SCIENTIFIC NOTEBOOK

612-1E

by

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INITIAL ENTRIES

Scientific Notebook: #612E

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Title: TPA 5.0 Code Development

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2 - S. Mohanty
3 - R. Rice
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5 - O. Pensado
6 - R. Benke
7 - P. LaPlante
8 - G. Adams
9 - B. Winfrey
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15 - J. Menchaca
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17 - O. Povetko

Objective:
        This scientific notebook will document the work performed in the development
of the TPA 5.0 code. The TPA code is designed to estimate total-system performance
measures of an annual individual dose or risk expected to be specified in the EPA
standard and the NRC conforming regulations. The TPA code is a combination of and

executive driver, a set of consequence modules, and a library of utility modules. Consequence modules simulate physical processes and events such as unsaturated zone infiltration , evolution of the near-field thermal-hydrologic environment, failure of the drip shield and waste packages, dissolution and release of waste, transport of waste in the groundwater system, extraction of groundwater, and consumption of groundwater. This scientific notebook contains an initial entry section within Chapter 1 followed by the technical content for all subsequent chapters prepared by the participants. These participants receive tasking from the project manager and work under his guidance as it pertains to the stated objective..

Oct. 10, 2003   Transport logic for Neftran

The following e- mail was sent to C. Grossman on Oct. 9, 2003.

```
Chris,

Sorry for the delay.  Here is a brief summary of the UZ transport logic.  Note
that far field subarea infiltration is used here with no consideration for
reflux.

1.  For each time step find the layer with the highest matrix fraction as
permitted by infiltration and conductivity considerations.
    matrix fraction = conductivity / infiltration
    (Although the lowest matrix fraction is the more conservative value, it was
found to be excessively conservative since this value is
applied to all layers simultaneously, and in most cases would effectively bypass
any matrix layers present.)

2.  Limit the matrix fraction to <= 1.0.

3.  Determine a fracture fraction for the time step.
    fracture fraction = 1.0 - matrix fraction

4.  For each time step divide the Curies per year, entering the UZ from the
invert, into matrix and fracture parts, using the fractions
above.

5.  For each time step apply the permanent loss colloid filter factor to the
matrix fraction only, leaving the fracture fraction unchanged.

6.  For each time step, find velocity in each layer.
    velocity  = infiltration / (porosity * saturation?)

7.  Constrain velocities in each layer to yield at least 5 year travel time in
the layer.

8.  For each time step find GWTT for each layer.
```

```
9.  For each layer use trapezoidal integration to determine the average travel
time over the simulation period and again for  the compliance
period.

10.  Select the minimum (more conservative value) as the average GWTT for that
layer.

11.  Write the velocity file.  The velocity changes with time due to changes in
the infiltration.. However,  velocity changes are accepted
only when the variation is greater than or equal to a user specified fraction
(0.4 base case) of the previous velocity.

12.  Remove layers whose average travel time is not at least 10 years OR not at
least 10% of the total average travel time for all layers.

13.  If no stratigraphic layers are retained, the UZ is by passed and the EBS
releases are transferred directly to the SZ.

ron j
```

Oct. 10, 2003   Linear dose at 10,000 years

Run 1: initial failure @ 11000, no scenarios => 0 dose

Run 2: initial failure @ 0, no scenarios, defective fraction =10^{-8} => 0 dose

Run 3: initial failure @ 0, no scenarios, defective fraction =.25 => 2.622e-2 rem/yr

Run 4: initial failure @ 0, no scenarios, defective fraction =.5 => 5.245e-2 rem/yr

Run 5: initial failure @ 0, no scenarios, defective fraction =1.0 => 1.04e-1 rem/yr

So it is linear, and heuristically we can say that:

```
dose =  (% initial failure) mrem/yr
```

Oct. 14, 2003   TPA 5.0q

TPA 5.0q was put in *../dev/...* and compiled on **spock**.

Nov. 5, 2003   Software Validation Report (SVR) & SVTRs

B. Brient agrees that the SVR prepared for the NRC should be submitted to the QA records to supercede the SVTRs originally submitted to the QA files, since the CDs were compressed onto one platter for the SVR. Both submissions are internally consistent, but the data locations on the CDs do not agree between the submissions. The only content changes were the addition of successful test evaluations replacing failed tests in the original submission.

Nov. 12, 2003   Cvolc

The dispersion fraction may need to be set to 0.01 for the base case of **cvolc** runs.

Nov. 12, 2003   Beowulf

The **beowulf** cluster uses SUSE Linux-9 at address 129.162.79.54 for the OSO machine.

Nov. 12, 2003   Dose limits

Total dose limit = 15mrem/year.

Ground water dose limit = 4mrem/year.

Nov. 12, 2003   Spent Fuel Dissolution limits.

The highest practical, in a sensitivity study computational sense, spent fuel dissolution rate, removes the fuel in 100 years.

Nov. 12, 2003   Burn up

35% BWR => 0.35 *   8407 = 2942.5 W/MTHM
65% PWR => 0.65 * 10510 = 6831.5 W/MTHM

2942.5 + 6831.5 = 9774. W/MTHM

9774 * 9.76 MTHM/WP = 95394 W/WP = 19 kW/m @ 5m/WP

Dec. 8, 2003   TPA 4.1jpd Source Code Release to NV

Here are some points from the telecon with NRC about the NV FOIA request.

NV has TPA 4.1jpd executable only.

Most software today is vended as executable only.

Tim is opposed to sending source code for TPA5.0 current version to NV.

FOIA usually implies immediate release of information.

Most comments are not marginalia.

TPA5.0 is being cleaned up for LSN.

The software compilation process was explained.

The use of "CC" at the beginning of a comment was clarified.

Chris G. supplied a coding example from ashplume.f. It contained the Suzuki correction comment.

The source code would be about 4000 pages in landscape mode.

NV does not pay for the review effort. They pay for media only.

Removing all comments would be considered antagonistic, even though the original request did not specify the inclusion of comments.

NV is looking for the TPA Achilles' heel and something to challenge.

NV may appeal the NRC's approach to this FOIA compliance.

All redacted material will need an Exemption 5 basis.

Should TPA 4.1jpd be considered a draft version?

Some comments that no longer apply may imply that the code is also misapplied.

Some example redactions from OGC are requested.

Ad hoc examples:
This code is no longer used.
Known to have bugs.
Models in it are not validated.

Redactions should include location, number of lines/words, and basis for exemption of material and are indicated in brackets with phrases such as :
  - Information redacted per Exemption 5.

12-12-03 is due date for NRC response.

Embarrassment is not grounds for withholding comments.

FOIA Exemption 5 deals with pre-decisional, deliberative and opinion oriented comments.

A disclaimer could read:
Comments are outdated, potentially misleading, and factually incorrect. A newer version with these comments updated will be supplied.

Dec. 9, 2003   TPA Source Code for LSN

K. Compton is planning an IM for 3-15-04 to deliver an LSN version of 5.0r source code.

Dec. 9, 2003   MTIHM in burnup.dat file.

M. Smith sent the following e-mail:

```
A google search on the internet gives many cases for
"metric tons of initial heavy metal."   If Jim used
ORIGEN, then I would check with Oleg to see if he knows
what values are output from ORIGEN (maybe several and
that wouldn't help).   It's not definitive, but here is
one definition that was given from an EPA report about
high-level waste inventories:

Information in this chapter describes fuel inventories
either in terms of metric tons of initial heavy metal
(MTIHM) or in terms of metric tons of heavy metal (MTHM)
depending on the metric used in the source document. The
former term (MTIHM) is useful since it is a metric that
is independent of fuel burnup, while the latter term
(MTHM) is useful since it is a metric that is consistent
with the repository regulatory limit (i.e., 70,000 MTHM).
Heavy metal refers to the mass of actinide elements
(elements with atomic numbers greater than 89) in the
fuel. Generally, the initial heavy metal is mostly
uranium. Differences between MTIHM and MTHM are small.


Hope this helps.

--Mike
```

Dec. 12, 2003   **Differing Professional View**   Examples from ONMSS

 Differing Professional View Regarding Modeling Chemical Consequence Effects for Determining Safety Requirements at the Proposed Mixed-Oxide Fuel Fabrication Facility

A Differing Professional View (DPV), filed December 19, 2002, with the Office of Nuclear Material Safety and Safeguards (NMSS), raised concerns regarding Modeling Chemical Consequence Effects for Determining Safety Requirements at the Proposed-Mixed Oxide (MOX) Fuel Fabrication Facility. The principal issues the DPV identified were: (1) Chemical consequences to MOX facility workers, the public, and the environment may be significantly understated if NRC allows use of the ARCON 96 automated scientific code, and therefore approaches for adequate safety measures and safety controls may not be implemented; (2) NMSS should establish a position on the use of codes, estimation techniques, and parameters that is consistent, peer-reviewed, conservative, provides adequate assurances of safety, and is defensible; and (3) the staff should have a formal approach for reconciling codes and methodologies that produce significantly different estimates of consequences.

An ad hoc panel appointed by the Director, NMSS, to review the DPV issued a report on September 30, 2003. The panel concluded that: (1) The ARCON 96 automated scientific code is a suitable tool for analyzing potential chemical consequences for a MOX fabrication facility; (2) Suitable documentation exists to guide NRC development, endorsement, and acceptance of automated scientific codes. The ARCON 96 code is documented sufficiently for license reviewers to ascertain suitability of the code for its specific application at the MOX facility; and (3) Different results are possible when different codes are applied to the same phenomena. Rather than reconcile these differences, it is more important that license reviewers using or reviewing codes and their license-specific application results have a sufficient understanding of each code's suitability for its specific use to determine which code is appropriate (i.e., more reasonable) for the intended use.

