + 1.0d0
          elseif (time .le. 1000.0d0) then
            time = time + 10.0d0
          elseif (time .le. 10000.0d0) then
            time = time + 100.0d0
          elseif (time .le. 100000.0d0) then
            time = time + 1000.0d0
          elseif (time .le. 1000000.0d0) then
            time = time + 10000.0d0
          endif
    enddo

    close(iebspacnuc)
    stop
```

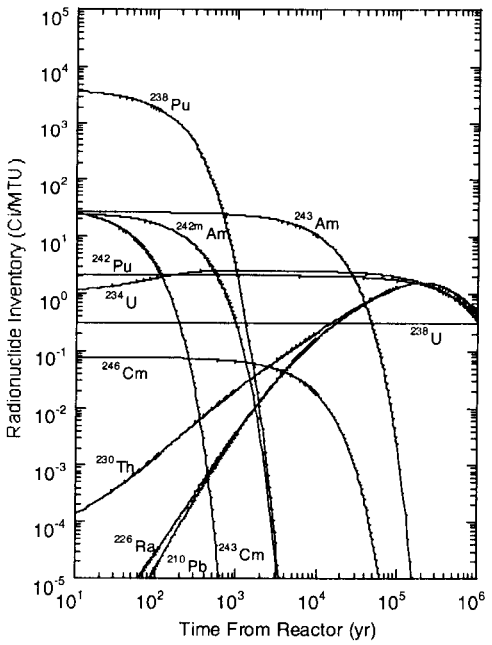
The plots shown above for the inventory as a function of time were updated, modified to match figure 3-9 in the TPA Version 3.2 Code User's Guide, and emailed to S. Mohanty. The plots are shown below.

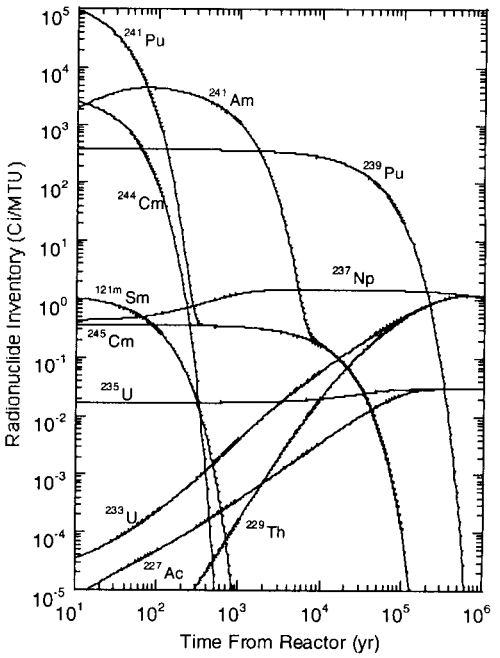
8/29/00 - 9/13/00 Performed Importance Analysis Debugging, Code Modifications, and





Code Testing, Including Interaction with CNWRA Staff (specific details





of this work are provided

subsequently):

Received instructions from R. Janetzke to develop a test plan for the Importance Analysis features that were added to version 4.0. The following test plan was developed and faxed to R. Janetzke for his review and approval on 9/1/00. (R. Janetzke approved of the test plan, but recommended comparing the *lhs.out* files, in addition to the ones listed. The following test plan includes these changes.)

****

TPA Version 4.1 Test Plan: PA-SCR-322

Task Description: Activate importance analysis

Reason for Change: Enable the generation of sub-system, barrier, and component importance analysis

---

Analyst: Robert Rice **Date:** 8/31/00

Controlled Version: **Version 4.0 Released April 3,2000 (see the SCR322\v40 directory)**
Modified Version: **Version 4.1 modified source code for Importance Analysis from R. Janetzke via email attachment on 8/29/00 (see the SCR322\source directory)**

(Note: all tests are conducted for one realization and 201 time steps for 10,000 yr using the basecase *tpa.inp* input file)

Flag 1: ImportanceAnalysisFlag(yes=1,no=0)
Description: This is the master flag to control the importance analysis process. If this flag is zero all importance analysis is skipped regardless of the other component flag values.

Test 1. Run Versions 4.0 and 4.1 with their accompanying *tpa.inp* files with all append files ON, and ImportanceAnalysisFlag(yes=1,no=0) = 0 and all Importance Analysis flags inactive.

Purpose: Because Versions 4.0 and 4.1 should have the same results using their accompanying *tpa.inp* files, this test verifies the modifications introduced in Version 4.1 do not change the output with the importance analysis OFF.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file *filecomp.bat*)
- *tpa.inp*
- all **.res* files
- all **.tpa* files
- all append files (**.ech*, **.rlt*, and **.cum*)
- *lhs.out*

Pass/Fail Criteria:

The results in all output files should be the same except for the time and date of the run. See the *filecomp.out* file for the differences between these two runs.

Documentation of Testing:

This test is stored in the SCR322/flag1/test1 directory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Test 2. Run Versions 4.0 and 4.1 with their accompanying tpa.inp files for 10,000 yr with all append files ON, ImportanceAnalysisFlag(yes=1,no=0) = 1 (ON), and all other flags with the barriers inactive.

Purpose: Because Versions 4.0 and 4.1 should have the same results using their accompanying *tpa.inp* files, this test verifies the modifications introduced in Version 4.1 do not change the output. Moreover, with only the importance analysis flag = 1 (ON) and all other importance analysis flags inactive, there should be no difference in the results for Versions 4.0 and 4.1.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file *filecomp.bat*)
- *tpa.inp*
- all *.*res* files
- all *.*tpa* files
- all append files (*.*ech*, *.*rlt*, and *.*cum*)
- *lhs.out*

Pass/Fail Criteria:

The results in all output files should be the same except for the time and date of the run. See the *filecomp.out* file for the differences between these two runs.

Documentation of Testing:

This test is stored in the SCR322/flag1/test2 directory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Test 3. Run versions 4.0 and 4.1 with their accompanying *tpa.inp* files for 10,000 yr with all append files ON, ImportanceAnalysisFlag(yes=1,no=0) = 0 (OFF) but all other importance analysis components active.

Purpose: Because Versions 4.0 and 4.1 should have the same results using their accompanying *tpa.inp* files, this test verifies the modifications introduced in Version 4.1 do not change the output. Moreover, with the importance analysis flag = 0 (OFF) and all other components active, there should be no difference in the results for Versions 4.0 and 4.1.

TPA Output Files to Compare:

(use the "fc" DOS command in WINDOWS NT 4.0 with the script file filecomp.bat)
- tpa.inp
- all *.res files
- all *.tpa files
- all append files (*.ech, *.rlt, and *.cum)
- *lhs.out*

Pass/Fail Criteria:

The results in all output files should be the same except for the time and date of the run. See the *filecomp.out* file for the differences between these two runs.

Documentation of Testing:

This test is stored in the SCR322/flag1/test3 directory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Testing for Flags 2-24

Description: Each of these flags will be examined individually with one test to ensure that the values specified in the *ia.dat* file for each flag is properly transferred from the *tpa.inp* file to the *cp.tpa* file. The following information lists the (1) *ia.dat* file with the parameter values and the flag name and (2) the *tpa.inp* file parameter names that should be modified in the *cp.tpa* file for each of the flags.

Listing of *ia.dat*:

```
TITLE: Importance Analysis data for the TPA code using the IA option.
TITLE: Developed for TPA 4.1 on 8-02-00.
**
  SUBSYSTEM = 'SubsystemNaturalStudy'
**
  BARRIER   = 'BarrierBiosphereStudy'
**
  Component = 'ComponentPrecipitationStudy'
**
  parameter = 'WastePackageFlowMultiplicationFactor'
  value     = 1.11111
**
  parameter = 'SubAreaWetFraction'
  value     = 2.22222
**
  BARRIER   = 'BarrierUpperUnsaturatedZoneStudy'
**
  Component = 'ComponentTivaCanyonStudy'
**
  parameter = 'ElevationOfGroundSurface[m]'
  value     = 3.33333
**
  parameter = 'MassDensityofYMRock[kg/m^3]'
  value     = 4.44444
**
  parameter = 'SpecificHeatofYMRock[J/(kg-K)]'
  value     = 5.55555
**
  parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
  value     = 6.66666
**
  parameter = 'EmissivityOfDriftWall[-]'
  value     = 7.77777
**
  parameter = 'CritChlorideConcForFirstLayer[mol/L]'
  value     = 8.88888
**
  parameter = 'CritChlorideConcForSecondLayer[mol/L]'
  value     = 9.99999
```

```
**
  BARRIER   = 'BarrierLowerUnsaturatedZoneStudy'
**
  Component = 'ComponentTSwStudy'
**
  parameter = 'TSw_Thickness_1SubArea[m]'
  value     = 10.10101
**
  parameter = 'TSw_Thickness_2SubArea[m]'
  value     = 11.11111
**
  parameter = 'TSw_Thickness_3SubArea[m]'
  value     = 12.12121
**
  parameter = 'TSw_Thickness_4SubArea[m]'
  value     = 13.13131
**
  parameter = 'TSw_Thickness_5SubArea[m]'
  value     = 14.14141
**
  parameter = 'TSw_Thickness_6SubArea[m]'
  value     = 15.15151
**
  parameter = 'TSw_Thickness_7SubArea[m]'
  value     = 16.16161
**
  parameter = 'TSw_Thickness_8SubArea[m]'
  value     = 17.17171
**
  Component = 'ComponentCHnvStudy'
**
  parameter = 'CHnvThickness_1SubArea[m]'
  value     = 18.18181
**
  parameter = 'CHnvThickness_2SubArea[m]'
  value     = 19.19191
**
  parameter = 'CHnvThickness_3SubArea[m]'
  value     = 20.20202
**
  parameter = 'CHnvThickness_4SubArea[m]'
  value     = 21.21212
**
  parameter = 'CHnvThickness_5SubArea[m]'
  value     = 22.22222
**
  parameter = 'CHnvThickness_6SubArea[m]'
  value     = 23.23232
**
  parameter = 'CHnvThickness_7SubArea[m]'
  value     = 24.24242
**
  parameter = 'CHnvThickness_8SubArea[m]'
  value     = 25.25252
**
  Component = 'ComponentCHnzStudy'
**
  parameter = 'CHnzThickness_1SubArea[m]'
  value     = 26.26262
**
  parameter = 'CHnzThickness_2SubArea[m]'
  value     = 27.27272
**
```

```
  parameter = 'CHnzThickness_3SubArea[m]'
  value     = 28.28282
**
  parameter = 'CHnzThickness_4SubArea[m]'
  value     = 29.29292
**
  parameter = 'CHnzThickness_5SubArea[m]'
  value     = 30.30303
**
  parameter = 'CHnzThickness_6SubArea[m]'
  value     = 31.31313
**
  parameter = 'CHnzThickness_7SubArea[m]'
  value     = 32.32323
**
  parameter = 'CHnzThickness_8SubArea[m]'
  value     = 33.33333
**
  Component = 'ComponentPPwStudy'
**
  parameter = 'PPw_Thickness_1SubArea[m]'
  value     = 34.34343
**
  parameter = 'PPw_Thickness_2SubArea[m]'
  value     = 35.35353
**
  parameter = 'PPw_Thickness_3SubArea[m]'
  value     = 36.36363
**
  parameter = 'PPw_Thickness_4SubArea[m]'
  value     = 37.37373
**
  parameter = 'PPw_Thickness_5SubArea[m]'
  value     = 38.38383
**
  parameter = 'PPw_Thickness_6SubArea[m]'
  value     = 39.39393
**
  parameter = 'PPw_Thickness_7SubArea[m]'
  value     = 40.40404
**
  parameter = 'PPw_Thickness_8SubArea[m]'
  value     = 41.41414
**
  Component = 'ComponentUCFStudy'
**
  parameter = 'UCF_Thickness_1SubArea[m]'
  value     = 42.42424
**
  parameter = 'UCF_Thickness_2SubArea[m]'
  value     = 43.43434
**
  parameter = 'UCF_Thickness_3SubArea[m]'
  value     = 44.44444
**
  parameter = 'UCF_Thickness_4SubArea[m]'
  value     = 45.45454
**
  parameter = 'UCF_Thickness_5SubArea[m]'
  value     = 46.46464
**
  parameter = 'UCF_Thickness_6SubArea[m]'
  value     = 47.47474
```