A Director's Decision issued on October 3, 2003, found that some of the DPV views had merit, and agreed with the review panel 's recommendations. The Director requested that the staff: (1) Ensure that sufficient information has been docketed to demonstrate the reasonableness of the site-specific application of the ARCON 96 code for safety-related decisionmaking; (2) Implement guidance to ensure that managers and staff involved with development, endorsement, use, or acceptance review of automated scientific codes are familiar with relevant sections of NRC Management Directives, NUREG/BR-0167, and Software Quality Assurance Program and Guidelines; and (3) Issue guidance to ensure that staff have a sufficient understanding of relevant automated scientific codes to determine which code is appropriate (i.e., reasonable) for the intended use.

Differing Professional View Regarding Technical Safety Requirements for Instrumentation Setpoints and Allowable Values at Portsmouth Gaseous Diffusion Plant

A Differing Professional View (DPV) filed November 6, 2002, with the Office of Nuclear Material Safety and Safeguards (NMSS) raised concerns regarding technical safety requirements for

instrumentation setpoints and allowable values at the Portsmouth Gaseous Diffusion Plant in Piketon, Ohio. The DPV identified three issues: (1) Portsmouth setpoints in plant procedures are not consistent with Limiting Control Setting values in the Technical Safety Requirements (TSRs); (2) Portsmouth allowable values in the plant are not consistent with allowable values in the TSR; and (3) staff actions (addressing specific examples used to support inspection findings concerning plant-wide problems in lieu of addressing broader open issues) lack technical/regulatory basis and undermine/negate adequate resolution of unresolved issues.

An ad hoc panel appointed by the Director, NMSS, to review the DPV, issued a report on August 28, 2003. Although the DPV panel was not unanimous in its decision, the panel disagreed with the DPV position on several levels. The panel found that: (1) the applicable instrument standard (ANSI/ISA - S67.04 - 1988) did not prevent the approach taken by the certificate-holder; (2) the TSRs' purposes are still met; (3) NRC still maintains adequate regulatory authority of the safety-related setpoints; (4) Quality Assurance Requirements apply to procedures and setpoints; (5) Region III closed the Inspection Follow-up Item appropriately.

The minority view stated that: (1) changes to TSRs (e.g., setpoints, allowable values) must be submitted to NRC for review and approval. The panel majority agreed, but concluded that TSRs were not changed. No limiting control settings were changed–only procedural limits more limiting than limit control settings. (2) The change control process (10 CFR 70.68) cannot be used by Portsmouth because the regulation specifically excludes its use for changing TSRs. The panel majority agreed, but concluded that TSRs were not changed. (3) The DPV concerns are risk-significant. The panel majority disagreed, concluding that, to be risk-significant, the DPV's proposed changes in the NRC position should show a significant increase in the margin of safety by reducing the likelihood or consequences of an accident. The panel majority found that no evidence had been provided to support a change in likelihood or consequences, and that the Certificate holder is apparently operating with more safety margin than the TSRs require.

However, the panel found that inspection procedure 92701, *Follow-up*, was not referenced by the inspection program as described in Manual Chapter (MC) 2630. The panel recommended that MC 2630 be updated accordingly, and that the staff consider revising NRC Inspection Manual Chapter MC 2630 or the inspection procedure to include guidance to the inspector on the scope of follow-up for inspection open items. The panel recommended no change in any staff position, in either licensing or inspection.

A Director's Decision was issued on September 3, 2003, agreeing with the review panel majority's conclusions and recommendations. The Director requested that the staff take into consideration the review panel's conclusions and recommendations in future changes to inspection guidance.

Dec. 15, 2003   MTIHM

The following was received from O. Povetko:

```
DOE's abbreviation MWd/MTIHM means (megawatt days per metric tons of initial
heavy metal). For irradiated heavy metal they use term "postirradiated heavy
```

```
metal loading". Interpretation of MTIHM as ...irradiated heavy metal... would
lead to ambiguity as we discussed before. The former interpretation is pretty
clear and in case of U+Th loadings it is not an equivalent to "MTU".

Oleg.
```

Dec. 22, 2003　NFENV Relative Humidity

Only the lower bound of the delequesence RH is sampled, not the RH itself. The upper bound is 100%.

Feb. 6, 2004　XP Make

Four compile switches used on LF90 are not available on LF95: -nbind, -nwrap, -04, and -vax.

Several new switches are available: -ap, -in, -trap, -vsw.

The GETENV function in zportpc.f is now a subroutine call in LF95.

Feb. 9, 2004　Findelev.f

Findelev.f is not used in the TPA code.

Feb. 10, 2004　Filemerge

The following command line can be useful when creating a script file using `filemerge`:

```
filemerge myfile.f ../test/myfile.f;mv filemerge.out myfile.f;read temp
```

Feb. 16, 2004   TPA runs

Maximum GS dose for cfsv1kr10a18k100y is 99. rem/yr. Maximum GW dose is 1.1 rem/yr.

The highest dose for a cfsv100r10a18k1ky direct release only and wind direction uniform from -180 to 0 run of TPA 5.0s was 424.2 rem/yr at realization 53 of 100.

Feb. 23, 2004   Fortran comments

A script for the collection of Fortran comments on the Sun follows:

```
echo
# Useage: >comments tpadir output
# where tpadir($1) = root directory for TPA source code.
#       output($2) = local output file name.
#
if test -f $2
then
     echo $2  output file exists.
     exit 1
fi
#
if test -d $1
then
     cd $1
else
     echo $1 directory not found.
     exit 1
fi
#
     touch ../$2
     grep -i "^[c]" *.f >> ../$2
     grep -i ! *.f >> ../$2
#
#
if test -d ccdf
then
     cd ccdf
else
     echo $1/ccdf directory not found.
     exit 1
fi
#
     grep -i "^[c]" *.f >> ../../$2
     grep -i ! *.f >> ../../$2
```

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```
     cd ..
#
if test -d codes
then
     cd codes
else
     echo $1/codes directory not found.
     exit 1
fi
#
     grep -i "^[c]" *.f >> ../../$2
     grep -i ! *.f >> ../../$2
#
if test -d gentpa
then
     cd gentpa
else
     echo $1/codes/gentpa directory not found.
     exit 1
fi
#
     grep -i "^[c]" *.f >> ../../../$2
     grep -i ! *.f >> ../../../$2
     cd ..
#
if test -d itym/src
then
     cd itym/src
else
     echo $1/codes/itym/src directory not found.
     exit 1
fi
#
     grep -i "^[c]" *.f >> ../../../../$2
     grep -i ! *.f >> ../../../../$2
     cd ../../..
#
```

Mar. 1, 2004   FTP

The following was sent to C. Grossman and Jun Li (jli7@ncsu.edu):

```
TPA source files for the SUN platform have been placed on ftp.swri.edu.

FTP file access info:

HOST: ftp.swri.edu
NAME: anonymous
DIRECTORY: /pub/incoming
MODE: binary
FILENAME:
tpa41jpd.tar
```

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```
tpa41j4k.tar is a Unix tar file of the source, object and executable TPA
4.1jpd files.
```

Mar. 2 2004   McCartin Comments

During the last KTI meeting T. McCartin announced that he was looking into a couple of potentially abnormal behaviors of the TPA 4.1jp code.

1. 30% of the realizations of a 100 realiztion run show no flow for the volcanic scenario in 10k years.

2. Changing the WP flow mult factor from 1.0 to 1.3 affects the reflux.

These results were not reproduced with 4.1jp.   The runs do show all realizations produce flow at least during reflux although about 10% have 0 flow after that for the remainder of the 10k year period.

Changing the WP flow mult factor did not affect the reflux.

He also mentioned that water is flowing at 160C in 5.0. This behavior was verified and was reproduced in both 4.1jp and 5.0s.

Mar. 16, 2004   GINO

Use of GINO requires the -**MOD** and -**LIBPATH** *lf95* switches. The **.lib* files must be listed by name in the command line if they are used. The <u>%GINO%</u> environment variable may aid in the construction of command lines also.

The following will work for a simple test file:

```
>lf95 @%GINO%\edginbld.bat tg.f90
```

Mar. 19, 2004   GENII / TPA5.0s1

NRC reported an error in the code when run for direct release only from 1 to 100 realizations on realization number 12. The RITEXP routine in GENII produces asterisks for TC99 values in genv.out (file number 13). This is caused by the use of the -dbl switch in the LF95 command to convert to double precision in the **Automake** configuration files *Mkenv.fig* and *Mkenvin.fig*. The compiler enables 3 digit exponents with -dbl for double precision values and the FORMAT statement is not compatible with these exponents and requires 2 digit exponents. TPA version 5.0s1is generated with the updated **.fig* files.

Mar. 25, 2004   Testing

A meeting was held today with O. Pensado, G. Adams, and C. Scherer on automated testing of the TPA code. The following items were agreed on, as desirable characteristics for TPA testing.

1. Testing should be automated.
2. All testing should be performed on both the Sun and PC.
3. A site visit should be made to NRC for all IM or major releases well in advance of the delivery date to perform some or all of the tests in their environment of compilers and hardware.
4. A 1024 realization run should be included.
5. The code should be modified to produce a tpa_min.inp and tpa_max.inp test input files.
6. All model and mode switches should be exercised.
7. A test mode should be added to the code to only sample one parameter at a time and continue execution until all of the sampled parameters have been exercised.
8. Accommodate some sort of convergence test.
9. Modify the Pre-Processor to automate as much of the above testing as possible.
10. Move deadlines up by 2 weeks so that a full week can be devoted to automated test runs and an additional week can be used for modifications dictated by the test results.

Mar. 30, 2004   Testing

An additional item for testing:

11. Encourage the use of the PC version on local PA workstations.

April 1, 2004   Drip Shield Corrosion

R. Codell announced that no drip shield corrosion is expected in 10,000 years.

May 4, 2004   Volcanic Events

S. Mohanty says that volcanic events should be limited to the first 10,000 years even if the simulation time is greater than 10,000 years, in order to provide similar event profiles for both types of runs. This aids in comparing the results.