```
**
  parameter = 'UCF_Thickness_7SubArea[m]'
  value     = 48.48484
**
  parameter = 'UCF_Thickness_8SubArea[m]'
  value     = 49.49494
**
  Component = 'ComponentBFwStudy'
**
  parameter = 'BFw_Thickness_1SubArea[m]'
  value     = 50.50505
**
  parameter = 'BFw_Thickness_2SubArea[m]'
  value     = 51.51515
**
  parameter = 'BFw_Thickness_3SubArea[m]'
  value     = 52.52525
**
  parameter = 'BFw_Thickness_4SubArea[m]'
  value     = 53.53535
**
  parameter = 'BFw_Thickness_5SubArea[m]'
  value     = 54.54545
**
  parameter = 'BFw_Thickness_6SubArea[m]'
  value     = 55.55555
**
  parameter = 'BFw_Thickness_7SubArea[m]'
  value     = 56.56565
**
  parameter = 'BFw_Thickness_8SubArea[m]'
  value     = 57.57575
**
  BARRIER   = 'BarrierSaturatedZoneStudy'
**
  Component = 'Component_STFF_SAV_Study'
  parameter = 'DistanceToTuffAlluviumInterface[km]'
  value     = 58.58585
**
  BARRIER   = 'BarrierReceptorGroupStudy'
**
  Component = 'ComponentWellWaterStudy'
**
  parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
  value     = 59.59595
**
  parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
  value     = 60.60606
**
  SUBSYSTEM = 'SubsystemEngineeredStudy'
**
  BARRIER   = 'BarrierDriftStudy'
**
  Component = 'ComponentBackfillStudy'
  parameter = 'EmplacementBackfillThickness[m]'
  value     = 61.61616
**
  Component = 'ComponentDripShieldStudy'
  parameter = 'DripShieldThickness[m]'
  value     = 62.62626
**
  BARRIER   = 'BarrierWastePackageStudy'
**
```

```
  Component = 'ComponentInnerContainerStudy'
  parameter = 'InnerWPThickness[m]'
  value     = 63.63636
**
  Component = 'ComponentOuterContainerStudy'
  parameter = 'OuterWPThickness[m]'
  value     = 64.64646
**
```

Listing of parameter names and values to check for flags 2-24 :

Flag 2: SubsystemNaturalStudy

```
  parameter = 'WastePackageFlowMultiplicationFactor'
  value     = 1.11111
  parameter = 'SubAreaWetFraction'
  value     = 2.22222
  parameter = 'ElevationOfGroundSurface[m]'
  value     = 3.33333
  parameter = 'MassDensityofYMRock[kg/m^3]'
  value     = 4.44444
  parameter = 'SpecificHeatofYMRock[J/(kg-K)]'
  value     = 5.55555
  parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
  value     = 6.66666
  parameter = 'EmissivityOfDriftWall[-]'
  value     = 7.77777
  parameter = 'CritChlorideConcForFirstLayer[mol/L]'
  value     = 8.88888
  parameter = 'CritChlorideConcForSecondLayer[mol/L]'
  value     = 9.99999
  parameter = 'TSw_Thickness_1SubArea[m]'
  value     = 10.10101
  parameter = 'TSw_Thickness_2SubArea[m]'
  value     = 11.11111
  parameter = 'TSw_Thickness_3SubArea[m]'
  value     = 12.12121
  parameter = 'TSw_Thickness_4SubArea[m]'
  value     = 13.13131
  parameter = 'TSw_Thickness_5SubArea[m]'
  value     = 14.14141
  parameter = 'TSw_Thickness_6SubArea[m]'
  value     = 15.15151
  parameter = 'TSw_Thickness_7SubArea[m]'
  value     = 16.16161
  parameter = 'TSw_Thickness_8SubArea[m]'
  value     = 17.17171
  parameter = 'CHnvThickness_1SubArea[m]'
  value     = 18.18181
  parameter = 'CHnvThickness_2SubArea[m]'
  value     = 19.19191
  parameter = 'CHnvThickness_3SubArea[m]'
  value     = 20.20202
  parameter = 'CHnvThickness_4SubArea[m]'
  value     = 21.21212
  parameter = 'CHnvThickness_5SubArea[m]'
  value     = 22.22222
  parameter = 'CHnvThickness_6SubArea[m]'
  value     = 23.23232
  parameter = 'CHnvThickness_7SubArea[m]'
  value     = 24.24242
  parameter = 'CHnvThickness_8SubArea[m]'
  value     = 25.25252
  parameter = 'CHnzThickness_1SubArea[m]'
  value     = 26.26262
```

```
parameter = 'CHnzThickness_2SubArea[m]'
value     = 27.27272
parameter = 'CHnzThickness_3SubArea[m]'
value     = 28.28282
parameter = 'CHnzThickness_4SubArea[m]'
value     = 29.29292
parameter = 'CHnzThickness_5SubArea[m]'
value     = 30.30303
parameter = 'CHnzThickness_6SubArea[m]'
value     = 31.31313
parameter = 'CHnzThickness_7SubArea[m]'
value     = 32.32323
parameter = 'CHnzThickness_8SubArea[m]'
value     = 33.33333
parameter = 'PPw_Thickness_1SubArea[m]'
value     = 34.34343
parameter = 'PPw_Thickness_2SubArea[m]'
value     = 35.35353
parameter = 'PPw_Thickness_3SubArea[m]'
value     = 36.36363
parameter = 'PPw_Thickness_4SubArea[m]'
value     = 37.37373
parameter = 'PPw_Thickness_5SubArea[m]'
value     = 38.38383
parameter = 'PPw_Thickness_6SubArea[m]'
value     = 39.39393
parameter = 'PPw_Thickness_7SubArea[m]'
value     = 40.40404
parameter = 'PPw_Thickness_8SubArea[m]'
value     = 41.41414
parameter = 'UCF_Thickness_1SubArea[m]'
value     = 42.42424
parameter = 'UCF_Thickness_2SubArea[m]'
value     = 43.43434
parameter = 'UCF_Thickness_3SubArea[m]'
value     = 44.44444
parameter = 'UCF_Thickness_4SubArea[m]'
value     = 45.45454
parameter = 'UCF_Thickness_5SubArea[m]'
value     = 46.46464
parameter = 'UCF_Thickness_6SubArea[m]'
value     = 47.47474
parameter = 'UCF_Thickness_7SubArea[m]'
value     = 48.48484
parameter = 'UCF_Thickness_8SubArea[m]'
value     = 49.49494
parameter = 'BFw_Thickness_1SubArea[m]'
value     = 50.50505
parameter = 'BFw_Thickness_2SubArea[m]'
value     = 51.51515
parameter = 'BFw_Thickness_3SubArea[m]'
value     = 52.52525
parameter = 'BFw_Thickness_4SubArea[m]'
value     = 53.53535
parameter = 'BFw_Thickness_5SubArea[m]'
value     = 54.54545
parameter = 'BFw_Thickness_6SubArea[m]'
value     = 55.55555
parameter = 'BFw_Thickness_7SubArea[m]'
value     = 56.56565
parameter = 'BFw_Thickness_8SubArea[m]'
value     = 57.57575
parameter = 'DistanceToTuffAlluviumInterface[km]'
```

```
value     = 58.58585
parameter = 'DistanceToTuffAlluviumInterface[km]'
value     = 58.58585
parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
value     = 59.59595
parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
value     = 60.60606
```

Flag 3: BarrierBiosphereStudy

```
parameter = 'WastePackageFlowMultiplicationFactor'
value     = 1.11111
parameter = 'SubAreaWetFraction'
value     = 2.22222
```

Flag 4: ComponentPrecipitationStudy

```
parameter = 'WastePackageFlowMultiplicationFactor'
value     = 1.11111
parameter = 'SubAreaWetFraction'
value     = 2.22222
```

Flag 5: BarrierUpperUnsaturatedZoneStudy

```
parameter = 'ElevationOfGroundSurface[m]'
value     = 3.33333
parameter = 'MassDensityofYMRock[kg/m^3]'
value     = 4.44444
parameter = 'SpecificHeatofYMRock[J/(kg-K)]'
value     = 5.55555
parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
value     = 6.66666
parameter = 'EmissivityOfDriftWall[-]'
value     = 7.77777
parameter = 'CritChlorideConcForFirstLayer[mol/L]'
value     = 8.88888
parameter = 'CritChlorideConcForSecondLayer[mol/L]'
value     = 9.99999
```

Flag 6: ComponentTivaCanyonStudy

```
parameter = 'ElevationOfGroundSurface[m]'
value     = 3.33333
parameter = 'MassDensityofYMRock[kg/m^3]'
value     = 4.44444
parameter = 'SpecificHeatofYMRock[J/(kg-K)]'
value     = 5.55555
parameter = 'ThermalConductivityofYMRock[W/(m-K)]'
value     = 6.66666
parameter = 'EmissivityOfDriftWall[-]'
value     = 7.77777
parameter = 'CritChlorideConcForFirstLayer[mol/L]'
value     = 8.88888
parameter = 'CritChlorideConcForSecondLayer[mol/L]'
value     = 9.99999
```

Flag 7: BarrierLowerUnsaturatedZoneStudy

```
parameter = 'TSw_Thickness_1SubArea[m]'
value     = 10.10101
parameter = 'TSw_Thickness_2SubArea[m]'
value     = 11.11111
parameter = 'TSw_Thickness_3SubArea[m]'
value     = 12.12121
parameter = 'TSw_Thickness_4SubArea[m]'
value     = 13.13131
```

```
parameter = 'TSw_Thickness_5SubArea[m]'
value     = 14.14141
parameter = 'TSw_Thickness_6SubArea[m]'
value     = 15.15151
parameter = 'TSw_Thickness_7SubArea[m]'
value     = 16.16161
parameter = 'TSw_Thickness_8SubArea[m]'
value     = 17.17171
parameter = 'CHnvThickness_1SubArea[m]'
value     = 18.18181
parameter = 'CHnvThickness_2SubArea[m]'
value     = 19.19191
parameter = 'CHnvThickness_3SubArea[m]'
value     = 20.20202
parameter = 'CHnvThickness_4SubArea[m]'
value     = 21.21212
parameter = 'CHnvThickness_5SubArea[m]'
value     = 22.22222
parameter = 'CHnvThickness_6SubArea[m]'
value     = 23.23232
parameter = 'CHnvThickness_7SubArea[m]'
value     = 24.24242
parameter = 'CHnvThickness_8SubArea[m]'
value     = 25.25252
parameter = 'CHnzThickness_1SubArea[m]'
value     = 26.26262
parameter = 'CHnzThickness_2SubArea[m]'
value     = 27.27272
parameter = 'CHnzThickness_3SubArea[m]'
value     = 28.28282
parameter = 'CHnzThickness_4SubArea[m]'
value     = 29.29292
parameter = 'CHnzThickness_5SubArea[m]'
value     = 30.30303
parameter = 'CHnzThickness_6SubArea[m]'
value     = 31.31313
parameter = 'CHnzThickness_7SubArea[m]'
value     = 32.32323
parameter = 'CHnzThickness_8SubArea[m]'
value     = 33.33333
parameter = 'PPw_Thickness_1SubArea[m]'
value     = 34.34343
parameter = 'PPw_Thickness_2SubArea[m]'
value     = 35.35353
parameter = 'PPw_Thickness_3SubArea[m]'
value     = 36.36363
parameter = 'PPw_Thickness_4SubArea[m]'
value     = 37.37373
parameter = 'PPw_Thickness_5SubArea[m]'
value     = 38.38383
parameter = 'PPw_Thickness_6SubArea[m]'
value     = 39.39393
parameter = 'PPw_Thickness_7SubArea[m]'
value     = 40.40404
parameter = 'PPw_Thickness_8SubArea[m]'
value     = 41.41414
parameter = 'UCF_Thickness_1SubArea[m]'
value     = 42.42424
parameter = 'UCF_Thickness_2SubArea[m]'
value     = 43.43434
parameter = 'UCF_Thickness_3SubArea[m]'
value     = 44.44444
parameter = 'UCF_Thickness_4SubArea[m]'
```

```
value     = 45.45454
parameter = 'UCF_Thickness_5SubArea[m]'
value     = 46.46464
parameter = 'UCF_Thickness_6SubArea[m]'
value     = 47.47474
parameter = 'UCF_Thickness_7SubArea[m]'
value     = 48.48484
parameter = 'UCF_Thickness_8SubArea[m]'
value     = 49.49494
parameter = 'BFw_Thickness_1SubArea[m]'
value     = 50.50505
parameter = 'BFw_Thickness_2SubArea[m]'
value     = 51.51515
parameter = 'BFw_Thickness_3SubArea[m]'
value     = 52.52525
parameter = 'BFw_Thickness_4SubArea[m]'
value     = 53.53535
parameter = 'BFw_Thickness_5SubArea[m]'
value     = 54.54545
parameter = 'BFw_Thickness_6SubArea[m]'
value     = 55.55555
parameter = 'BFw_Thickness_7SubArea[m]'
value     = 56.56565
parameter = 'BFw_Thickness_8SubArea[m]'
value     = 57.57575
```

Flag 8: ComponentTSwStudy

```
parameter = 'TSw_Thickness_1SubArea[m]'
value     = 10.10101
parameter = 'TSw_Thickness_2SubArea[m]'
value     = 11.11111
parameter = 'TSw_Thickness_3SubArea[m]'
value     = 12.12121
parameter = 'TSw_Thickness_4SubArea[m]'
value     = 13.13131
parameter = 'TSw_Thickness_5SubArea[m]'
value     = 14.14141
parameter = 'TSw_Thickness_6SubArea[m]'
value     = 15.15151
parameter = 'TSw_Thickness_7SubArea[m]'
value     = 16.16161
parameter = 'TSw_Thickness_8SubArea[m]'
value     = 17.17171
```

Flag 9: ComponentCHnvStudy

```
parameter = 'CHnvThickness_1SubArea[m]'
value     = 18.18181
parameter = 'CHnvThickness_2SubArea[m]'
value     = 19.19191
parameter = 'CHnvThickness_3SubArea[m]'
value     = 20.20202
parameter = 'CHnvThickness_4SubArea[m]'
value     = 21.21212
parameter = 'CHnvThickness_5SubArea[m]'
value     = 22.22222
parameter = 'CHnvThickness_6SubArea[m]'
value     = 23.23232
parameter = 'CHnvThickness_7SubArea[m]'
value     = 24.24242
parameter = 'CHnvThickness_8SubArea[m]'
value     = 25.25252
```

Flag 10: ComponentCHnzStudy

```
parameter = 'CHnzThickness_1SubArea[m]'
value     = 26.26262
parameter = 'CHnzThickness_2SubArea[m]'
value     = 27.27272
parameter = 'CHnzThickness_3SubArea[m]'
value     = 28.28282
parameter = 'CHnzThickness_4SubArea[m]'
value     = 29.29292
parameter = 'CHnzThickness_5SubArea[m]'
value     = 30.30303
parameter = 'CHnzThickness_6SubArea[m]'
value     = 31.31313
parameter = 'CHnzThickness_7SubArea[m]'
value     = 32.32323
parameter = 'CHnzThickness_8SubArea[m]'
value     = 33.33333
```

Flag 11: ComponentPPwStudy

```
parameter = 'PPw_Thickness_1SubArea[m]'
value     = 34.34343
parameter = 'PPw_Thickness_2SubArea[m]'
value     = 35.35353
parameter = 'PPw_Thickness_3SubArea[m]'
value     = 36.36363
parameter = 'PPw_Thickness_4SubArea[m]'
value     = 37.37373
parameter = 'PPw_Thickness_5SubArea[m]'
value     = 38.38383
parameter = 'PPw_Thickness_6SubArea[m]'
value     = 39.39393
parameter = 'PPw_Thickness_7SubArea[m]'
value     = 40.40404
parameter = 'PPw_Thickness_8SubArea[m]'
value     = 41.41414
```

Flag 12: ComponentUCFStudy

```
parameter = 'UCF_Thickness_1SubArea[m]'
value     = 42.42424
parameter = 'UCF_Thickness_2SubArea[m]'
value     = 43.43434
parameter = 'UCF_Thickness_3SubArea[m]'
value     = 44.44444
parameter = 'UCF_Thickness_4SubArea[m]'
value     = 45.45454
parameter = 'UCF_Thickness_5SubArea[m]'
value     = 46.46464
parameter = 'UCF_Thickness_6SubArea[m]'
value     = 47.47474
parameter = 'UCF_Thickness_7SubArea[m]'
value     = 48.48484
parameter = 'UCF_Thickness_8SubArea[m]'
value     = 49.49494
```

Flag 13: ComponentBFwStudy

```
parameter = 'BFw_Thickness_1SubArea[m]'
value     = 50.50505
parameter = 'BFw_Thickness_2SubArea[m]'
value     = 51.51515
parameter = 'BFw_Thickness_3SubArea[m]'
value     = 52.52525
```

```
parameter = 'BFw_Thickness_4SubArea[m]'
value     = 53.53535
parameter = 'BFw_Thickness_5SubArea[m]'
value     = 54.54545
parameter = 'BFw_Thickness_6SubArea[m]'
value     = 55.55555
parameter = 'BFw_Thickness_7SubArea[m]'
value     = 56.56565
parameter = 'BFw_Thickness_8SubArea[m]'
value     = 57.57575
```

Flag 14: BarrierSaturatedZoneStudy

```
parameter = 'DistanceToTuffAlluviumInterface[km]'
value     = 58.58585
```

Flag 15: Component_STFF_SAV_Study

```
parameter = 'DistanceToTuffAlluviumInterface[km]'
value     = 58.58585
```

Flag 16: BarrierReceptorGroupStudy

```
parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
value     = 59.59595
parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
value     = 60.60606
```

Flag 17: ComponentWellWaterStudy

```
parameter = 'WellPumpingRateAtReceptorGroup10km[gal/day]'
value     = 59.59595
parameter = 'WellPumpingRateAtReceptorGroup20km[gal/day]'
value     = 60.60606
```

Flag 18: SubsystemEngineeredStudy

```
parameter = 'EmplacementBackfillThickness[m]'
value     = 61.61616
parameter = 'DripShieldThickness[m]'
value     = 62.62626
parameter = 'InnerWPThickness[m]'
value     = 63.63636
parameter = 'OuterWPThickness[m]'
value     = 64.64646
```

Flag 19: BarrierDriftStudy

```
parameter = 'EmplacementBackfillThickness[m]'
value     = 61.61616
parameter = 'DripShieldThickness[m]'
value     = 62.62626
```

Flag 20: ComponentBackfillStudy

```
parameter = 'EmplacementBackfillThickness[m]'
value     = 61.61616
```

Flag 21: ComponentDripShieldStudy

```
parameter = 'DripShieldThickness[m]'
value     = 62.62626
```

Flag 22: BarrierWastePackageStudy

```
parameter = 'InnerWPThickness[m]'
value     = 63.63636
parameter = 'OuterWPThickness[m]'
```

```
value      = 64.64646
```

Flag 23: ComponentInnerContainerStudy

```
parameter = 'InnerWPThickness[m]'
value     = 63.63636
```

Flag 24: ComponentOuterContainerStudy

```
parameter = 'OuterWPThickness[m]'
value     = 64.64646
```

Purpose: The values specified in the *tpa.inp* file for the subsystem, barrier, or component should be written to the *cp.tpa* file, since this change should only affect the constant parameters in *cp.tpa*.

TPA Output Files to Compare:

The following files will be checked for flags 2-24.
- *lhs.inp*
- *lhs.out*
- *cp.tpa*

Pass/Fail Criteria:

The *lhs.inp* and *lhs.out* files should be the same for version 4.0 and 4.1. The *cp.tpa* file should contain the above values for each of the parameters listed in each test.

Documentation of Testing:

These tests are stored in the SCR322/flagX subdirectory, where X equals 2 to 24. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Flag Combination

Test 1. Run Versions 4.0 and 4.1 with their accompanying tpa.inp files for 10,000 yr with all append files ON, ImportanceAnalysisFlag(yes=1,no=0) = 1 (ON) in both versions, and all other flags with the barriers inactive, except for the following: ComponentOuterContainerStudy, BarrierWastePackageStudy, and ComponentUCFStudy

Purpose: The values specified in the *tpa.inp* file for the subsystem, barrier, or component should be written to the *cp.tpa* file, since this change should only affect the constant parameters in *cp.tpa*.

TPA Output Files to Compare:

The following files will be checked.
- *lhs.inp*
- *lhs.out*
- *cp.tpa*

Pass/Fail Criteria:

The *lhs.inp* and *lhs.out* files should be the same for version 4.0 and 4.1. The *cp.tpa* file should contain the above values for each of the parameters listed in each test.

Documentation of Testing:

These tests are stored in the SCR322/comb/test1 subdirectory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Test 2. Run Versions 4.0 and 4.1 with their accompanying tpa.inp files for 10,000 yr with all append files ON, ImportanceAnalysisFlag(yes=1,no=0) = 1 (ON) in both versions, and all other flags with the barriers inactive, except for the following: BarrierSaturatedZoneStudy, BarrierLowerUnsaturatedZoneStudy, and SubsystemNaturalStudy

Purpose: The values specified in the *tpa.inp* file for the subsystem, barrier, or component should be written to the *cp.tpa* file, since this change should only affect the constant parameters in *cp.tpa*.

TPA Output Files to Compare:

The following files will be checked.
- *lhs.inp*
- *lhs.out*
- *cp.tpa*

Pass/Fail Criteria:

The *lhs.inp* and *lhs.out* files should be the same for version 4.0 and 4.1. The *cp.tpa* file should contain the above values for each of the parameters listed in each test.

Documentation of Testing:

These tests are stored in the SCR322/comb/test2 subdirectory. The Version 4.0 output is stored in the SCR322/v40 directory. All testing output files are archived on a CD.

Approved by: _____ **Date:** 10/19/05

****

Received the TPA source code and data files via email attachment from R. Janetzke on 8/29/00. These files were either modified or added to the TPA code to conduct Importance Analysis. These files are (note that the "ia" or "i" portion of the file names was dropped for compiling and running the TPA code; also note that the iareader.f file corresponds to the ia.f file in version 4.0):

dcagwia.f
ebsfaili.f
ebsrelia.f
execia.f
ia.dat
ia1.i

iareader.f
nfenvia.f
readeria.f
sampleri.f
seismoia.f
szftia.f
tpaia.inp
uzftia.f

While compiling the version 4.0 code with the above files, there were some compilation errors. From the *exec.f*, *ebsrel.f*, *ebsfail.f*, *sampler.f*, *szft.f*, and *uzft.f* files, lines were commented out that were related to **.log* files and IEEE which were added for the UNIX code development (this was recommended by R. Janetzke). Also, found that in *ia.f*, the following changes were required to compile and run the code and to copy the new data file *ia.dat* to the working directory (the following is a file comparison between the v4.0 and the IA file received from R. Janetzke):

```
Comparing files iareader.f and ..\IA.F
***** iareader.f

    character*60 name
***** ..\IA.F

cc rwr 8/31/00 added to copy ia.f from data
    integer zportsh
    external zportsh
    character*80 command
    include 'path.i'

    character*60 name
*****

***** iareader.f
    external igetunitnumber

***** ..\IA.F
    external igetunitnumber

cc rwr 8/29/00 added to avoid compile errors on the pc
    logical lexist

*****

***** iareader.f
    if (iaflag .ne. 0) then
      iaunit = igetunitnumber('exec    ')
***** ..\IA.F
    if (iaflag .ne. 0) then
```

```
cc rwr 8/31/00 added copy for the ia.f file from data
      call clearchar(80,command)
      command = 'cp ' // dpath // 'data/ia.dat .'
      istatus=zportsh(command)
      if( istatus .ne. 0 ) then
        print *, ' ***>>> Error in ia.f <<<*** '
        print *, ' not able to copy ia.f'
        print *, ' istatus .ne. 0 '
        print *, ' istatus = sh( ', command, ' )'
        print *, ' istatus = ', istatus
        stop
      endif

      iaunit = igetunitnumber('exec    ')
*****


***** iareader.f
      cparamvalue = ''
      return
***** ..\IA.F
      cparamvalue = ''
cc rwr 9/11/00 debug    add the following line because clineid is reset for some reason
      clineid = 'VALUE'
      return
*****
```

NOTE: There are three changes in the *ia.f* file: (1) adding copy-related statements which will copy the *ia.dat* file from the data subdirectory to the working directory (requested by R. Janetzke); (2) adding a logical declaration for variable *lexist*; and (3) adding clineid='VALUE' (for some reason the assignment of clineid to 'VALUE' is lost.

In addition to changes in the *ia.f* file, the *sampler.f* file was modified by commenting out the "close" statements (closing *sp.tpa* and *cp.tpa*). These two statements were introduced as part of the Importance Analysis modifications. However, by closing these files, the *exec.f* file is not able to write to these files and an error message is written to the screen during TPA code execution. The comparison file for *sampler.f* follows.