For faulting events, however, the faulting event time should not be limited to the first 10,000 years, but should have a range of the full simulation period.

May 12, 2004   Screened Colloids. SCR 486

Version 5.0s was reported by Buck at NRC to produce a step increase in total dose at the last time step of the 10,000 year period. This was caused by the code disallowing releases from the SZ prior to the UZ release. The colloid contribution was moved to the parent nuclide before they were screened for SZ release. As a result the screening was based on the time of the parent from the UZ rather than on the time of the colloid release.

This behavior had little effect on the peak dose since the last time step is not subject to screening and was calculated correctly in all cases.

May 24, 2004   TPA on Shared PC network

The following e-mail was received form IMS:

A new share (named "TPA_Share") has been created on Vermont. You should be able to read and write to it (\\Vermont\TPA_Share). All other users have read-only access.

June 10, 2004   GENII Leach Rate

The following e-mail was received from C. Scherer:

```
I get an invalid operation flag raised when I run this one.  Could you run
this tpa.inp (Volcanism = 1, and Direct Release Only = 1, Number of
Realizations = 1000, Start & Stop Realization = 668) with the debugger and
see what it points to?  Maybe it's just another potential divide by zero
that isn't taken care of.
```

This is due to the lack of precision in the GENII data transfer files between envin.e and env.e. This was caused by the sum of the lambda for decay (AL) and the leaching factor (AB) being equal for two consecutive members of a decay chain. In this case it was U232 an Th232 in genv.in chain number 19. A contributing factor is that the variability was severely constrained due to the few significant digits in the data transfer files. The gftrans.dat file uses 2 significant digits for the leaching factor and the env.in file uses 3 significant digits for the LEACHT parameter.   The ALT variable comes from the file grmdlib.dat. The (ALT + LEACHT) in env.in for U232 equals the (ALT + LEACHT) for Th232. The module chain.f in env.e takes the difference between these sums and uses it for the denominator when determining A(), one of the coefficients that determine the activity of each nuclide. The resulting divide by the difference of zero caused the error. Chain.f is unmodified from the GENII code and was received from PNL with the bug.

July 24,   2004   Lahey LF95

Useful compile switches for LF95 are -ap, -chk, -chkglobal, -fix, -g, -in, -info, -pca, -trace, -trap, -w, -zero, and -dbl.

July 24, 2004   mechfail / nfenv

SCR480 and SCR481 will require a new calling sequence for the EXEC module.

UZFLOW   (output: qm3peryrinsa)

HAZARDCRVE   (output: timeofseismicevents,
                          output: typeofseismicevents)

SEISMO   (input: timeofseismicevents,
            input: typeofseismicevents,
            output: drift_radius,
            output: bfthick,
            output: seismicfailwpsubarea,
            output: seismicfaildssubarea)

NFENV   (input: bfthick,
            input: drift_radius,
            output: temprep,
            output: tempwp,
            output: relhumwp,
            output: qm3peryrperwpinsamisswp,
            output: qm3peryrperwpinsahitwp,
            output: flconcentration)

DSFAIL   (input: seismicfailwpsubarea,
            input: seismicfaildssubarea,
            input: flconcentration,
            output: ds_thickness,
            output: ds_corrosion,
            output: dsfailuretime,
            output: dsfailureflag,
            output: dsfailcorrected [variable to coordinate mechanical and
            corrosion DS failures])

SEISMO   (input: timeofseismicevents,

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input: typeofseismicevents,
input: ds_thickness,
input: ds_failure_time,
input: bfthick,
output: seismicfailwpsubarea,
output: seismicfaildssubarea)

NFENV2   (input: qm3peryrperwpinsahitwp,
input: relhumwp,
input: temprep,
input: dsfailuretime,
input: dsfailcorrected ,
output: co3,
output: ph,
output: cl,
output: no3,
output: delta_ecrit)

EBSFAIL   (input: temprep,
input: tempwp,
input: relhumwp,
input: ph,
input: cl,
input: delta_ecrit,
output: corrosionfailwp)

FAULTO   (output: faultfailwp)

VOLCANO (output: volcanicfailwp,
output: amtuejected)

CUMFAIL   (input: corrosionfailwp,
input: sesimicfailwpsubarea,
input: faultfailwp,
input: vocanicfailwp,
output: cumfailwp)

EBSREL   (input: sesimicfaildssubarea,
          input: qm3peryrwpinsahitwp,
          output ciperyrinsaintoloweruz,
          output: wp_fill_time)

Questions: Does each subarea have a different drift radius?
             If so, does this affect the repository temperature?

Aug. 13, 2004   Volcano

Both volcano models 1 & 2 should use the
NumberofMagmaInducedMechanicalFauluresRemainingInDrift[] parameter and
not the dike geometry when failing packages for the groundwater pathway. See
following e-mail:

```
Looks like you're using the EDA-II design here, which has some large
differences from LA footprint for total area, MTU/WP and MTU/acre.

In VOLCANO, we need to represent 1-10 WP released by a volcanic
conduit 5-50m diameter. This is done by using dividing WP load (mtu)
by the average mass loading (mtu/acre), then deriving the appropriate
areas to represent 1-10 WP.

The current LA design footprint is 5485614 m2
Total Waste is 70044 MTU
Thus, have a waste loading of 1.28e-2 MTU / m2

If WP load is 7.89 MTU/WP, then 1-10 WP = 618-6180 m2

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

If changes occur in the area of the repository, total MTU emplaced, or
MTU/WP, then the volcanic conduit diameters must be changed in VOLCANO
for TPA.INP to reflect the appropriate effective diameters.

These parameters need to be consistent in TPA.INP, or else the
volcanic releases are wrong.

In looking at the VOLCANO.F code to track this down, though, I think
```

```
I've uncovered another problem. For indirect (i.e., intrusive)
release, if the geometric model is selected (VolcanoModel=1), then the
code appears to calculate the # of WP failed during intrusive event
with the dike geometry model. In changes for TPA 4.1, this model was
supposed to be disabled as this geometry calculation is simply
incorrect for evaluating this source term. Assuming a rigid dike
geometry grossly underestimates the number of failed WP during an
intrusive event.  Thus,
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[] should always
be sampled, regardless of VolcanoModel=1 or 2. This parameter does not
depend on the "dogleg" flow through the drift, which only affects the
direct release source term (i.e., pass to ASHPLUME).

Please verify my suspicion that for VolcanoModel=1, VOLCANO is passing
to EBSREL (?) the number of WP failed during intrusive event (i.e.,
source for hydrologic transport, not to ASHPLUME) is being calculated
by the dike length and width relationships. If so, this is incorrect
and should be changed so this pass to EBSREL(?) is from sampling
NumberOfMagmaInducedMechanicalFailuresRemainingInDrift[] for all
conditions of VolcanoModel.

For WP source to ASHPLUME, the # of WP should remain dependent on
VolcanoModel. For VolcanoModel=1, use the DiameterOfVolcanicCone
relationshps. For VolcanoModel=2, sample the
NumberOfWPsEntrainedByEjecta[]

Thanks-
Britt
```

Aug. 16, 2004   Reflux termination time

T. McCartin verified via telecon that he noticed a blip at 10k years when the reflux model is turned off. He suggests a tpa.inp user selected time for reflux termination may help this.

Aug. 17, 2004   Near-Field Relative Humidity for Pre-Closure

R. Fedors suggests a change for the pre-closure relative humidity calculation; that is to use the ground surface temperature rather than the repository temperature for the relative humidity calculation.   This could require that the ground surface temperature definition (a constant AAT0) be moved from UZFLOW to the tpa.inp file.

Aug. 19, 2004   Calc_kd, calc_rd

The following was received from P. Bertetti:

```
Summary of Meeting on Radionuclide Transport Parameters and Coding in TPA

We reviewed a number of topics concerning possible modifications to parameters
used in calculating radionuclide Kds and Rds (especially those in which
Turner's method is used - Am, Np, Pu, Th and U) and reviewed possible changes
to the code to correct deficiencies or weak technical bases.  This summary
includes what I believe to be the most important points and provides a point
of view that reflects the consensus of opinion expressed at the meeting.

1.    coefkdeq.dat

The data file (coefkdeq.dat) used to provide coefficients to calculate Ka'
values for subsequent use in calculation of Kd and Rd needs to be updated.
The original curve fits of surface complexation model results include residual
errors that results in a significant mismatch between the SCM curves and TPA-
produced versions of the curves.  Although this is most evident for Np, the
problem affects Pu and U as well.  These errors can be reduced significantly
by re-fitting the SCM curves and producing and updated coefficient file.
Corrections have been made for Np and will be made for U and Pu in the next
few weeks (Bertetti).  TPA staff will need to incorporate the modified
coefkdeq.dat into the final verison of TPA 5.0.

2.    Surface area calculations

The effective specific surface areas of the various hydrogeologic layers in
the TPA code are used in the calculation and conversion of Ka' to Kd for Am,
Np, Pu, Th and U.  Specific surface areas are calculated using a relationship
found in Arthur (1996), which uses an idealized geometric representation of
pore spaces to estimate surface area of whole rock with known porosity and
density.  The relationship was originally utilized for consolidated
crystalline rock.

a.    A single constant value is used to represent the pore size distribution
      of the rock layers within TPA. A more appropriate and defensible method
      should include a distribution of pore sizes based on measurements.  The
      current value of 0.05 × 10⁻⁶ m does produce reasonable surface area
      values for tuff layers.

b.    The pore size value for tuffs is probably not appropriate for the
      alluvium (SAV layer in TPA) and is not consistent with observations of
      in Fortymile Wash alluvium, yet the constant value is used for SAV.  A
      recent analysis of surface area for well cuttings and sonic core samples
      suggest that we can produce a defensible distribution of surface area
      values for the SAV.  Modifications to the TPA code will be required to
      introduce this new parameter and to modify the surface area calculation
      for this layer.

c.    The values used for porosity and density in the surface area calculation
```

need to be reviewed. The relationship in Arthur appears to call for
total porosity and bulk density. Instead, grain density values are used
in the code. Also, the code uses effective porosity in the calculation
for alluvium. It appears that the tuff values in the code represent
total porosity. The code could be modified to include a bulk density
calculation (grain density * (1-porosity)) similar to that used in the
Kd calculation. This modification should be incorporated into TPA 5.0.