```
Comparing files sampler.f and ..\SAMPLER.F
***** sampler.f
          call printtitlessp(iunitcp,iunitsp)
          close (iunitcp)
          close (iunitsp)
cc         if(1+1 .eq. 2) STOP
***** ..\SAMPLER.F
          call printtitlessp(iunitcp,iunitsp)
cc rwr debug          close (iunitcp)
cc rwr debug          close (iunitsp)
```

```
cc        if(1+1 .eq. 2) STOP
*****
```

Once the above modifications were introduced into the TPA souce code, the testing was conducted according to the test plan listed previously. All input, data, and output files (for SCR-322) are archived on a CD that was sent to R. Janetzke together with a summary of the test results.

The test results for flag1 (tests 1-4), flags 2-24, and combinations tests 1 and 2, are located in the directories described in the test plan. A comparison between the test cases and version 4.0 was automatically performed using the "fc" command in a DOS Window with the *filecomp.bat* file. The output file (*filecomp.out*) was examined to verify that the parameters in the *ia.dat* file were correctly written to *sp.tpa*, *lhs.out*, and *cp.tpa*.

The results from all tests show that the values in *ia.dat* for all flags and combinations of flags described in the test plan were correctly written to the *sp.tpa*, *lhs.out*, and *cp.tpa* files (see the *filecomp.out* file in each test subdirectory). Thus, for the tests described in the test plan, the testing results indicate the modifications for Importance Analysis were correctly implemented.

9/1/00 - 9/10/00 **Participated with CNWRA Staff to Develop the Implementation in the TPA Code for Determining Compliance with the EPA Standard; also, Modified and Tested Changes to the TPA Code Related to this Implementation (specific details of this work are provided subsequently):**

The implementation of calculations in the TPA code for determining groundwater concentrations and dose was developed through scoping activities with P. Laplante, J. Weldy, and M. Smith starting in the middle of July 2000. From these scoping activities, an SCR was developed and submitted to R. Janetzke and S. Mohanty for their input and ultimate approval of the modifications and approach. The SCR is provided below.

SOFTWARE CHANGE REPORT (SCR)

SCR No. (*Software Developer Assigns*): PA-SCR-4xx	**Software Title and Version:** TPA 4.0	**Project No:** 20-01402-772
Affected Software Module(s), Description of Problem(s): The modified source code files are *dcagw.f*, *nuclides.dat*, *tpa.inp*, *tpanames.dbs*, *exec.f*, and *invent.f*. A new include file (*inventp.i*) and dose factor data file (*organdf.dat*) will be added and a new output file will be written (*epa_dose.out*). Also, the screen print will be changed to show the new results. These changes will enhance the capabilities of the TPA code to evaluate the safety case presented in the Department of Energy's Total System Performance Assessment by computing values according to the proposed rule for the Individual Protection Standard and the Groundwater Protection Standards in the Environmental Radiation Standard for Yucca Mountain as described in the Federal Register (40 CFR Part 197, v. 64, n. 166, August 27, 1999).		

Change Requested by: P. LaPlante Date: 7-19-00	**Change Authorized by** (*Software Developer*): R. Janetzke Date: 7-31-00
Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): The *dcagw.f* source code will be modified to use new parameters specified in the *tpa.inp* file for the dilution volume and fraction of the plume captured in computing groundwater concentrations (note that the present methodology used to calculate groundwater concentrations and doses in *dcagw.f* will not be affected). Values for these parameters are described in the Federal Register (40 CFR Part 197, v. 64, n. 166, August 27, 1999). Release rates from the *szft.f* module will be used in this calculation. Using these groundwater concentrations, the following output will be computed, however because of the large amount of information generated only a part of these values will be written to output files and to the screen print: (1) peak dose will be calculated and compared to the 15 mrem/yr individual standard; (2) the dose for combined beta and photon emitting radionuclides to each of seven organs and to the whole body will be computed using dose factors in a new data file (*organdf.dat*) and the total dose to each organ and the whole body will be compared to the groundwater limit of 4 mrem/yr; (3) the Ra-226 activity in the groundwater will be compared to the groundwater limit of 5 picocuries per liter; (4) the gross alpha activity in the groundwater will be compared to the groundwater limit 15 picocuries per liter; and (5) the total uranium groundwater concentration will be determined. Additionally, a flag will be introduced to the *tpa.inp* file which will activate or suppress these calculations.	
Implemented by: J. Weldy and R. Rice	**Date:** 7-31-00 (work initiated)
Description of Acceptance Tests: Acceptance testing will involve running the TPA code with and without these modifications and comparing the output. All output in the **.res* and **.tpa* should not change. Values in the new output file (*epa_dose.out*) should be checked for their correctness using hand calculations.	
Tested by:	**Date:**

CNWRA Form TOP-5 (01/99)

After a tele-conference call with R. Janetzke, S. Mohanty, and J. Weldy on September 1, an approach was agreed on that would involve a basic implementation of EPA Standard calculations. The implementation included the modifications in the above SCR with the addition of writing the *epa_dose.out* file (whose name was changed to *epa_ave.out*) and *epapktim.out* . This file contains the peak value for the EPA Standard for each realization in the same categories as in the average for all realization information in *epa_ave.out*. A listing of these files with the headers is provided below.

Listing of *epapktim.out*

Input file tpa.inp as supplied with TPA Version 4.0 Code.

Base case

TPA 4.0, Job started: Tue Sep 05 16:44:15 2000
Peak Concentration/Dose (Scaled) and Time of the Peak

for Each Realization Using the EPA Standard

realization	gross alpha	uranium		
radon226	Lung	Gonad	R Marrow	Breast
B Surface	Whole Body	Thyroid	Total Dose	Remainder
unitless	scaled conc	time	scaled conc	time
scaled conc	time	scaled dose	time	scaled dose
time	scaled dose	time	scaled dose	time
scaled dose	time	scaled dose	time	scaled dose
time	scaled dose	time	scaled dose	time
1	5.61832E-05	8.00000E+04	2.78203E-04	8.00000E+04
6.76870E-06	8.00000E+04	7.61473E-03	8.00000E+04	7.70774E-03
8.00000E+04	7.62762E-03	8.00000E+04	7.65473E-03	8.00000E+04
7.65318E-03	8.00000E+04	2.92762E+00	7.63288E+04	1.25743E-01
8.00000E+04	9.84895E-02	7.63288E+04	2.63737E-02	7.63288E+04

Listing of *epa_ave.out*

Input file tpa.inp as supplied with TPA Version 4.0 Code.

Base case

TPA 4.0, Job started: Tue Sep 05 16:44:15 2000
Average Dose (Scaled) Over All Realizations

Determined Using the EPA Standard

time	gross alpha	uranium	radon226	Gonad
Breast	Lung	R Marrow	B Surface	Thyroid
Remainder	Whole Body	Total Dose		
yr	scaled conc	scaled conc	scaled conc	scaled dose
scaled dose	scaled dose	scaled dose	scaled dose	scaled dose
scaled dose	scaled dose	scaled dose		
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
3.67117E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
7.51714E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.15462E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		

1.57672E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.01891E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.48216E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.96747E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
3.47588E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
4.00851E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
4.56649E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
5.15104E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
5.76343E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
6.40498E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
7.07707E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
7.78117E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
8.51879E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
9.29154E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.01011E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.09492E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.18376E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.27684E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.37435E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.47650E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		

1.58352E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.69563E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.81308E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.93612E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.06503E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.20007E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.34154E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.48974E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.64500E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.80766E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
2.97806E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
3.15657E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
3.34359E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
3.53951E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
3.74475E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
3.95978E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
4.18504E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
4.42102E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
4.66824E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
4.92724E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		

5.19856E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
5.48281E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
5.78059E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
6.09255E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
6.41936E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
6.76173E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
7.12041E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
7.49616E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
7.88981E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
8.30220E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
8.73423E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
9.18683E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
9.66098E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.01577E+04	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00		
1.06781E+04	3.18201E-23	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	1.03097E-22		
1.12232E+04	1.11081E-19	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	3.59901E-19		
1.17944E+04	8.24924E-18	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
0.00000E+00	0.00000E+00	2.67275E-17		
1.23927E+04	1.57046E-16	0.00000E+00	0.00000E+00	3.08556E-12
3.08556E-12	3.08556E-12	3.08556E-12	3.08556E-12	3.08556E-12
3.32499E-12	3.15894E-12	8.42537E-13		
1.30195E+04	1.49075E-15	0.00000E+00	0.00000E+00	1.14359E-08
1.14359E-08	1.14359E-08	1.14359E-08	1.14359E-08	1.14613E-08
1.23233E-08	1.17086E-08	3.12099E-09		
1.36761E+04	9.26094E-15	1.20316E-19	0.00000E+00	1.17077E-07
1.19624E-07	1.17433E-07	1.18173E-07	1.18120E-07	3.28480E-05
1.26826E-07	1.10262E-06	2.93194E-07		

1.43640E+04	4.35953E-14	8.15030E-12	1.87466E-16	8.31148E-07
8.66697E-07	8.36121E-07	8.46436E-07	8.45699E-07	4.57596E-04
9.04906E-07	1.45654E-05	3.87253E-06		
1.50847E+04	2.03357E-13	5.84544E-10	1.07087E-13	1.07190E-06
1.31997E-06	1.10654E-06	1.17857E-06	1.17342E-06	3.18915E-03
1.22103E-06	9.68209E-05	2.57387E-05		
1.58397E+04	1.43457E-12	4.54898E-09	2.62817E-12	1.04814E-06
1.79463E-06	1.15222E-06	1.36909E-06	1.35357E-06	9.59649E-03
1.33142E-06	2.89182E-04	7.68748E-05		
1.66306E+04	8.25504E-12	1.80725E-08	1.97883E-11	7.28207E-07
1.21744E-06	7.96220E-07	9.38513E-07	9.28309E-07	6.29162E-03
9.21267E-07	1.89634E-04	5.04157E-05		
1.74592E+04	3.43649E-11	4.13134E-08	8.95788E-11	1.68077E-06
1.91540E-06	1.71315E-06	1.78158E-06	1.77665E-06	3.02119E-03
1.88171E-06	9.23853E-05	2.45711E-05		
1.83272E+04	1.01713E-10	6.75787E-08	2.70956E-10	3.02822E-06
3.65901E-06	3.11601E-06	3.29940E-06	3.28627E-06	8.11550E-03
4.98095E-06	2.47146E-04	6.57199E-05		
1.92366E+04	2.34263E-10	9.59750E-08	6.21298E-10	7.71033E-06
9.41698E-06	7.94824E-06	8.44410E-06	8.40864E-06	2.20586E-02
7.79057E-05	6.90714E-04	1.83681E-04		
2.01893E+04	4.61691E-10	1.37695E-07	1.19974E-09	2.52316E-05
2.68989E-05	2.54634E-05	2.59483E-05	2.59136E-05	2.20437E-02
3.81879E-04	7.93168E-04	2.11096E-04		
2.11873E+04	8.36497E-10	1.89137E-07	2.10504E-09	3.59015E-05
3.71936E-05	3.60804E-05	3.64568E-05	3.64298E-05	1.75296E-02
5.72847E-04	7.22080E-04	1.92319E-04		
2.22329E+04	1.43430E-09	2.41919E-07	3.45154E-09	5.50894E-05
5.60368E-05	5.52197E-05	5.54964E-05	5.54766E-05	1.36358E-02
9.05927E-04	7.17937E-04	1.91418E-04		
2.33282E+04	2.35718E-09	2.97475E-07	5.33669E-09	3.96534E-05
4.03287E-05	3.97453E-05	3.99433E-05	3.99292E-05	9.73972E-03
6.52206E-04	5.14545E-04	1.37226E-04		
2.44757E+04	3.76087E-09	3.53397E-07	7.85131E-09	1.82786E-05
1.87510E-05	1.83420E-05	1.84812E-05	1.84715E-05	6.56937E-03
2.96415E-04	2.98349E-04	7.95759E-05		
2.56779E+04	5.89181E-09	4.12458E-07	1.10740E-08	1.43445E-04
1.43768E-04	1.43487E-04	1.43583E-04	1.43577E-04	8.01222E-03
2.41366E-03	1.06049E-03	2.83369E-04		
2.69372E+04	9.15266E-09	4.74057E-07	1.50909E-08	1.86045E-04
1.86274E-04	1.86074E-04	1.86143E-04	1.86139E-04	7.95556E-03
3.13531E-03	1.30376E-03	3.48460E-04		
2.82566E+04	1.42072E-08	5.37294E-07	2.00193E-08	1.33184E-04
1.33353E-04	1.33204E-04	1.33256E-04	1.33253E-04	5.76889E-03
2.24408E-03	9.35417E-04	2.50080E-04		
2.96388E+04	2.21262E-08	6.03540E-07	2.60238E-08	8.82690E-05
8.83991E-05	8.82842E-05	8.83244E-05	8.83228E-05	4.06514E-03
1.48650E-03	6.26977E-04	1.67707E-04		
3.10867E+04	3.45315E-08	6.70228E-07	3.31297E-08	5.67023E-05
5.68095E-05	5.67142E-05	5.67479E-05	5.67471E-05	2.92519E-03
9.53955E-04	4.11895E-04	1.10290E-04		
3.26037E+04	5.39679E-08	7.36404E-07	4.14195E-08	3.56127E-05
3.57065E-05	3.56228E-05	3.56525E-05	3.56525E-05	2.18744E-03
5.98130E-04	2.68906E-04	7.21568E-05		
3.41928E+04	8.43235E-08	8.01020E-07	5.10277E-08	2.40183E-05
2.41036E-05	2.40271E-05	2.40545E-05	2.40552E-05	1.76849E-03
4.02543E-04	1.89904E-04	5.11559E-05		
3.58577E+04	1.31385E-07	8.63009E-07	6.19637E-08	1.71449E-05
1.72245E-05	1.71530E-05	1.71787E-05	1.71801E-05	1.51100E-03
2.86621E-04	1.42804E-04	3.87321E-05		

3.76018E+04	2.03701E-07	9.21394E-07	7.42741E-08	1.33810E-05
1.34563E-05	1.33884E-05	1.34130E-05	1.34152E-05	1.35485E-03
2.23177E-04	1.16567E-04	3.19633E-05		
3.94289E+04	3.13638E-07	9.75376E-07	8.79992E-08	1.14046E-05
1.14765E-05	1.14116E-05	1.14352E-05	1.14383E-05	1.25824E-03
1.89900E-04	1.02363E-04	2.85294E-05		
4.13431E+04	4.78787E-07	1.02435E-06	1.03149E-07	1.02453E-05
1.03143E-05	1.02519E-05	1.02747E-05	1.02787E-05	1.19006E-03
1.70409E-04	9.36943E-05	2.67509E-05		
4.33484E+04	7.23908E-07	1.06800E-06	1.19715E-07	9.48598E-06
9.55249E-06	9.49226E-06	9.51440E-06	9.51936E-06	1.13776E-03
1.57659E-04	8.77920E-05	2.59682E-05		
4.54491E+04	1.08301E-06	1.10630E-06	1.37664E-07	8.90615E-06
8.97050E-06	8.91210E-06	8.93370E-06	8.93971E-06	1.09466E-03
1.47928E-04	8.31912E-05	2.59000E-05		
4.76499E+04	1.60238E-06	1.13943E-06	1.56956E-07	8.43603E-06
8.49839E-06	8.44165E-06	8.46279E-06	8.46991E-06	1.05727E-03
1.40036E-04	7.93871E-05	2.65614E-05		
4.99555E+04	2.34323E-06	1.16767E-06	1.77508E-07	8.06022E-06
8.12074E-06	8.06547E-06	8.08624E-06	8.09453E-06	1.02420E-03
1.33486E-04	7.61781E-05	2.80971E-05		
5.23709E+04	3.38617E-06	1.19134E-06	1.99252E-07	8.65770E-06
8.71648E-06	8.66255E-06	8.68302E-06	8.69255E-06	9.95406E-04
1.33698E-04	7.57748E-05	3.13576E-05		
5.49013E+04	4.83442E-06	1.21073E-06	2.22118E-07	9.18110E-06
9.23826E-06	9.18552E-06	9.20577E-06	9.21658E-06	9.69448E-04
1.33801E-04	7.53748E-05	3.59303E-05		
5.75522E+04	6.81753E-06	1.22612E-06	2.46024E-07	1.20726E-05
1.21282E-05	1.20765E-05	1.20966E-05	1.21088E-05	9.47879E-04
1.49198E-04	8.12729E-05	4.39131E-05		
6.03293E+04	9.49591E-06	1.23752E-06	2.70890E-07	1.44293E-05
1.44832E-05	1.44327E-05	1.44526E-05	1.44661E-05	9.25812E-04
1.61434E-04	8.58514E-05	5.37952E-05		
6.32386E+04	1.30613E-05	1.24399E-06	2.96611E-07	1.90930E-05
1.91451E-05	1.90958E-05	1.91156E-05	1.91305E-05	9.05555E-04
1.88483E-04	9.64656E-05	6.81585E-05		
6.62865E+04	1.77405E-05	1.24294E-06	3.23045E-07	2.17194E-05
2.17696E-05	2.17215E-05	2.17412E-05	2.17576E-05	8.81832E-04
2.02669E-04	1.01759E-04	8.47094E-05		
6.94795E+04	2.37927E-05	1.22953E-06	3.49957E-07	6.04193E-05
6.05070E-05	6.04262E-05	6.04572E-05	6.04743E-05	1.40157E-03
2.45945E-04	1.56288E-04	1.18818E-04		
7.28245E+04	3.15168E-05	1.93816E-05	4.08202E-07	8.15520E-04
1.03424E-03	8.46104E-04	9.09580E-04	9.05068E-04	2.81147E+00
1.11145E-03	8.52785E-02	2.27772E-02		
7.63288E+04	4.16611E-05	1.54695E-04	1.63031E-06	2.21968E-03
2.44376E-03	2.25096E-03	2.31604E-03	2.31148E-03	2.92762E+00
3.04003E-02	9.84895E-02	2.63737E-02		
8.00000E+04	5.61832E-05	2.78203E-04	6.76870E-06	7.61473E-03
7.70774E-03	7.62762E-03	7.65473E-03	7.65318E-03	1.39581E+00
1.25743E-01	8.47140E-02	2.28410E-02		

The files that were modified were sent via email attachment to R. Janetzke. These files were listed in the SCR (i.e., *dcagw.f*, *nuclides.dat*, *tpa.inp*, *tpanames.dbs*, *exec.f*, and *invent.f.*). Additionally, the files *inventp.i, execc.i,* and *organdf.dat* are new files.

The file comparison files are provided below:

Listing of differences in *dcagw.f.*

```
Comparing files dcagw.f and DCAGW.ORIGINAL.F
***** dcagw.f

cc    jrw 7/27/00 added for groundwater protection
      dimension aconc(ntim), rconc(ntim), uconc(ntim)
      dimension aconcsum(ntim), rconcsum(ntim), uconcsum(ntim)
      dimension rnconc(ntim, 43)
      character*80 aline
***** DCAGW.ORIGINAL.F

      character*80 aline
*****

***** dcagw.f

cc rwr 9/6/00 modified for groundwater protection calculations
      integer gwpc
      character*6 nucname(43)
      common / dcagw25 / gwpc
      common / dcagw26 / ipumpgwp
      common / dcagw27 / ifrplumegwp
      common / dcagw28 / numberreal,durationcp
      common / dcagw29 / dosefactor(43,8)
      dimension epadose(43,ntim,8)
      dimension epadoseave(ntim,8)
      dimension epadosesum(ntim,8)
      dimension epadosetotal(ntim)
      dimension epadosetotalsum(ntim)
      dimension epapktim(12,2)
      dimension epasf(5)
      include 'inventp.i'
      include 'execc.i'

      external maplist
***** DCAGW.ORIGINAL.F

      external maplist
*****

***** dcagw.f

cc jrw 7/21/00 modified to incorporate groundwater protection calculation

***** DCAGW.ORIGINAL.F


cc jrw 1/31/00 modified for user input switch to pluvial DCF values
cc jrw 1/31/00 modified for pluvial pump rates at 20 km

*****

***** dcagw.f
        call clearchar( 60, name )
        name = 'GroundwaterProtectionCalc(yes=1,no=0)'
        igwpc = ispquery( name )
        gwpc  = ivaluesp(igwpc)

***** DCAGW.ORIGINAL.F
        call clearchar( 60, name )
        name = 'PluvialWellPumpingRateAtReceptorGroup20km[gal/day]'
        ipluvpump20 = ispquery( name )
```

```
*****

***** dcagw.f
        call clearchar( 60, name )
        name = 'WellPumpingRateGroundwaterProtection[gal/day]'
        ipumpgwp = ispquery( name )

        call clearchar( 60, name )
        name = 'FractionPlumeCaptureGroundwaterProtection'
        ifrplumegwp = ispquery( name )

cc jrw 1/31/00 modified for user input switch to pluvial DCF values
cc jrw 1/31/00 modified for pluvial pump rates at 20 km

        call clearchar( 60, name )
        name = 'PluvialWellPumpingRateAtReceptorGroup20km[gal/day]'
        ipluvpump20 = ispquery( name )

        call clearchar( 60, name )
        name = 'PluvialSwitchTime[yr]'
***** DCAGW.ORIGINAL.F
        call clearchar( 60, name )
        name = 'PluvialSwitchTime[yr]'
*****

***** dcagw.f

cc rwr 9/6/00 modified for groundwater protection calculations
        if (gwpc .eq. 1) then
          call clearchar( 60, name )
          name = 'NumberOfRealizations'
          inumberreal = ispquery( name )
          numberreal =  ivaluesp ( inumberreal )

          call clearchar( 60, name )
          name = 'DurationOfCompliancePeriod[yr]'
          idurationcp = ispquery( name )
          durationcp =  valuesp ( idurationcp )

          ireadorgandf = igetunitnumber('dcagw   ')
          call clearchar(80,command)
          command = 'cp ' // dpath // 'data/organdf.dat .'
          istatus=zportsh(command)
          if(istatus .ne. 0) then
            print *, ' ***>>> Error in DCAGW <<<*** '
            print *, ' Failure copying organdf.dat'
            print *, ' command = ', command
            print *, ' Status = ', istatus
            STOP
          endif

          iline=1
          open (unit=ireadorgandf,file='organdf.dat',status='old')
  182     continue
          read (ireadorgandf, '(a80)', end=910, err=911) aline
          iline = iline+1
          if (aline(1:2) .eq. 'TI' .or.
     &      aline(1:2) .eq. 'ti' .or.
     &      aline(1:2) .eq. '**' )   go to 182
          backspace(ireadorgandf)
          do iorgandf = 1,43
```

```
            read (ireadorgandf, 184) nucname(iorgandf),
     &        dosefactor(iorgandf,1), dosefactor(iorgandf,2),
     &        dosefactor(iorgandf,3), dosefactor(iorgandf,4),
     &        dosefactor(iorgandf,5), dosefactor(iorgandf,6),
     &        dosefactor(iorgandf,7), dosefactor(iorgandf,8)
          enddo
          do iorgandf = 1,5
            read(ireadorgandf,'(d8.2)' ) epasf(iorgandf)
          enddo
          do iini1 = 1, ntim
            uconcsum(iini1)=0.0d0
            aconcsum(iini1)=0.0d0
            rconcsum(iini1)=0.0d0
            epadosetotalsum(iini1) = 0.0d0
            do iini2 = 1,8
              epadoseave(iini1,iini2) = 0.0d0
            enddo
          enddo

        endif
  184   format(3x,a6,2x,d8.2,7(8x,d8.2))
        close(ireadorgandf)

        ikey =39231
***** DCAGW.ORIGINAL.F

        ikey =39231
*****

***** dcagw.f

cc jrw 07/21/00 next two lines added to implement groundwater protection

        pumpgwp = valuesp (ipumpgwp)
        frplumegwp = valuesp (ifrplumegwp)

        aqthickness5km = valuesp (iaqthickness5km )
***** DCAGW.ORIGINAL.F

        aqthickness5km = valuesp (iaqthickness5km )
*****

***** dcagw.f

cc jrw 7/21/00 added to implement groundwater protection
      pumpgwp = ( pumpgwp*365.25d0 / 264.172d0)

      if( dist .lt. cutoffpt ) then
***** DCAGW.ORIGINAL.F

      if( dist .lt. cutoffpt ) then
*****

***** dcagw.f

cc rwr 9/6/00 modified for groundwater protection calculations
cc            initialize
        do iinit1 = 1, ntim
          uconc(iinit1)=0.0d0
          aconc(iinit1)=0.0d0
          rconc(iinit1)=0.0d0
```

```
          epadosetotal(iinit1) = 0.0d0
          do iinit2 = 1,8
            epadosesum(iinit1,iinit2) = 0.0d0
            do iinit3 = 1,nnucl
              epadose(iinit3,iinit1,iinit2) = 0.0d0
            enddo
          enddo
        enddo
        do iinit1 = 1,12
          do iinit2 = 1,2
            epapktim(iinit1,iinit2) = 0.0d0
          enddo
        enddo

        do j=1,ntim
cc jrw 02/02/00 modified to implement user-specified time of climate change
***** DCAGW.ORIGINAL.F

        do j=1,ntim

cc jrw 02/02/00 modified to implement user-specified time of climate change
*****

***** dcagw.f
            endif

           remperyrpernuclgw(j,k)=dcf(ik)*ciperyrallsafromsz(j,k) /
     &       dilutionvolume * fractionmasscaptured

cc rwr 9/6/00 modified for groundwater protection calculations
cc    jrw 7-14-00 calculate uranium and gross alpha concentrations in the water
cc    and convert to units of pCi/L (Ci/m3 * 1e9 = pCi/L)
           if (gwpc.eq.1) then
             rnconc(j,k)=ciperyrallsafromsz(j,k)/pumpgwp*frplumegwp*1e9
             do ifind = 1,43
               if (nucname(ifind) .eq. names(k)) then
                 ifound = ifind
                 goto 194
               endif
             enddo
  194        continue
             if (idecaytype(ifound).eq.4) then
                uconc(j)=uconc(j)+rnconc(j,k)
             elseif (idecaytype(ifound) .eq. 2 .or.
     &         idecaytype(ifound) .eq. 3) then
               aconc(j)=aconc(j)+rnconc(j,k)
               if (idecaytype(ifound).eq.3) then
                 rconc(j)=rconc(j)+rnconc(j,k)
               endif
             elseif (idecaytype(ifound) .eq. 1) then
cc rwr 9/6/00 note the following conversion
cc            to change from pCi/L to mrem/yr, multiply
cc            rnconc(pCi/L) by 2 L/d, 365 d/yr, 1.0d5 mrem/Sv,
cc            3.7d10 Bq/Ci, and 1.0d-12 Ci/pCi and the dose factor (Sv/Bq)
               do kkk = 1,8
                 epadose(j,k,kkk) = rnconc(j,k)*2.0d0*365.25d0*
     &             dosefactor(ifound,kkk)*1.0d5*3.7d10*1.0d-12
               enddo
             endif
           endif
```

```
cc rwr 9/6/00 determine the total dose using tpa code dw dcfs
            epadosetotal(j) = epadosetotal(j)+rnconc(j,k)*
     &              dwdcf(j,ik)*1.0d-6
        enddo

        do isumall1 = 1, 8
          do isumall2 = 1, nnucl
            epadosesum(j,isumall1) = epadosesum(j,isumall1) +
     &       epadose(j,isumall2,isumall1)
          enddo
        enddo
***** DCAGW.ORIGINAL.F
            endif
            remperyrpernuclgw(j,k)=dcf(ik)*ciperyrallsafromsz(j,k) /
     &       dilutionvolume * fractionmasscaptured
        enddo
*****