3.   Effective porosity for alluvium

The code uses alluvium effective porosity in calculations to determine surface
area and Rd.   Total porosity should be used.   The Rd calculation should be
modified accordingly to include a scaling factor or alternate parameter
distribution for alluvium porosity.   Modifications to the surface area
calculation would not be required if alluvium surface area is sampled directly
as suggested above.

4.   pH and CO_2 distributions

pH and CO_2 distributions produced by the TPA code are slightly different than
the distribution produced by the Perfect et al. data set. Because of other
issues, it is difficult to analyze the importance of this difference. Recent
chemical analyses of Fortymile Wash groundwaters suggest that adding those
values might shift the pH and CO_2 range toward the values that TPA currently
produces. There are some differences in estimated dose when the new range is
implemented, but the differences do not appear to be significant. The
parameter range should be updated, but only after other issues are dealt with.

5.   Intermediate analysis results

It is difficult to conduct intermediate analyses because the code does not
produce a set of stored values for surface area, Kd, and Rd. Recent
modifications have been made by Janetzke et al. to provide such output, but it
is not available to most versions of TPA 5.0.

Aug. 23, 2004   TPA 5.0.1 Validation

The following modules have been modified to the extent where validation is
suggested:

Exec.f
Invent.f
Nfenv.f
Numrecip.f
Ebsrel.f/releaset.f
ebsfail.f

Weldfail.f
Seismo2.f/dsfail.f/dsfailt.f,equivdiam.f
Uzft.f
Szft.f
Volcano.f
Ashplume.f
Ashrmovo.f
Dcags.f

Aug. 27, 2004   MOU - GEOLEM topics

    Connect to alternative databases as supposed to GIS only
    Representative Use Cases
    Deployment
    Junit Testing
    Error handling/management
    Management of data persistance
    Thread safety
    Interoperability / C interface
    Performance
    Reliability
    Scalability related to simultanous access (e.g. for Web applications)
    Connect to alternative GIS
    Direct programmatic access
    Defining and implementing compound command specs
    Schema Building Tools (was 'organize library & schema')
    re-use of schemas (was 'model to schema mapping')
    Standard naming of spatial operations (simple/compound commands)
    XML validation Scheme/DTD
    Transaction Management
    Visualization linkage and User interaction

Aug. 27, 2004   Emplacement Time,

O. Povetko said that since the burnup.dat file does not have an entry for zero years
that the emplacement time should be set at 2034 A. D. for the files that have and
effective date of 2033.

Aug. 28, 2004   Some considerations for million year runs.

Ashrmovo.f has maxsimulationtime parameter of 100000.
Nfenv.f has about 20 arrays dimensioned by years simulated.
Ebsrel.f has 3 arrays dimension by 100000.
Need new climate history.
Exec.f has 73 arrays dimensioned by maxntime. 38 of which are double
dimensioned with subarea or nuclides.

Sep. 1, 2004   NEFMKS

T. McCartin concurred today that a minimum ground water travel time for the UZ
layers could be set to 20 years instead of 10 years.

He also suggested to use:

AverageCalendarYearAssumedForEmplacement[A.D.]

as the reference year for the *burnup.dat* and *nuclide.dat* files.

Sep. 7, 2004   DLLs

Use the following for LF95:

>LF95 -dll prog.f90
>dumpbin /exports prog.dll

Goldsim requires at least one output value declared both on the Goldsim side and
on the Fortran side.

Sep. 8, 2004   SCR484

New table from Carol:

[Blank to next page.]

Matrix							
Unsaturated Zone				**Saturated Zone (Alluvium)**			
Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source
matrix porosity	Φ	-	sampled	matrix porosity	Φ	-	sampled
matrix grain density	ρ	kg/m^3	sampled	matrix grain density	ρ	kg/m^3	sampled
matrix pore radius	r	m	sampled	matrix pore radius	r	m	sampled
specific surface area	ssa	m^2/kg	$= \dfrac{3\,\Phi}{\rho\,r}$	specific surface area	ssa	m^2/kg	$= \dfrac{3\,\Phi}{\rho\,r}$
K$_a$	K$_a$	mL/m^2	table lookup	K$_a$	K$_a$	mL/m^2	table lookup
Kd	Kd	m^3/kg	$= K_a\,ssa\,(10^{-6}\,\frac{m^3}{mL})$; or sampled	Kd	Kd	m^3/kg	$= K_a\,ssa\,(10^{-6}\,\frac{m^3}{mL})$
				moisture content	n	kg/m^3	1
				mobile Rd immobile Rd	Rd$_m$ Rd$_i$	m^3/kg	$= 1 + \dfrac{\rho(1-\Phi)}{n}\,Kd$; or sampled
modify Rd to approximate effect of reversibles:							
colloid concentration	Cc	kg/m3	sampled	colloid concentration	Cc	kg/m3	1.0d-03
surface area factor	F	-	590	surface area factor	F	-	590
colloid retardation factor	R$_c$	m3/kg	sampled	colloid retardation factor	R$_c$	m3/kg	sampled
radionuclide partitioning coefficient	K$_0$	-	$= C_c \times F \times Kd$	radionuclide partitioning coefficient	K$_0$	-	$= C_c \times F \times Kd$
effective retardation	R^{eff}	m3/kg	$= (Rd + (K_0 \times R_c)) \div (1 + K_0)$	effective retardation mobile	R$^{eff}_m$	m3/kg	$= (Rd_m + (K_0 \times R_c)) \div (1 + K_0)$
				effective retardation immobile	R$^{eff}_i$	m3/kg	$= Rd_i \div (1.d0 + K_0)$
mass transfer factor		-	0.0d0	mass transfer factor tuff		-	$= 1.0d0 \div (1.0d0 + K_0)$
				mass transfer factor alluvium		-	0.0d0

Fracture							
Unsaturated Zone				**Saturated Zone (Tuff)**			
Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source
specific surface area	ssa	m^2/kg	1	specific surface area	ssa	m^2/kg	1
K_a	K_a	mL/m^2	table lookup	K_a	K_a	mL/m^2	table lookup
Kd	Kd	m^3/kg	$= K_a \, ssa \left(10^{-6} \frac{m^3}{mL}\right)$	Kd	Kd	m^3/kg	$= K_a \, ssa \left(10^{-6} \frac{m^3}{mL}\right)$
fracture aperture	A	m	sampled	fracture aperture	A	m	sampled
Rd	Rd	m^3/kg	$= 1 + \dfrac{2}{A} K_a\,;$ or sampled	mobile RD immobile RD	Rd_m Rd_i	m^3/kg	$= 1 + \dfrac{2}{A} K_a\,;$ or sampled
modify Rd to approximate effect of reversibles:							
colloid concentration	Cc	kg/m3	sampled	colloid concentration	Cc	kg/m3	sampled
surface area factor	F	-	590	surface area factor	F	-	590
colloid retardation factor	R_c	m3/kg	sampled	colloid retardation factor	R_c	m3/kg	sampled
radionuclide partitioning coefficient	K_0	-	$= 2.0d5 \times A \times C_c \times$ $(Rd - 1.0d0)$	radionuclide partitioning coefficient	K_0	-	$= C_c \times F \times Kd$
effective retardation	R^{eff}	m3/kg	$= (Rd + (K_0 \times R_c)) \div$ $(1.0d0 + K_0)$	effective retardation mobile	R^{eff}_m	m3/kg	$= (Rd_m + (K_0 \times R_c)) \div$ $(1 + K_0)$
				effective retardation immobile	R^{eff}_i	m3/kg	1.0d0
mass transfer factor		-	0.0d0	mass transfer factor tuff		-	$= 1.0d0 \div$ $(1.0d0 + K_0)$
				mass transfer factor alluvium		-	0.0d0

Sep. 9, 2004   Uzflow

The following e-mail was received from R. Fedors:

```
I recommend that the testing of the new tpa.inp parameters
GroundSurfaceTemperature and CurrentAnnualPrecipitation should not include
evaluation of net infiltration results when these new parameters are
significantly adjusted. The ITYM code uses  these parameters in its
independent calculation of the maydtbl.dat external file. An inconsistency
likely arises if only the TPA 5.1 parameters of GroundSurfaceTemperature and
CurrentAnnualPrecipitation are changed without changing them in ITYM.

The intent of making the annual average precipitation and temperature at
```

```
start (modern climate) tpa.inp parameters, instead of them being hardcoded
as was previously done, was to make this information available to other
modules. The temperature is used by nfenv and the precipitation is used by a
biosphere module.

Also as part of the SCR 488, the relative humidity calculation for
preclosure was changed. The approximate relative humidity values for the
range of waste package temperatures during the preclosure are:
     Twp=60 C then RH=0.03 (3%)
     Twp=90 C then RH=0.008 (0.8%)
     Twp=97 C then RH=0.0064 (0.64%)

--Randy
```

Sep. 14, 2004 Long term runs for TPA4.1jpd

Modification required for long term runs.