***** dcagw.f
            endif
           remperyrpernuclgw(j,k)=dcf(ik)*ciperyrallsafromsz(j,k) /
     &       dilutionvolume * fractionmasscaptured

cc rwr 9/6/00 modified for groundwater protection calculations
cc    jrw 7-14-00 calculate uranium and gross alpha concentrations in the water
cc    and convert to units of pCi/L (Ci/m3 * 1e9 = pCi/L)
           if (gwpc.eq.1) then
             rnconc(j,k)=ciperyrallsafromsz(j,k)/pumpgwp*frplumegwp*1e9
             do ifind = 1,43
               if (nucname(ifind) .eq. names(k)) then
                 ifound = ifind
                 goto 195
               endif
             enddo
  195        continue
             if (idecaytype(ifound).eq.4) then
                uconc(j)=uconc(j)+rnconc(j,k)
             elseif (idecaytype(ifound) .eq. 2 .or.
     &         idecaytype(ifound) .eq. 3) then
               aconc(j)=aconc(j)+rnconc(j,k)
               if (idecaytype(ifound).eq.3) then
                 rconc(j)=rconc(j)+rnconc(j,k)
               endif
             elseif (idecaytype(ifound) .eq. 1) then
cc rwr 9/6/00 note the following conversion
cc            to change from pCi/L to mrem/yr, multiply
cc            rnconc(pCi/L) by 2 L/d, 365 d/yr, 1.0d5 mrem/Sv,
cc            3.7d10 Bq/Ci, and 1.0d-12 Ci/pCi and the dose factor (Sv/Bq)
               do kkk = 1,8
                 epadose(j,k,kkk) = rnconc(j,k)*2.0d0*365.25d0*
     &             dosefactor(ifound,kkk)*1.0d5*3.7d10*1.0d-12
               enddo
             endif

cc rwr 9/6/00 determine the total dose using tpa code dw dcfs
             epadosetotal(j) = epadosetotal(j)+rnconc(j,k)*
     &         dwdcf(j,ik)*1.0d-6
           endif
        enddo

        if (gwpc.eq.1) then
```

```
          do isumall1 = 1, 8
            do isumall2 = 1, nnucl
              epadosesum(j,isumall1) = epadosesum(j,isumall1) +
     &          epadose(j,isumall2,isumall1)
            enddo
          enddo
        endif
      endif
***** DCAGW.ORIGINAL.F
            endif
            remperyrpernuclgw(j,k)=dcf(ik)*ciperyrallsafromsz(j,k) /
     &       dilutionvolume * fractionmasscaptured
        enddo
      endif
*****

***** dcagw.f
      enddo


cc rwr 9/6/00 modified for groundwater protection calculation
cc            determine peak and time of peak in the compilance period
      if (gwpc.eq.1) then
        do ipeak = 1,ntim
          if (tim(ipeak) .le. durationcp) then
            if(epapktim(1,1) .lt. aconc(ipeak)) then
              epapktim(1,1)=aconc(ipeak)
              epapktim(1,2)=tim(ipeak)
            endif
            if(epapktim(2,1) .lt. uconc(ipeak)) then
              epapktim(2,1)=uconc(ipeak)
              epapktim(2,2)=tim(ipeak)
            endif
            if(epapktim(3,1) .lt. rconc(ipeak)) then
              epapktim(3,1)=rconc(ipeak)
              epapktim(3,2)=tim(ipeak)
            endif
            do ipeak2 = 1,8
              if(epapktim(ipeak2+3,1) .lt. epadosesum(ipeak,ipeak2)) then
                epapktim(ipeak2+3,1)=epadosesum(ipeak,ipeak2)
                epapktim(ipeak2+3,2)=tim(ipeak)
              endif
            enddo
            if(epapktim(12,1) .lt. epadosetotal(ipeak)) then
              epapktim(12,1)=epadosetotal(ipeak)
              epapktim(12,2)=tim(ipeak)
            endif
          endif
        enddo
        do isetduration = 1,12
          if(epapktim(isetduration,2) .le. 1.0d-5)
     &       epapktim(isetduration,2) = durationcp
        enddo
      endif

cc rwr 9/6/00 determine the total dose over all realizations (use tpa dcfs)
        if (gwpc.eq.1) then
          do isumall = 1,ntim
            aconcsum(isumall) = aconcsum(isumall) + aconc(isumall)
            rconcsum(isumall) = rconcsum(isumall) + rconc(isumall)
            uconcsum(isumall) = uconcsum(isumall) + uconc(isumall)
```

```
            epadosetotalsum(isumall) = epadosetotalsum(isumall) +
     &        epadosetotal(isumall)
          enddo

cc rwr 9/6/00 modified for groundwater protection calculation
cc            accumulate for determining average, then divide
cc            by number of realizations
          do isumall1 = 1,8
            do isumall2 = 1,ntim
              epadoseave(isumall2,isumall1) =
     &          epadoseave(isumall2,isumall1) +
     &          epadosesum(isumall2,isumall1)
            enddo
          enddo
      write(iwriteepapktim,'(5x,i5,5x,24(1pe14.5,2x))')irl,
     &  epapktim(1,1)/epasf(1),epapktim(1,2),epapktim(2,1)/epasf(2),
     &  epapktim(2,2),epapktim(3,1)/epasf(3),epapktim(3,2),
     &  epapktim(4,1)/epasf(4),epapktim(4,2),epapktim(5,1)/epasf(4),
     &  epapktim(5,2),epapktim(6,1)/epasf(4),epapktim(6,2),
     &  epapktim(7,1)/epasf(4),epapktim(7,2),epapktim(8,1)/epasf(4),
     &  epapktim(8,2),epapktim(9,1)/epasf(4),epapktim(9,2),
     &  epapktim(10,1)/epasf(4),epapktim(10,2),epapktim(11,1)/epasf(4),
     &  epapktim(11,2),epapktim(12,1)/epasf(5),epapktim(12,2)
      if (irl .eq. numberreal) then
        do iaverage1 = 1,8
          do iaverage2 = 1,ntim
            epadoseave(iaverage2,iaverage1) =
     &      epadoseave(iaverage2,iaverage1)/dble(numberreal)
          enddo
        enddo
        do iaverage = 1,ntim
          if(tim(iaverage) .le. durationcp) then
            aconcsum(iaverage) = aconcsum(iaverage)/dble(numberreal)
            rconcsum(iaverage) = rconcsum(iaverage)/dble(numberreal)
            uconcsum(iaverage) = uconcsum(iaverage)/dble(numberreal)
            epadosetotalsum(iaverage) =
     &        epadosetotalsum(iaverage)/dble(numberreal)
            write(iwriteepa_ave,'(13(1pe14.5,2x))')tim(iaverage),
     &        aconcsum(iaverage)/epasf(1),uconcsum(iaverage)/epasf(2),
     &        rconcsum(iaverage)/epasf(3),
     &        (epadoseave(iaverage,jj)/epasf(4),jj=1,8),
     &        epadosetotalsum(iaverage)/epasf(5)
          endif
        enddo
        close(iwriteepa_ave)
        close(iwriteepapktim)
      endif
      endif

      return
***** DCAGW.ORIGINAL.F
      enddo

      return
*****

***** dcagw.f


cc rwr 9/6/00 modified for groundwater protection calculations
910   continue
```

```
      print *, ' ***>>> Error in DCAGW <<<*** '
      print *, ' Error reading organdf.dat '
      print *, ' end of file reached unexpectedly'
      print *, ' look on line = ', iline
      print *, '  '
      STOP

911   continue
      print *, ' ***>>> Error in DCAGW <<<*** '
      print *, ' can not read from organdf.dat'
      print *, ' check the format '
      print *, ' look on line = ', iline
      print *, '  '
      STOP


      end
***** DCAGW.ORIGINAL.F

      end
*****
```

Listing of differences in *exec.f.*

```
Comparing files exec.f and EXEC.ORIGINAL.F
***** exec.f

cc rwr 9/6/00 modified for groundwater protection calculations
      include 'execc.i'

      include 'inventb.i'
***** EXEC.ORIGINAL.F

      include 'inventb.i'
*****

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

cc rwr 9/6/00 modified for groundwater protection calculations
      call clearchar( 60, name )
      name = 'GroundwaterProtectionCalc(yes=1,no=0)'
      iigwpcalc = ispquery( name )
      igwpcalc  = ivaluesp( iigwpcalc )
      if (igwpcalc .eq. 1) then
        call clearchar( 24, filename)
        call clearchar( 160, mes1)
        call clearchar( 160, mes2)
        iwriteepapktim = igetunitnumber('exec    ')
        filename ='epapktim.out'
        mes1 = ' Peak Concentration/Dose (Scaled) and Time of the Peak'
        mes2 = ' for Each Realization Using the EPA Standard  '
        call writehead(iwriteepapktim,title1,title2,datetim,mes1,mes2,
     &                 filename)
        ilength = 25*16+5
        call clearchar(ilength,columnheader1)
        call clearchar(ilength,columnheader2)
        do i = 1,13
          if ( i .eq. 1 ) then
            columnheader1(3:13) = 'realization'
```

```
        columnheader2(3:13) = '  unitless '
      elseif ( i .eq. 2 ) then
        columnheader1(25:35) = 'gross alpha'
        columnheader2(20:40) = 'scaled conc      time'
      elseif ( i .eq. 3 ) then
        columnheader1(59:66) = 'uranium '
        columnheader2(54:71) = 'scaled conc   time'
      elseif ( i .eq. 4 ) then
        columnheader1(91:98)='radon226'
        columnheader2(86:103)='scaled conc   time'
      elseif ( i .eq. 5 ) then
        columnheader1(123:130)='  Gonad '
        columnheader2(118:135)='scaled dose   time'
      elseif ( i .eq. 6 ) then
        columnheader1(155:162)=' Breast '
        columnheader2(150:167)='scaled dose   time'
      elseif ( i .eq. 7 ) then
        columnheader1(187:194)='   Lung '
        columnheader2(182:199)='scaled dose   time'
      elseif ( i .eq. 8 ) then
        columnheader1(219:226)='R Marrow'
        columnheader2(214:231)='scaled dose   time'
      elseif ( i .eq. 9 ) then
        columnheader1(251:259)='B Surface'
        columnheader2(246:264)='scaled dose    time'
      elseif ( i .eq. 10) then
        columnheader1(283:290)=' Thyroid'
        columnheader2(278:295)='scaled dose   time'
      elseif ( i .eq. 11) then
        columnheader1(315:323)='Remainder'
        columnheader2(310:328)='scaled dose    time'
      elseif ( i .eq. 12) then
        columnheader1(346:355)='Whole Body'
        columnheader2(341:360)='scaled dose     time'
      elseif ( i .eq. 13) then
        columnheader1(378:387)='Total Dose'
        columnheader2(373:392)='scaled dose     time'
      endif
    enddo
    write(iwriteepapktim,'(a)')
&     (columnheader1(1:400))
    write(iwriteepapktim,'(a)')
&     (columnheader2(1:402))


    call clearchar( 24, filename)
    call clearchar( 160, mes1)
    call clearchar( 160, mes2)
    iwriteepa_ave = igetunitnumber('exec    ')
    filename ='epa_ave.out'
    mes1 = ' Average Dose (Scaled) Over All Realizations '
    mes2 = ' Determined Using the EPA Standard  '
    call writehead(iwriteepa_ave,title1,title2,datetim,mes1,mes2,
&                  filename)
    ilength = 13*16+5
    call clearchar(ilength,columnheader1)
    call clearchar(ilength,columnheader2)
    do i = 1,13
      if ( i .eq. 1 ) then
        columnheader1(5:12) = '  time  '
        columnheader2(5:12) = '   yr   '
```

```
          elseif ( i .eq. 2 ) then
            columnheader1(19:29) = 'gross alpha'
            columnheader2(19:29) = 'scaled conc'
          elseif ( i .eq. 3 ) then
            columnheader1(37:44) = 'uranium '
            columnheader2(35:45) = 'scaled conc'
          elseif ( i .eq. 4 ) then
            columnheader1(53:60)='radon226'
            columnheader2(51:61)='scaled conc'
          elseif ( i .eq. 5 ) then
            columnheader1(69:76)='  Gonad '
            columnheader2(67:77)='scaled dose'
          elseif ( i .eq. 6 ) then
            columnheader1(85:92)=' Breast '
            columnheader2(83:93)='scaled dose'
          elseif ( i .eq. 7 ) then
            columnheader1(101:108)='   Lung '
***** EXEC.ORIGINAL.F

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='npkdoset.res'
      mes1 = ' Peak Dose and Corresponding Time by Nuclide'
      mes2 = ' Values for Each Vector '
      call writehead(iunitnpkdoset,title1,title2,datetim,mes1,mes2,
     &               filename)

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='npkdst_c.res'
      mes1 = ' Peak Dose and Corresponding Time by Nuclide' //
     &       ' for Compliance Period'
      mes2 = ' Values for Each Vector '
      call writehead(iunitnpkdoset_c,title1,title2,datetim,mes1,mes2,
     &               filename)

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='totdose.res'
      mes1 = ' Total Dose for All Pathways, All Nuclides, and All Times'
      mes2 = ' Including Dilution Volume - Values for Each Vector '
      call writehead(iunittotdose,title1,title2,datetim,mes1,mes2,
     &               filename)