Uz_parms.i limit should be changed from 1001 to 2001.
Maxseismicevents in *exec.f* should be set to 10,000
The format for writing the second column in *ebstrh.dat* in *ebsrel.f* should be changed to f7.0.
The format for writing **ETIME** for *nefii.inp* in **prenefmks**() and **prenefmksa**() should be changed to f10.0.
Wpflow.def should be extended to 1000000 years.
Tefkti.inp should be extended to 1000000 years.
A new module (**climategenerator**()?)should be written to create the *climato2.dat* file on the fly for each realization, by adding appropriate parameters to the tpa.inp file.
Format for writing #**RATES** in *nefmks.f* into *nefii.dis* should be changed to I8.
Parameter **maxnumdis** in *uzft.f* should be set to 999999.

Sept. 24, 2004   ASHREMOB Cross Reference

From Joe Sylvester:

Variable names for **ashremob** subroutine.

Variable Name	Symbol	Reference
abnmassldinth	$S_{ash,out-H} * \exp(-\lambda_r t)$	n/a
abnmassldintl	$S_{ash,out-L} * \exp(-\lambda_r t)$	n/a
anumflowevents	$n_{deplete}$	6.2.1.2
areaasheol(isizeeruptable)	$a_{ash,e}$	Tbl 6-1
areaashflu(isizeeruptable)	$a_{ash,f}$	Tbl 6-1
areabasinfluv	$A_{basin,f}$	Tbl 6-2
areaeolianregion	A_{eolian}	Tbl 6-2
atemp	$tim(1)$	-
ciperghlw(maxntime,43)	$SA_k(t)$	Step 52

29

concentfactoreoli	c_e	eq 6-13
concentfactorfluv	c_f	eq. 6-6
concentfactorinit	c_i	eq 6-4
dcf(maxntime,43)	-	pre-existing (not used)
dcfde(43)	-	pre-existing read in only
dcfinga(43)	-	pre-existing read in only
dcfingp(43)	-	pre-existing read in only
dcfinh(43)	$BR * DCF_k$	step 53
dcfmlk(43)	-	pre-existing read in only
dilutfactoreoli	de	6.2.1.3
dilutfactorfluv	d_f	6.2.1.2
doseinh(maxtime,43)	$DOSE_k(t)$	step 54
durationfluvial	$t_{duration,f}$	6.2.1.2
endtimefluvial	$toe + t_{duration,f}$	
gmashperm2te	$c_{HLW,f}$ (alias)	Tbl 6-1
hlwgmp3toth(maxntime)	$P_{out-H}(t)$	Eq. 2
hlwgmp3totl(maxntime)	$P_{out-L}(t)$	Eq. 4
hlwgpm3eoli(maxntime)	$H_e(t)$	6.2.1
hlwgpm3fluv(maxntime)	$H_f(t)$	6.2.1
hlwgpm3inth(maxntime)	$H_{i-H}(t)$	6.2.1
hlwgpm3intl(maxntime)	$H_{i-L}(t)$	6.2.1
hremiin(maxntime)	$H_{REMI,indoor}(t)$	Eq. 7
hremioff(maxntime)	$H_{REMI,offsite}(t)$	Eq. 8
hremiout(maxntime)	$H_{REMI,outdoor}(t)$	Eq 1
hrmei(maxntime)	$H_{REMI}(t)$	Eq. 9
ireal	TEPHRA realization index	6.2.1
massasheol(isizeeruptable)	$m_{ash,e}$	Tbl 6-1
massashfluv(isizeeruptable)	$m_{ash,f}$	Tbl 6-1
massashinit(isizeeruptable)	$c_{ash,f}$	Tbl 6-1
masshlweol(isizeeruptable)	$m_{HLW,e}$	Tbl 6-1
masshlwfluv(isizeeruptable)	$m_{HLW,f}$	Tbl 6-1
masshlwinit(isizeeruptable	$c_{HLW,f}$	Tbl 6-1

)

massloadashheavy	not used	compatibility w/checkvalues routine
massloadashlight	not used	compatibility w/checkvalues routine
massloadinheavy	$S_{ash,in-H}$	Tbl 6-2
massloadinlight	$S_{ash,in-L}$	Tbl 6-2
massloadoffsite	$S_{offsite}$	eq. 8
massloadoutheavy	$S_{ash,out-H}$	Tbl 6-2
massloadoutlight	$S_{ash,out-L}$	Tbl 6-2
occupancyinheavy	f_{in_H}	Tbl 6-2
occupancyinlight	f_{in_L}	Tbl 6-2
occupancyoffsite	$f_{offsite}$	eq. 8
occupancyout	$f_{in\_H} + f_{in\_L}$	eq. 6-1
occupancyoutheavy	f_{out_H}	6.2.1
occupancyoutlight	f_{out_L}	6.2.1
partmassloadeoli (maxntime)	$S_e(t)$	6.2.1.3
partmassloadfluv (maxntime)	$S_f(t)$	6.2.1.2
pluvswitch		pre-existing
portioneolh	$p_{e-H}(t)$	eq. 3
portioneoll	$p_{e-L}(t)$	eq. 5
portionflvh	$p_{f-H}(t)$	eq. 3
portionflvl	$p_{f-L}(t)$	eq. 5
portioninth	$p_{i-H}(t)$	eq. 3
portionintl	$p_{i-L}(t)$	eq. 5
proporteoli	$p_e(t)$	eq. 6
proportfluv	$p_f(t)$	eq. 6
proportinti	$p_i(t)$	eq. 6
reductionfactor	$\exp(-\lambda_r t)$	multiple referances
reductionfactor	$\exp(-\lambda_r t)$	n/a
reductionrate	λ_r	Tbl 6-2
resuspendabledepthcm	T_r	step 8
resuspendablefraction	$f_r(t)$	6.2.2.1

(maxntime)

rhoash	$\rho_{ash,i}$	step 5
rhoasheol	$\rho_{ash,e}$	Tbl 6-2
tempdnt1(maxntime)	-	used in calculation of $\mathbf{SA_k(t)}$
thickashm(maxntime)	$T_B(t)$ (in meters)	Step 7
thickness	$T_B(t)$ (in meters)	Step 7
thicknesseolcm	-	6.2.1.3
timebetweenflows	T_f	Tbl 6-2
toe	time of event	pre-existing
volashfluv	$v_{ash,f}$	6.2.1.2
volsediment	$v_{sediment,f}$	6.2.1.2
wgtfactoreolian	w_e	6.2.1.3
wgtfactorfluvial	w_f	6.2.1.2
wgtfactorinitial	w_i	6.2.1.1
yieldambsediment	$Y_{sediment,f}$	Tbl 6-2
yieldashfluv	$Y_{ash,f}$	Tbl 6-2

Notes:

Step Y refers to Razvan's pseudo code
Chapter 6 is from the "Risk Analysis for Risk Insights - Progress Report",
CNWRA 2004
"Tbl 6-X" refers to Chapter 6 table
"6.x.y.z" refers to paragraph of Chapter 6
"eq. 6-X" refers to equation from Chapter 6

"eq Z refers to equation in memo:
"Calculation of the Total Airborne Concentration of High-Level Waste for the Ash
Remobilization Model Abstraction"

Sept. 24, 2004   Razvan's Pseudo-Code

Pseudo-Code for Calculating the Airborne Concentration of High-Level Waste at the RMEI Location Through Time

When the AshEvolutionMode flag is set to a value of 1, the following loop is executed:

1.   Sample one of the n realizations of ASHPLUME_P code [$c_{HLW,i}$, $c_{ash,i}$, $m_{HLW,f}$, $m_{ash,f}$, $a_{ash,f}$, $m_{HLW,e}$, $m_{ash,e}$, $a_{ash,e}$], from Table 6_1. The selection is accepted if the index k of the realization wasn't previously selected ($k = 1, n$).

2.   Calculate c_i using eq. 6-4.

3.   Get $S_{ash,out-H}$ from TPA Input file .

4.   Set $\rho_{ash,i}$ = AshBulkDensity[g/cm^3] parameter of ASHRMOVO.

5.   Calculate $T_{B-0} = c_{ash,i} / (\rho_{ash,i} \times 10000)$.

6.   Set λ_B = RelativeRateOfBlanketRemoval[yr^{-1}] parameter of ASHRMOVO.

7.   Calculate $T_B(t) = T_{B-0} \exp(-\lambda_B(t-t_{event}))$.

8.   Get T_R from TPA Input file (parameter name: DepthOfResuspendableLayer[cm]).

9.   If $T_B(t) \leq T_R$ calculate $f_R(t) = T_B(t)/T_R$, else $f_R(t) = 1$.

10.   Get $\lambda_{r(t)}$ from TPA Input file .

11.   Calculate $H_{i-H}(t)$ using eq. 6-2.

12.   Get w_i from TPA Input file.

13.   Get $S_{ash,out-L}$ from TPA Input file .

14.   Calculate $H_{i-L}(t)$ using eq. 6-3.

15.   Get $\rho_{ash,f}$ from TPA Input file.

16.   Calculate $v_{ash,f}$ using eq. 6-8.

17.   Get $Y_{ash,f}$ from TPA Input file.

18.   Calculate $n_{deplete}$ using eq. 6-10.

19.   Get $Y_{sediment,f}$ from TPA Input file.

20.   Get $A_{basin,f}$ from TPA Input file.

21.   Calculate $v_{sediment,f}$ using eq. 6-9.

22.   Calculate d_f using eq. 6-7.

23.   Get T_f from TPA Input file.

24.   Calculate c_f using eq. 6-6.

25.   Calculate $t_{duration,f}$ using eq. 6-11.

26.   Get $S_f(t)$ equal to the
        AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3] parameter
        from TPA Input   file if $t \le t_{duration,f}$, and zero otherwise.

27.   Get w_f from TPA Input file.

28.   Calculate $H_f(t)$, $t \in [t_0 , t_{max}]$, using eq. 6-5.

29.   Get $A_{eolian,e}$ from TPA Input file.

30.   Get $\rho_{ash,e}$ from TPA Input file.

31.   Calculate d_e using eq. 6-14.

32.   Calculate c_e using eq. 6-13.

33.   Get w_e from TPA Input file.

34.   Set $S_e(t=0)$ equal to the
        AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3] parameter
        from TPA Input file .

35.   Get λ_r = RateOfReductionOfMassLoadingFactor[1/yr] from TPA Input file.

36.   Calculate $S_e(t) = S_e(t=0) \, exp(-\lambda_r \, t)$ for $t \in [t_0 , t_{max}]$.

37.   Calculate $H_e(t)$, $t \in [t_0 , t_{max}]$, using eq. 6-12.

38.   Get f_{out-H}, f_{out-L} from TPA Input file.

39.   Calculate $H_{RMEI-outdoor}(t)$, $t \in [t_0 , t_{max}]$, using eq. 6-1.

40.   If $t \le t_{duration}$, $S_f(t) = S_{ash,out-L}$, otherwise $S_f(t) = 0.0$.

41.   Calculate $P_{out\text{-}H}(t)$ using eq. 2 .

42.   Calculate $p_{i\text{-}H}(t)$, $p_{f\text{-}H}(t)$, and $p_{e\text{-}H}(t)$ using eq. 3 .

43.   If $t \leq t_{duration}$, $S_f(t) = S_{ash,out\text{-}L}$, otherwise $S_f(t) = 0.0$.

44.   Calculate $P_{out\text{-}L}(t)$ using eq. 4

45.   Calculate $p_{i\text{-}L}(t)$, $p_{f\text{-}L}(t)$, and $p_{e\text{-}L}(t)$ using eq. 5 .

46.   Calculate $p_i(t)$, $p_f(t)$, and $p_e(t)$ using eq. 6 .

47.   Get $f_{in\text{-}H}$ and $f_{in\text{-}H}$ from TPA Input file.

48.   Calculate $H_{RMEI\text{-}indoor}(t)$, using eq. 7.

49.   Get $f_{offsite}$ and $S_{offsite}$ from TPA Input file.

50.   Calculate $H_{RMEI\text{-}offsite}(t)$ using eq. 8.

51.   Calculate $H_{RMEI}(t)$ using eq. 9.

52.   Let $k = 1$ (1-st radionuclide).

53.   Get $SA_k(t)(Ci/g_{HLW})$ from the INVENT module.

54.   Get $BR \times DCF_k$ from *gs_cb_ad.dat* or *gs_pb_ad.dat* (where BR = breathing rate (m^3/yr), DCF_k = dose conversion factor for inhalation for radionuclide k (rem/Ci))

55.   Calculate the inhalation dose for radionuclide k: $DOSE_k(t) = BR \times DCF_k \times H_{RMEI}(t) \times SA_k(t)$

56.   Let $k = k+1$.

57.   Go to 52. Repeat 52 to 56 until $DOSE_k(t)$ is calculated for all the radionuclides.

58.   Calculate the total inhalation dose: $DOSE(t) = \sum DOSE_k(t)$.

59.   Go to 1 for a new realization.

NOTES:

I.   The first set of parameters sampled at 1. is randomly sampled from the n entries of

Table 6_1.

II.   If $n \geq rmax$, ($rmax$ = total number of realizations), the following *rmax-1* sets are non-repetitively sampled from Table 6_1.

III.   The non-repetitive sampling is ensured by recording for each realization the index value k, and adding it to the list of the previous indices of selected sets of parameters.

IV.   If $n < rmax$, after every n executions of loop 1.-36., the record of indices k is cleared, and the executions of 1.-36. resume and continue as described at I, II, III.

V.   Equations 6-x refer to " Ash Remobilization Modeling for Extrusive Volcanism", and equations 1 to 9 refer to "Calculation of the Total Airborne Concentration of High-Level Waste for the Ash Remobilization Model Abstraction " (Roland, 08/31/04).

Sep. 28, 2004   Matrix - Fracture Kd Rd Table

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Matrix											
Unsaturated Zone				Saturated Zone (Tuff)				Saturated Zone (Alluvium)			
Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source
matrix porosity	Φ	-	sampled	matrix porosity (effective)	Φ	-	sampled	matrix porosity (effective)	Φ	-	sampled for flow calculations
total porosity	Φ_T	-	Not used	total porosity	Φ_T	-	Not used	total porosity	Φ_T	-	sampled
matrix grain density	ρ	kg/m^3	sampled	matrix grain density	ρ	kg/m^3	sampled	matrix grain density	ρ	kg/m^3	Not used
matrix pore radius	r	m	sampled	matrix pore radius	r	m	sampled	matrix pore radius	r	m	Not used
specific surface area	ssa	m^2/kg	$= \dfrac{3\,\Phi}{\rho\,r}$	specific surface area	ssa	m^2/kg	$= \dfrac{3\,\Phi}{\rho\,r}$	specific surface area	ssa	m^2/kg	sampled
K$_a$	K$_a$	mL/m^2	table lookup	K$_a$	K$_a$	mL/m^2	table lookup	K$_a$	K$_a$	mL/m^2	table lookup
Kd	Kd	m^3/kg	$= K_a \times ssa \times$ $(10^{-6}\,\dfrac{m^3}{mL})$; or sampled	Kd	Kd	m^3/kg	$= K_a \times ssa \times$ $(10^{-6}\,\dfrac{m^3}{mL})$	Kd	Kd	m^3/kg	$= K_a \times ssa \times$ $(10^{-6}\,\dfrac{m^3}{mL})$

Matrix											
Unsaturated Zone				**Saturated Zone (Tuff)**				**Saturated Zone (Alluvium)**			
Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source
				moisture content	n	kg/m^3	1	moisture content	n	kg/m^3	1
				mobile Rd immobile Rd	Rd$_m$ Rd$_i$	m^3/kg	$= 1 + \dfrac{\rho(1-\Phi)}{n} Kd;$ or sampled	mobile Rd immobile Rd	Rd$_m$ Rd$_i$	m^3/kg	$= 1 + \dfrac{\rho(1-\Phi_T)}{n} Kd;$ or sampled
modify Rd to approximate effect of reversibles:											
colloid concentration	Cc	kg/m3	sampled	colloid concentration	Cc	kg/m3	1.0d-03	colloid concentration	Cc	kg/m3	1.0d-03
surface area factor	F	-	590	surface area factor	F	-	590	surface area factor	F	-	590
colloid retardation	R$_c$	m3/kg	sampled	colloid retardation factor	R$_c$	m3/kg	sampled	colloid retardation factor	R$_c$	m3/kg	sampled
radionuclide partitioni	K$_0$	-	$= C_c \times F \times Kd$	radionuclide partitioning	K$_0$	-	$= C_c \times F \times Kd$	radionuclide partitioning	K$_0$	-	$= C_c \times F \times Kd$
effective retardation	R^{eff}	m3/kg	$= (Rd + (K_0 \times R_c)) \div (1 + K_0)$	effective retardation mobile	R$^{eff}_m$	m3/kg	$= (Rd_m + (K_0 \times R_c)) \div (1 + K_0)$	effective retardation mobile	R$^{eff}_m$	m3/kg	$= (Rd_m + (K_0 \times R_c)) \div (1 + K_0)$

Matrix											
Unsaturated Zone				**Saturated Zone (Tuff)**				**Saturated Zone (Alluvium)**			
Quantity	**Symbol**	**Units**	**Source**	**Quantity**	**Symbol**	**Units**	**Source**	**Quantity**	**Symbol**	**Units**	**Source**
				effective retardation immobile	R^{eff}_i	m3/kg	$= Rd_i \div (1.d0 + K_0)$	effective retardation immobile	R^{eff}_i	m3/kg	$= Rd_i \div (1.d0 + K_0)$
mass transfer factor		-	0.0d0	mass transfer factor tuff		-	$= 1.0d0 \div (1.0d0 + K_0)$	mass transfer factor tuff		-	$= 1.0d0 \div (1.0d0 + K_0)$
				mass transfer factor alluvium		-	0.0d0	mass transfer factor alluvium		-	0.0d0

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| Fracture | | | | | | | | | | | |
| Unsaturated Zone | | | | Saturated Zone (Tuff) | | | | Saturated Zone (Alluvium) | | | |
Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source
specific surface area	ssa	m^2/kg	1	specific surface area	ssa	m^2/kg	1				
K_a	K_a	mL/m^2	table lookup	K_a	K_a	mL/m^2	table lookup				
Kd	Kd	m^3/kg	$= K_a \times ssa \times (10^{-6}\frac{m^3}{mL})$	Kd	Kd	m^3/kg	$= K_a \times ssa \times (10^{-6}\frac{m^3}{mL})$				
fracture aperture	A	m	sampled	fracture aperture	A	m	sampled				
Rd	Rd	m^3/kg	$=1+\frac{2}{A}K_a;$ or sampled	mobile RD immobile RD	Rd_m Rd_i	m^3/kg	$=1+\frac{2}{A}K_a;$ or sampled				
modify Rd to approximate effect of reversibles:											
colloid concentration	Cc	kg/m3	sampled	colloid concentration	Cc	kg/m3	sampled				
surface area factor	F	-	590	surface area factor	F	-	590				

Fracture											
Unsaturated Zone				**Saturated Zone (Tuff)**				**Saturated Zone (Alluvium)**			
Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source	Quantity	Symbol	Units	Source
colloid retardation factor	R_c	m3/kg	sampled	colloid retardation factor	R_c	m3/kg	sampled				
radionuclide partitioning	K_0	-	$= 2.0d5 \times A \times C_c \times (Rd - 1.0d0)$	radionuclide partitioning coefficient	K_0	-	$= C_c \times F \times Kd$				
effective retardation	R^{eff}	m3/kg	$= (Rd + (K_0 \times R_c)) \div (1.0d0 + K_0)$	effective retardation mobile	R^{eff}_m	m3/kg	$= (Rd_m + (K_0 \times R_c)) \div (1 + K_0)$				
				effective retardation immobile	R^{eff}_i	m3/kg	1.0d0				
mass transfer factor		-	0.0d0	mass transfer factor tuff		-	$= 1.0d0 \div (1.0d0 + K_0)$				
				mass transfer factor alluvium		-	0.0d0				

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Sep 30, 2004   Scientific Notebook

* = Contributing chapters for last 12 months.