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='totdos_c.res'
      mes1 = ' Total Dose for All Pathways, All Nuclides,' //
     &       ' for Compliance Period'
      mes2 = ' Including Dilution Volume - Values for Each Vector '
      call writehead(iunittotdose_c,title1,title2,datetim,mes1,mes2,
     &               filename)
```

```
      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='airpkdos.res'
      mes1=' Air Release Total Peak Dose and Peak Time with Doses '
      mes2=' for Each Nuclide at Peak Time - Values for Each Vector'
      call writehead(iunitairpkdos,title1,title2,datetim,mes1,mes2,
     &               filename)

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='arpkds_c.res'
      mes1=' Air Release Total Peak Dose and Peak Time with Doses ' //
     &     'for Compliance Period'
      mes2=' for Each Nuclide at Peak Time - Values for Each Vector'
      call writehead(iunitairpkdos_c,title1,title2,datetim,mes1,mes2,
     &               filename)

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='gwpkdos.res'
      mes1=' Groundwater Total Peak Dose and Peak Time with Doses '
      mes2=' for Each Nuclide at Peak Time - Values for Each Vector'
      call writehead(iunitgwpkdos,title1,title2,datetim,mes1,mes2,
     &               filename)

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='gwpkds_c.res'
      mes1=' Groundwater Total Peak Dose and Peak Time with Doses ' //
     &     'for Compliance Period'
      mes2=' for Each Nuclide at Peak Time - Values for Each Vector'
      call writehead(iunitgwpkdos_c,title1,title2,datetim,mes1,mes2,
     &               filename)

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='nearfld.res'
      mes1=' Near Field WP Temp, RH, and Cl Averaged for All Subareas'
      mes2=' Printed for Each 10th Time and Each Vector'
      call writehead(iunitnearfld,title1,title2,datetim,mes1,mes2,
     &               filename)

      call clearchar( 24, filename)
      call clearchar( 160, mes1)
      call clearchar( 160, mes2)

      filename ='gwttuzsz.res'
*****
```

Listing of differences in *invent.f.*

```
Comparing files invent.f and INVENT.ORIGINAL.F
***** invent.f

cc rwr 9/6/00 modified for groundwater protection calculations
cc            dimension new integer array in the new include file
      include 'inventp.i'

      dimension time(2)
***** INVENT.ORIGINAL.F

      dimension time(2)
*****

***** invent.f
     &      wmole(iNucIndex), halflife(iNucIndex), epalim(iNucIndex),
     &      cipermtuat10yr(iNucIndex), idecaytype(iNucIndex)
cc rwr 9/6/00 modified for groundwater protection calculations
cc            changed previous line to read decay information
cc     &      cipermtuat10yr(iNucIndex)
      enddo
***** INVENT.ORIGINAL.F
     &      wmole(iNucIndex), halflife(iNucIndex), epalim(iNucIndex),
     &      cipermtuat10yr(iNucIndex)
      enddo
*****

***** invent.f

cc rwr 9/6/00 modified for groundwater protection calculations
cc   100 format(i5,3(3xa6),3x,a2,3x,d7.1,3x,d7.3,3x,d7.2,3x,d8.2)
  100 format(i5,3(3xa6),3x,a2,3x,d7.1,3x,d7.3,3x,d7.2,3x,d8.2,3x,i5)

***** INVENT.ORIGINAL.F

  100 format(i5,3(3xa6),3x,a2,3x,d7.1,3x,d7.3,3x,d7.2,3x,d8.2)

*****
```

Listing of differences in *nuclides.dat.*

```
Comparing files nuclides.dat and NUCLIDES.ORIGINAL.DAT
***** nuclides.dat
** rwr added new initial inventories 3/28/00
** rwr added flag to indicate decay information received from J. Weldy
**     for groundwater protection calculations: (1) beta/gamma,
**     (2) alpha, (3) radon, and (4) uranium (9/5/00)
**      idx = Nuclide index
***** NUCLIDES.ORIGINAL.DAT
** rwr added new initial inventories 3/28/00
**      idx = Nuclide index
*****

***** nuclides.dat
** CPMTU@10 = cipermtuat10yr
**    DECAY = decay information (see above) rwr 9/6/00
**      --- = unitless
***** NUCLIDES.ORIGINAL.DAT
** CPMTU@10 = cipermtuat10yr
**      --- = unitless
*****
```

```
***** nuclides.dat
43
**idx,     NIS,    NIS2,    NIS3, NES,    wmole, halflife,   epalim,  CPMTU@10,
DECAY
**---      ---,     ---,     ---, ---,  [g/mol],     [yr], [Ci/MTU],  [Ci/MTU],
  ---
   01      U238    U238     U238      U   238.0d0   4.468d9      0.10   3.15d-01
     4
   02     Cm246    Cm246    CM246     Cm   246.0d0   4.731d3      0.10   7.62d-02
     2
   03     Pu242    Pu242    PU242     Pu   242.0d0   3.869d5      0.10   2.10d+00
     2
   04    Am242m   Am242m   AM242M    Am   242.0d0   1.520d2      0.10   2.48d+01
     1
   05     Pu238    Pu238    PU238     Pu   238.0d0   8.774d1      0.10   3.77d+03
     2
   06      U234    U234     U234      U   234.0d0   2.445d5      0.10   1.18d+00
     4
   07     Th230    Th230    TH230     Th   230.0d0   7.700d4      0.01   1.37d-04
     2
   08     Ra226    Ra226    RA226     Ra   226.0d0   1.600d3      0.10   4.11d-07
     3
   09     Pb210    Pb210    PB210     Pb   210.0d0   2.230d1      1.00   5.67d-08
     1
   10     Cm243    Cm243    CM243     Cm   243.0d0   2.850d1      0.10   2.55d+01
     2
   11     Am243    Am243    AM243     Am   243.0d0   7.380d3      0.10   2.64d+01
     2
   12     Pu239    Pu239    PU239     Pu   239.0d0   2.406d4      0.10   3.69d+02
     2
   13      U235    U235     U235      U   235.0d0   7.038d8      0.10   1.71d-02
     4
   14     Pa231    Pa231    PA231     Pa   231.0d0   3.277d4      0.10   2.69d-05
     2
   15     Ac227    Ac227    AC227     Ac   227.0d0   2.177d1      0.10   7.51d-06
     1
   16     Cm245    Cm245    CM245     Cm   245.0d0   8.499d3      0.10   3.66d-01
     2
   17     Pu241    Pu241    PU241     Pu   241.0d0   1.440d1   1000.00   9.22d+04
     1
   18     Am241    Am241    AM241     Am   241.0d0   4.322d2      0.10   2.08d+03
     2
   19     Np237    Np237    NP237     Np   237.0d0   2.140d6      0.10   4.34d-01
     2
   20      U233    U233     U233      U   233.0d0   1.585d5      0.10   3.44d-05
     4
   21     Th229    Th229    TH229     Th   229.0d0   7.339d3      0.10   2.75d-07
     2
   22     Cm244    Cm244    CM244     Cm   244.0d0   1.811d1   1000.00   2.68d+03
     2
   23     Pu240    Pu240    PU240     Pu   240.0d0   6.537d3      0.10   5.44d+02
     2
   24      U236    U236     U236      U   236.0d0   2.341d7      0.10   2.81d-01
     4
   25      U232    U232     U232      U   232.0d0   7.200d1      0.10   3.93d-02
     4
   26     Sm151    Sm151    SM151     Sm   151.0d0   8.999d1      1.00   4.28d+02
     1
   27     Cs137    Cs137    CS137     Cs   137.0d0   3.000d1      1.00   9.15d+04
     1
```

```
   28     Cs135    Cs135     CS135     Cs    135.0d0    2.300d6       1.00    5.36d-01
     1
   29      I129     I129      I129      I    129.0d0    1.570d7       0.10    3.57d-02
     1
   30     Sn126    Sn126     SN126     Sn    126.0d0    1.000d5       1.00    8.85d-01
     1
   31    Sn121m   Sn121m    SN121M     Sn    121.0d0    4.997d1       1.00    1.04d+00
     1
   32    Ag108m   Ag108m    AG108M     Ag    108.0d0    4.180d2       1.00    1.26d-02
     1
   33     Pd107    Pd107     PD107     Pd    107.0d0    6.496d6       1.00    1.31d-01
     1
   34      Tc99     Tc99      TC99     Tc     99.0d0    2.130d5      10.00    1.45d+01
     1
   35      Mo93     Mo93      MO93     Mo     93.0d0    3.498d3       1.00    1.51d-02
     1
   36      Nb94     Nb94      NB94     Nb     94.0d0    2.030d4       1.00    8.48d-01
     1
   37      Zr93     Zr93      ZR93     Zr     93.0d0    1.530d6       1.00    2.47d+00
     1
   38      Sr90     Sr90      SR90     Sr     90.0d0    2.912d1       1.00    6.25d+04
     1
   39      Se79     Se79      SE79     Se     79.0d0    1.100d6       1.00    4.58d-01
     1
   40      Ni63     Ni63      NI63     Ni     63.0d0    9.200d1       1.00    3.72d+02
     1
   41      Ni59     Ni59      NI59     Ni     59.0d0    8.000d4       1.00    2.44d+00
     1
   42      Cl36     Cl36      CL36     Cl     36.0d0    3.010d5       1.00    1.15d-02
     1
   43       C14      C14       C14      C     14.0d0    5.729d3       0.10    1.44d+00
     1

***** NUCLIDES.ORIGINAL.DAT
43
**idx,      NIS,     NIS2,     NIS3, NES,    wmole, halflife,   epalim,  CPMTU@10
**---       ---,      ---,      ---, ---,  [g/mol],     [yr], [Ci/MTU],  [Ci/MTU]
   01       U238     U238      U238      U   238.0d0    4.468d9       0.10    3.15d-01
   02      Cm246    Cm246     CM246     Cm   246.0d0    4.731d3       0.10    7.62d-02
   03      Pu242    Pu242     PU242     Pu   242.0d0    3.869d5       0.10    2.10d+00
   04     Am242m   Am242m    AM242M     Am   242.0d0    1.520d2       0.10    2.48d+01
   05      Pu238    Pu238     PU238     Pu   238.0d0    8.774d1       0.10    3.77d+03
   06       U234     U234      U234      U   234.0d0    2.445d5       0.10    1.18d+00
   07      Th230    Th230     TH230     Th   230.0d0    7.700d4       0.01    1.37d-04
   08      Ra226    Ra226     RA226     Ra   226.0d0    1.600d3       0.10    4.11d-07
   09      Pb210    Pb210     PB210     Pb   210.0d0    2.230d1       1.00    5.67d-08
   10      Cm243    Cm243     CM243     Cm   243.0d0    2.850d1       0.10    2.55d+01
   11      Am243    Am243     AM243     Am   243.0d0    7.380d3       0.10    2.64d+01
   12      Pu239    Pu239     PU239     Pu   239.0d0    2.406d4       0.10    3.69d+02
   13       U235     U235      U235      U   235.0d0    7.038d8       0.10    1.71d-02
   14      Pa231    Pa231     PA231     Pa   231.0d0    3.277d4       0.10    2.69d-05
   15      Ac227    Ac227     AC227     Ac   227.0d0    2.177d1       0.10    7.51d-06
   16      Cm245    Cm245     CM245     Cm   245.0d0    8.499d3       0.10    3.66d-01
   17      Pu241    Pu241     PU241     Pu   241.0d0    1.440d1    1000.00    9.22d+04
   18      Am241    Am241     AM241     Am   241.0d0    4.322d2       0.10    2.08d+03
   19      Np237    Np237     NP237     Np   237.0d0    2.140d6       0.10    4.34d-01
   20       U233     U233      U233      U   233.0d0    1.585d5       0.10    3.44d-05
   21      Th229    Th229     TH229     Th   229.0d0    7.339d3       0.10    2.75d-07
   22      Cm244    Cm244     CM244     Cm   244.0d0    1.811d1    1000.00    2.68d+03
   23      Pu240    Pu240     PU240     Pu   240.0d0    6.537d3       0.10    5.44d+02
   24       U236     U236      U236      U   236.0d0    2.341d7       0.10    2.81d-01
```

```
  25     U232   U232     U232      U   232.0d0   7.200d1      0.10   3.93d-02
  26    Sm151   Sm151    SM151    Sm   151.0d0   8.999d1      1.00   4.28d+02
  27    Cs137   Cs137    CS137    Cs   137.0d0   3.000d1      1.00   9.15d+04
  28    Cs135   Cs135    CS135    Cs   135.0d0   2.300d6      1.00   5.36d-01
  29     I129   I129     I129      I   129.0d0   1.570d7      0.10   3.57d-02
  30    Sn126   Sn126    SN126    Sn   126.0d0   1.000d5      1.00   8.85d-01
  31   Sn121m  Sn121m   SN121M    Sn   121.0d0   4.997d1      1.00   1.04d+00
  32   Ag108m  Ag108m   AG108M    Ag   108.0d0   4.180d2      1.00   1.26d-02
  33    Pd107   Pd107    PD107    Pd   107.0d0   6.496d6      1.00   1.31d-01
  34     Tc99   Tc99     TC99     Tc    99.0d0   2.130d5     10.00   1.45d+01
  35     Mo93   Mo93     MO93     Mo    93.0d0   3.498d3      1.00   1.51d-02
  36     Nb94   Nb94     NB94     Nb    94.0d0   2.030d4      1.00   8.48d-01
  37     Zr93   Zr93     ZR93     Zr    93.0d0   1.530d6      1.00   2.47d+00
  38     Sr90   Sr90     SR90     Sr    90.0d0   2.912d1      1.00   6.25d+04
  39     Se79   Se79     SE79     Se    79.0d0   1.100d6      1.00   4.58d-01
  40     Ni63   Ni63     NI63     Ni    63.0d0   9.200d1      1.00   3.72d+02
  41     Ni59   Ni59     NI59     Ni    59.0d0   8.000d4      1.00   2.44d+00
  42     Cl36   Cl36     CL36     Cl    36.0d0   3.010d5      1.00   1.15d-02
  43      C14    C14      C14      C    14.0d0   5.729d3      0.10   1.44d+00