1 - Janetzke*
2 - Mohanty
3 - Rice*
4 - Scherer*
5 - Pensado
6 - Benke*
7 - LaPlante
8 - Adams*
9 - Winfrey
10 - Smith
11 - Lozano
12 - Wojcik*
13 - Osidele
14 - open
15 - Menchaca
16 - Portillo*

Nov. 8, 2004

The following e-mail regarding tpa4.1jpdls_beta3 was received from Marty:

```
I have several runs executing in parallel on both spock and idaho and have
done some runtime calculations with the results.

I am running differential analysis runs on Rob's beta3 code.
These are 328 single vector runs, where each subsequent vector has a parameter
incremented by 1% of its range.

It takes an average of 33 minutes per run on spock, which means that the total
run should take more that 7 days (7.52 days).

It takes an average of 23 minutes per run on idaho, which means that the total
run should take more that 5 days (5.24 days).

Jose M. "Marty" Menchaca
```

Nov. 15, 2004   TPA 4.1jpd

The MatrixKd for Cm246 in Chnv layer is 0 which causes NEFTRAN to abort for long simulation runs. Using values of 6000 seems to produce a successful run.

Tim's comment on the unintended behavior of the user defined dilution volume not being present in this version of the code seems not to be correct. TPA 4.1jpd was run on SPOCK and 4.1jp was run on ALBY and both runs show that the problem existed in these versions. The problem is that the user defined dilution volume is not recognized. This was corrected in 4.2q.

Nov. 15, 2004   MatrixKD for Cm

The following e-mail was received from P. Bertetti:

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

e.g. Runde, W. 2000. "The Chemical Interactions of Actinides in the
Environment". In Challenges in Plutonium Science, Vol II. Los Alamos Science,
No. 26. LA-UR-00-4100. Los Alamos, MN: Los Alamos National Laboratory. pp
392-411.
```

Nov. 17, 2004   TPA 4.1jpdls_beta4

Modules that required modification to accommodate more time steps are:

exec.f
Maxntime.i
Nintv.i
Releaset.f
Failt.f
Ebsfilt.f
SIZES.INC

Nov. 18, 2004   TPA 4.1jpdls_beta4

The incremental changes from beta3 to beta4 include:

1. Enabling user defined dilution volume at 3,000 acer-ft/yr (2,676,394 gal/d). Associated with this is the setting of the plume capture model to user defined with a fraction value of 1.0.

2. UZFT Kds for Cm set to the same as those for Am. This increases the number of sampled parameters from 330 to 337.

These changes give a change in results from 35 mrem/yr at 147,210 years to 65 mrem/yr at 148,810 years.

Nov. 29, 2004   SUN f77 V4.2

The SUN f77 V4.2 compiler cannot link the TPA 4.1jpdls_beta4 without causing a runtime error in **zportsh**. The modules link without error, but fail at run time. It was found that *zportunx.f* **zportsh** routine does not work when linked to modules greater than 166,290,903 bytes. This is not an absolute number be fluctuates with time or system resources. Modules larger than this have succeeded intermittently, with some correlation between the size of the module and the failure rate. Modules of size 166,325,463 fail the **zportsh** routine regularly. When the n3 parameter in '*reflux2.i*' include file is adjusted to alter the size of the *nfenv.o* file the failure mode can be induced (n3>767,600) or removed (n3<767,500). Values "in between" have intermittent success.   The behavior is typical of **scratchy1** but not exhibited on **spock**. This is apparently only a limitation when the system call is used since *releaset.e* runs OK even though it is 4 times larger than this configuration, but does not use **zportsh** calls.

Dec. 1, 2004   TPA4.1jpdls

The starting point for this version was V4.1jpd. The first cut at long term simulations was prepared by R. Rice and was stored on ALBY as tpa41jpdls on 10-

13-04.

Original version	Resulting version	Date	Files changed.
tpa41jpdls	tpa41jpdls_beta	10-28-04	automake.fig exec.f maxntime.i nintv.i tpa.inp uzft.f ebsfilt.f failt.v releaset.f sizes.in climato2.dat
tpa41jpdls_beta	tpa41jpdls_beta3	10-29-04	automake.fig exec.f nfenv.f tpa.inp tpanames.dbs
tpa41jpdls_beta3	tpa41jpdls_beta4	11-15-04	dcagw.f exec.f tpa.inp

Dec. 10, 2004   tpa.inp Parameters

The following was sent to R. Rice via e-mail.

```
Rob,

Here are my findings on the tpa.inp parameters.

1. AlluviumMatrixRD_SAV_Ni : Turner mentioned you may already have the
reference for this -  "Summary and Synthesis Report on Radionuclide
Retardation for the Yucca Mountain Site Characterization Project", Table 59,
```

page 175.

2. InnerDeltaEcritInh : Pensado is the source and the justification is that the base case does not take credit for the inner container.

3. OuterDeltaEcritInh : Pensado is the source, referencing a report in preparation "Passive and Localized Corrosion of Overpack Materials - Modeling and Experiments".

4. WeldDeltaEcritInh : Same as 3.

5. GapFractionForC14 : VJ says this really means "GapAndGrainBoundaryFraction", am waiting for a reference. Says that Mohanty said this is not an important parameter for the compliance period.

6. ArealMassLoading : This parameter is no longer in the tpa.inp file, but is calculated on the fly as a module variable.

7. EmissivityOfBackfill : Adams is the source and says that this value should be the same as EmissivityOfDriftWall (0.9) under the assumption that backfill is made up of former drift wall material.

8. FlagSeepageThreshold : Pensado is the source and the justification is that, use of the new model represents the current thinking of the staff.

9. SeepageThresholdT : Same as 8 with a value of 100.

10. SelectThermalModel : Adams is the source and thermal model 1 is selected to match the model used in TPA 4.1jpd.

Jan. 21, 2005   Some Definitions.

From Wes.

.   The Technical Operating Procedure (TOP)-018 on "Development and Control of Engineering and Scientific Software" defines software validation as a process that "Provides evidence of correct and successful implementation of the underlying theory and algorithms as outlined in the Software Requirements Description, Software Change Report, or other relevant documentation, such as user's manuals for acquired software. Software validation is a software testing process that is distinct from model validation."

2.   The TOP-018 definition of software validation is consistent with that provided in NUREG/BR-0167, which it cites. Namely, "the process of evaluating a software product at the end of the development process to ensure compliance with software requirements." NUREG-0856 provides a general definition as "assurance that a computer code correctly performs the operations specified in the numerical model." Thus, the definition used in

```
TOP-018 and described in the YM Team presentation is consistent with NRC
regulatory guidance.  Its clear aim is to test and assure that the
software-in layman's terms-does the arithmetic right.
```

```
3.    Model validation is a separate matter, per TOP-018 and as the term
is generally used in the profession.  TOP-018 defines model validation as
the "process of assuring that a mathematical model as embodied in a computer
code (software) is an adequate representation of the process or phenomenon
for the purpose for which it is intended."
```

```
4.    The TOP-018 definition of model validation is consistent with that
provided in NUREG-0856, which it cites.  Namely, "assurance that a model as
embodied in a computer code is a correct representation of the process or
system for which it is intended."  [Note that "correct" was replaced with
"adequate" in TOP-018 to avoid any implication that NRC requires a valid
model to be absolutely accurate.  A model needs only to be adequate or
sufficient for regulatory purposes.]  Thus, the definition used in TOP-018
is consistent with NRC regulatory guidance.  Its clear aim is to test and
assure that the actual model-the mathematical representation of the
real-world process or system-reasonably/adequately represents that
real-world process or system.
```

Jan. 24, 2005   Nuclides.dat

The following e-mail was received from O. Povetko:

```
According to DOE report, t=25 yrs corresponds to 2033 and the SNF parameters
were defined based on 84000 MTU baseline. In other words, it was
conservatively assumed that the average fuel was discharged from the reactor
at 2008 and emplaced at 2033. These inventories corresponding to the year
2033 are in nuclides.dat. For the bounding fuel, it's 2028 and 2033,
respectively.  If licensees' extensions are issued utilities may send to
repository younger fuel instead of the older one that has  been accounted
for in DOE estimates. In this case we will need to update nuclides.dat based
on newer information.

Oleg.
```

Jan. 26, 2005   VOLCANO

B. Hill has suggested to fail the intrusive failures with the extrusive ones until the number of WPs in a subarea is reached. Failures beyond this are assumed to be

extrusive only and their complement (i.e. the number remaining in subarea after the drift failures have been subtracted) is not subtracted from those remaining in the subarea. For the distribution model the range of failures remaining in drift should be normalized to a maximum of 9,445 packages based on a total repository package count of 11,184.

The model fails the ejected packages and makes them available to the direct release algorithm, but does not remove them from the repository for ground water calculations and treats them as 'failed in drift'. In this sense the ejected packages are double counted, but B. Hill posits that this is insignificant compared to the direct release dose.

A check of the volcanic failures for the event subarea can be made with:

(FailedInDriftFactor*nwpinsa + nejected)*[(nwpinsa-InititalFailures)/nwpinsa] should equal the number of volcanic failures printed to the screen.

Feb. 1, 2005   GENTPA

A summary of a discussion with P. LaPlante:

The modeling of different age groups will be retained. However, parameters for groups 1-4 may be deleted from the tpa.inp file. It is possible that groups 5 and 6 will be compared during some future analysis, so it is suggested to keep group 5 in the tpa.inp file (possibly commented out). This will leave the logic in place for the analyst to use the other age groups at some later time. It will be the analyst responsibility to provide justification for the parameters at that time.

Feb. 2, 2005 SNLLHS

Alpha and beta parameters must be greater than 0.5 and less than 22.

Feb. 7, 2005   Repository time line.

The following was considered during SCR553.