*****
```

Listing of differences in *tpa.inp*.

```
Comparing files tpa.inp and TPA.ORIGINAL.INP
***** tpa.inp
**
** rwr 9/6/00  the following 3 parameters in this new section
**             are  for groundwater protection calculations
**
**          ***>>> Groundwater Protection <<<***
**
iflag
GroundwaterProtectionCalc(yes=1,no=0)
1
**
***** TPA.ORIGINAL.INP
**
**          ***>>> UZFLOW  <<<***
**
uniform
ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
1.0, 10.0
**
uniform
MeanAveragePrecipitationMultiplierAtGlacialMaximum
1.5, 2.5
**
uniform
MeanAverageTemperatureIncreaseAtGlacialMaximum[degC]
-10, -5
**
*****

***** tpa.inp
constant
WellPumpingRateGroundwaterProtection[gal/day]
1.146e6
**
***** TPA.ORIGINAL.INP
```

```
constant
TimeStepForClimate[yr]
500.0
**
*****

***** tpa.inp
constant
FractionPlumeCaptureGroundwaterProtection
1.0
**
***** TPA.ORIGINAL.INP
constant
StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr]
0.0
**
constant
StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]
0.0
**
constant
CorrelationBetweenMAPAndMAT
-0.8
**
iconstant
ClimatePerturbationSet
1
**
*****

***** tpa.inp
**
**          ***>>> UZFLOW  <<<***
**
uniform
ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
1.0, 10.0
**
uniform
MeanAveragePrecipitationMultiplierAtGlacialMaximum
1.5, 2.5
**
uniform
MeanAverageTemperatureIncreaseAtGlacialMaximum[degC]
-10, -5
**
***** TPA.ORIGINAL.INP
**
**          ***>>> NFENV  <<<***
**
iflag
TabularTemperatureRHFlag(yes=1,no=0)
0
**
iconstant
nsetUsedToPickTempRHDataSet
1
**
*****

***** tpa.inp
```

```
constant
TimeStepForClimate[yr]
500.0
**
***** TPA.ORIGINAL.INP
constant
WPLength[m]
5.275
**
*****

***** tpa.inp
constant
StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr]
0.0
**
***** TPA.ORIGINAL.INP
constant
WPDiameter[m]
1.579
**
**csm1/24/2000
constant
EmplacementDriftDiameter[m]
5.5
**
**csm1/24/2000
constant
CircumferentialFractionNotCoveredByFloor[]
0.75
**csm1/24/2000
**
*****

***** tpa.inp
constant
StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]
0.0
**
***** TPA.ORIGINAL.INP
constant
EmplacementBackfillThickness[m]
0.6
**
*****

***** tpa.inp
constant
CorrelationBetweenMAPAndMAT
-0.8
**
***** TPA.ORIGINAL.INP
constant
DripShieldThickness[m]
0.02
**
**csm1/26/2000
constant
DripShieldEqvIntDia[m]
2.75
**csm1/26/2000
```

```
**
**  6/2/98 tpa3.2  name change for  UseReflux2
**
*****

***** tpa.inp
iconstant
ClimatePerturbationSet
1
**
**
**          ***>>> NFENV  <<<***
**
iflag
TabularTemperatureRHFlag(yes=1,no=0)
0
**
iconstant
nsetUsedToPickTempRHDataSet
1
**
***** TPA.ORIGINAL.INP
iconstant
SelectRefluxModel(1,2,3)
3
**
*****

***** tpa.inp
constant
WPLength[m]
5.275
**
***** TPA.ORIGINAL.INP
constant
LengthOfRefluxZone[m]
20
**
*****

***** tpa.inp
constant
WPDiameter[m]
1.579
**
**csm1/24/2000
constant
EmplacementDriftDiameter[m]
5.5
**
**csm1/24/2000
constant
CircumferentialFractionNotCoveredByFloor[]
0.75
**csm1/24/2000
**
***** TPA.ORIGINAL.INP
constant
MaximumFluxInRefluxZone[m/s]
1.0e-9
**
```

```
*****

***** tpa.inp
constant
EmplacementBackfillThickness[m]
0.6
**
***** TPA.ORIGINAL.INP
constant
PerchedBucketVolumePerSAarea[m3/m2]
0.5
**
*****

***** tpa.inp
constant
DripShieldThickness[m]
0.02
**
**csm1/26/2000
constant
DripShieldEqvIntDia[m]
2.75
**csm1/26/2000
**
**  6/2/98 tpa3.2  name change for  UseReflux2
**
iconstant
SelectRefluxModel(1,2,3)
3
**
***** TPA.ORIGINAL.INP
constant
Reflux2Thickness
100.0
**
*****

***** tpa.inp
constant
LengthOfRefluxZone[m]
20
**
***** TPA.ORIGINAL.INP
constant
Reflux2Porosity
0.14
**
*****

***** tpa.inp
constant
MaximumFluxInRefluxZone[m/s]
1.0e-9
**
***** TPA.ORIGINAL.INP
constant
Reflux2SatInit
0.9
**
*****
```

```
***** tpa.inp
constant
PerchedBucketVolumePerSAarea[m3/m2]
0.5
**
***** TPA.ORIGINAL.INP
constant
Reflux2SatResid
0.1
**
*****

***** tpa.inp
constant
Reflux2Thickness
100.0
***** TPA.ORIGINAL.INP
constant
Reflux2Period
100.0
*****

***** tpa.inp
constant
Reflux2Porosity
0.14
**
***** TPA.ORIGINAL.INP
constant
Reflux2LossI
0.1
**
*****

***** tpa.inp
constant
Reflux2SatInit
0.9
**
***** TPA.ORIGINAL.INP
constant
Reflux2LossD
0.1
**
** 1-22-00 EDA II design ****
**
*****

***** tpa.inp
constant
Reflux2SatResid
0.1
**
***** TPA.ORIGINAL.INP
constant
EmplacementDriftSpacing[m]
81.
**
*****

***** tpa.inp
```

```
constant
Reflux2Period
100.0
**
***** TPA.ORIGINAL.INP
constant
WPSpacingAlongEmplacementDrift[m]
6.1392
**
*****

***** tpa.inp
constant
Reflux2LossI
0.1
**
constant
Reflux2LossD
0.1
**
** 1-22-00 EDA II design ****
**
constant
EmplacementDriftSpacing[m]
81.
**
constant
WPSpacingAlongEmplacementDrift[m]
6.1392
**
constant
TotalWasteEmplacedInRepository[MTU]
***** TPA.ORIGINAL.INP
constant
TotalWasteEmplacedInRepository[MTU]
*****
```

Listing of differences in *tpanames.dbs.*

```
Comparing files tpanames.dbs and TPANAMES.ORIGINAL.DBS
***** tpanames.dbs
WellPumpingRateGroundwaterProtection[gal/day]                WPR_GWP
FractionPlumeCaptureGroundwaterProtection                    FPC_GWP
***** TPANAMES.ORIGINAL.DBS
*****
```

The modifications were tested in a one realization TPA run using the basecase *tpa.inp* file. For expediency, it is recognized and acknowledged by R. Janetzke that only developer testing was conducted and that these changes will be tested by non-developers (i.e, not by R. Rice). Furthermore, the EPA Standard determination is operational but not delivered in version 4.1, but will be fully implemented in the version 4.2 of the TPA code.

1/27/02

Performed simulations using TPA v4.1j to determine the effort required to conduct simulations to 500,000 yrs. The TPA simulations identified the needed changes and the changes were made to accomplish the desired simulation time. Additionally, simulations were conducted to verify the correctness of the TPA results. The findings from this work including the modified files were e-mailed to S. Mohanty, as requested.

The modified TPA files were climato2.dat,, exec,f, tpa.inp, and wpflow.def. The climato2.dat file was changed to encompass five 100,000 yr cycles, instead of one 100,000 yr cycle. The exec.f file was changed to increase the maximum number of seismic events from 1,000 to 5,000. The tpa.inp file was modified to increase the maximum time from 1e5 to 5e5. The wpflow.def file was modified to extend the maximum time from 100,000 to 500,00 yr.

3/08/02

Began activities related to SCR-388 for TPA 5.0 development (i.e., "Generate the SNLLHS input file such that only the input parameters that will be used during the run will be submitted to the SNLLHS code for sampling. This select submission will reduce the number of sampled parameters when not needed for a particular run" as stated in SCR-388). The completed activities included identifying all TPA "flags" (63 were identified), conducting the 63 TPA simulations with those "flags" activated, and preparing files with the parameters that were and were not needed with the different "flags" for each TPA simulation compared to the TPA basecase results. The TPA v.4.1j code was utilized for this developmental work.

Additionally, support was given to TPA 5.0 code development for other tasks during this time period. These tasks included (1) identification of the Reflux 1, 2, and 3 parameters and (2) TPA code capabilities for using alternative decay chains, such as 2 parents decaying to 1 daughter. The following table identifies the Reflux 1, 2, and 3 parameters from different TPA simulations.

tpa.inp parameter name (case 1)	Reflux 1, 2, 3 Parameter
LengthOfRefluxZone[m]	1
MaximumFluxInRefluxZone[m/s]	1
PerchedBucketVolumePerSAarea[m3/m2]	1
Reflux2Porosity	(should be 2 and 3)
Reflux2SatInit	(should be 2 and 3)
Reflux2SatResid	(should be 2 and 3)
EmplacementDriftSpacing[m]	not specific to reflux 1,2,3
WPSpacingAlongEmplacementDrift[m]	not specific to reflux 1,2,3
FractionOfCondensateRemoved[1/yr]	(should be 3)
FractionOfCondensateTowardRepository[1/yr]	(should be 3)
FractionOfCondensateTowardRepositoryRemoved[1/yr]	3
DensityOfWaterAtBoiling[kg/m^3]	3
EnthalpyOfPhaseChangeForWater[J/kg]	3
TemperatureGradientInVicinityOfBoilingIsotherm[K/m]	(should be 3)
BoilingPointOfWater[C]	(should be 1 and 3)

tpa.inp parameter name (case 2)

	Reflux 1, 2, 3 Parameter
Reflux2Thickness	2
Reflux2Period	2
Reflux2LossI	2
Reflux2LossD	2
EmplacementDriftSpacing[m]	not specific to reflux 1,2,3
WPSpacingAlongEmplacementDrift[m]	not specific to reflux 1,2,3
FractionOfCondensateRemoved[1/yr]	(should be 3)
FractionOfCondensateTowardRepository[1/yr]	(should be 3)
FractionOfCondensateTowardRepositoryRemoved[1/yr]	3
DensityOfWaterAtBoiling[kg/m^3]	3
EnthalpyOfPhaseChangeForWater[J/kg]	3
TemperatureGradientInVicinityOfBoilingIsotherm[K/m]	(should be 3)
ThermalConductivityofYMRock[W/(m-K)]	(should be 1 and 3)

For the TPA code capabilities to use alternative decay chains, it was concluded that the TPA code could model two parents decaying to one daughter by specifying two chains in the tpa.inp file, removing the error check for repeated radionuclides in "reader.f", and inserting logic in the TPA code to sum the inventories of the daughter in the two chains to determine the total inventory of the daughter. This information could be useful to model colloids in the TPA code.

3/22/02

Initiated work associated with testing the modified SNLLHS file according to the modifications listed in SCR-387. Upon compiling the SNLHS source code on a PC, it was discovered that the character strings "CDUM1" and "CDUM2" needed to be included in the CHARACTER definition statement and that the AMAX1 function needed to be changed to MAX. The changes were made by R. Janetzke and a revised version (TPA v.4.2a) was sent and received via email attachment. This version of the SNLLHS code (i.e., 3/19/02) is planned for use in the accepted test plan submitted to R. Janetzke for SCR-387.

A test plan for SCR-387 was submitted to R. Janetzke and after the comments were included in the test plan, the test plan was accepted.

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Entries into Scientific Notebook 170e (SN170e) for pages 94-97 have been made by Robert W. Rice.

Robert W. Rice — 3/22/02
(name) (date)

No original text entered into this Scientific Notebook has been removed.

Robert W. Rice — 3/22/02
(name) (date)

I have reviewed this scientific notebook in accordance with QAP-001 and find it in compliance. There is sufficient information that a qualified individual could repeat the activity.

James Winterle, manager — 11-1-05