```
Ideally the code should have independent controls for the following to permit
a complete barrier analysis:

1.  Active ventilation stop time (0-100 years assuming no backfill) relative
to WP emplacement time.
2.  Passive ventilation start/stop time (0-100 years assuming no backfill)
relative to WP emplacement time.
3.  Drip shield emplacement time (0-100 years) relative to WP emplacement
time, with a way to disable the DS corrosion model.
4.  Engineered backfill emplacement time (0-100 years) relative to WP
emplacement time .
5.  Enabling/disabling the natural backfill model.
```

Feb. 11, 2005   NFENV   tempin, tempsf

The following e-mail was received form G. Adams:

```
I left the code in Nfenv.f to calculate tempin,  the waste package inner wall
temperature and tempsf, maximum spent fuel temperature.  The tempsf array is
passed back to exec.f, but doesn't get printed anywhere or sent to any output.
The tempin value is only an intermediate result within nfenv, and also doesn't
get printed anywhere.

George
```

Feb. 13, 2005   UNIX2DOS

Unix2dos on ALBY: does not take source file names longer than 8.3 format.

Feb. 18, 2005   SCR530

Rob's files for long simulations are on GRYPHON at

d:\rrice\tpa500f_ls2\modified_files

and

d:\rrice\tpa500f_ls2\AAA_scientific_notebook.

Feb. 18, 2005 NEFTRAN

T. McCartin called to say he would prefer a flag for SZ to run normal NEFMKS or alternatively to run each leg with a separate NEFMKS run.   In the latter case he would also want a switch for each leg to select which legs to run individually. This would involve reformatting the *nefii.dis* file of the first leg run to look like *sotnef.dat* for input to the second or subsequent leg run. When running the SAV layer as a single leg a mixing zone leg of 50 meters with properties of the SAV layer should be added.   Three routines SZFT, SZSTFF, and SZSAV may be needed to handle the three cases. This mechanism may also help in UZFT where leg-to-leg transfer is turned off by matrix diffusion.

Mar. 7, 2005   DSFAIL

Notice was given to C. Grossman that the current version of the TPA code has the **mechfail** model that accounts for WP failure due to drip shield impingement, and that a version that includes temperature dependent material properties for the drip shield is under development for later use.

Mar. 9, 2005   C-14 parameters

The following e-mail was received form Marty Menchaca:

Here is the list of the C-14 related parameters that I deleted from TPA 5.0.0l.

RadiusOfSFGrain[m]
SubGrainFragmentRadiusAfterTransFrac[m]
ThicknessOfCladding[m]
SFC-14InventoryPerKgSF[ci]
CladC-14InventoryPerKgSF[ci]
ZyrOxideAndCrudC-14InvPerKgSF[ci]
GapAndGrainBoundaryInventoryPerKgSF[ci]

Mar. 10, 2005   Long Simulations. TPA V5.0.0n

Modules that required modification to accommodate more long simulations are:

exec.f
Maxntime.i
Nintv.i
SIZES.INC
uz_parms.i
Uzft.f
Seisadj.i
Reflux2.i
Failtadj.i
Nefmks.f
Nvenv.f
Reader.f

Data file changes:
tpa.inp
climato2.dat
wpflow.def
tpanames.dbs

Mar. 15, 2005 Long Simulations

Files that can retain small arrays if large number of times steps are not required are:

exec.f: kMaxTimeSteps = 501
exec.f: kMaxVectors = 1024
nintv.i: nintv = 2000
reflux2.i: n3 = 100000
uzft.f: maxnumdis = 99999

Mar. 31, 2005   Infilper.res

A note about file *infilper.res*. The data column headed with "avinfil [mm/yr]" is the total volumetric flow for all analyzed subareas divided by the total area for the analyzed subareas. The first value at time 0.0 will match the *tpa.inp* value of "areal average mean annual infiltration at start" only if the *climato2.dat* file has the first two values as 0.0 (so the interpolation will give a 0.0 value at time 0.0), and all the subareas are analyzed.

Mar. 31, 2005 Scientific Notebook

* = Contributing chapters for last 6 months.

1 - Janetzke*
2 - Mohanty
3 - Rice*
4 - Scherer*
5 - Pensado
6 - Benke*
7 - LaPlante
8 - Adams*
9 - Winfrey*
10 - Smith
11 - Lozano
12 - Wojcik*
13 - Osidele
14 - open
15 - Menchaca*
16 - Portillo
18 - LeNeveu*
19 - Nes

April 5, 2005   Appendix B - Auxiliary files

The following e-mail was sent to B. Winfrey.

```
Brandi,

FILENAME.DAT is OK.  It is the same one that was used in the validation of TPA
5.0s.

ia.dat is OK.  This is a special non-base case file that needs to be
configured manually for each sensitivity run.

repdes.dat is OK.  Data is from DOE via Britt Hill.  The file has been tested
under SCR 560.

tpanames.dbs is OK.  This is actually a hybrid file (both intermediate and
user supplied), and is modified at the users discretion.
```

April 6, 2005   Releaset.f runtimes.

The new releaset module from R. Codell that handles time dependent Fwet values takes about 1.2 minutes per realization for the base case. The old version took about 0.5 seconds per realization.

April 7, 2005   *TPA.INP* Scrub

A possible technique for scrubbing the *tpa.inp* parameters is:

1) list the occurrences of **ispquery()**.

2) the associated arguments should exist in a list of ***valuesp()** occurrences.

3) each *tpa.inp* parameter that is fully specified in the code as a completed character string should also exist in a list made from the **ispquery()** occurrences. Parameter names generated at run time will need to be checked manually.

The actual usage of a parameter during a run can be found in *spquery.tpa*.

A script to create a utility command file may be able to be created using repeated

53

lines like:

```
echo 'cat tpa50/exec.f |grep -i "[a-z]density"; echo echo'
echo echo; echo above line
```

By echoing the first line a marker will be placed in the output for the file currently being processed (or last processed).

April 8, 2005   Software Validation Test Plan (SVTP) TPA 5.0.1

The SVTP for 5.0.1 is contained in SCR548.

April 15, 2005   Glass WP

WP with glass waste form will comprise 50% of emplaced waste by volume. Each will contain 5 glass logs, which are about 2' in diameter and 10' long. Glas waste form does not have Am or PU radionuclides. Glass loses dimensional stability at 450C.

April, 21, 2005   TPA Rework

In addition to lack of input from T. McCartin on the new NEFMKS handler the changes specified in the following e-mail from P. LaPlante will cause code rework and a slip in schedule.

```
I talked to Ron and he has already implemented the changes to the code. In my
original note I may have overstated the case when I said we were "doing away
with" the capability to conduct age-dependent dose calculations. We have
currently maintained most of the code as before but have made mainly cosmetic
and simple changes to remove the age-dependent portions from view in order to
make the ICRP 72 implementation more transparent (to avoid confusing non
institutional memory-based users). Although the changes were somewhat
superficial, we did have to change the code from expecting the approx 50
additional input parameters associated with pre-adult age groups and these
parameters were marked as "comment lines" in tpa.inp (you still see them but
they are not functional unless the comment is removed). Thus, as now
implemented, the last round of changes would require a small code change to
bring back the full compliment of age-groups and some editing of tpa.inp.  So
```

```
if there is a desire to have the full age-dependent functionality in the code
without doing any code changes (I'll assume from the response that is what is
desired) then we need to change it back to the way it was.

I will now start drafting a new SCR to reverse all the code and tpa.inp
changes that impact the age-dependent functionality so that part of the code
looks and functions the way it was when we started and Ron can go back and
make the changes.  I will send the new SCR when it is ready to all interested
for another review prior to beginning the work again.
```

April 29, 2005   Subareas

The minimum roundoff error in "Total Buried Waste" (as listed in the screen print) is obtained when the subarea edges are slightly outward from the emplacement block edges when they are nearly co-linear.

April 29, 2005   Ventilation

The following e-mail was received from G. Ofoegbu:

```
Let's not over-use the term "passive ventilation".

DOE's current repository design calls for a preclosure/operational period of 100 yr, which
includes an initial 50-yr period during which forced ventilation (air flow of 15 m^3/s through
the emplacement drifts) will be used to control the thermal load. DOE has not defined any
ventilation for the second 50 yr period. The emplacement drifts (in fact, all the underground
openings) will be maintained during the 100 yr period to satisfy applicable regulatory
requirements. The term "passive ventilation" has now "crept in" to describe the second 50 yr
period, but DOE actually has not provided any definition of such ventilation (to the best of my
knowledge).

Regarding the invert structural system, DOE does not take any credit, therefore does not provide
any estimates, for any properties of the system beyond permanent closure. Any assumption of any
property, therefore, has to be justified by whoever makes the assumption. I think is better to
honor the DOE choice of not taking any credit for the invert structural system beyond permanent
closure.

gio
```

May 5, 2005   Glass Waste Form

The following e-mail was received from O. Povetko:

```
Shorter WPs can be included by approximate normalization to 5.2 m length.
```

```
CDSP WPs contain DSNF waste and HLW glass.
Mass of HLW in glass form: 4,667 MTHM or 6.67% of the total 70,000 MTHM in
repository.
(If Ron suggestion is realized then FractionOfRepositoryWasteInGlassForm
parameter should be < 0.067)
Mass of DSNF:2,333 MTHM.
Mass of DSNF and HLW combined: ~7000 MTHM.
Number of Long (~5.2 m) CDSP WPs: 1369
Number of Short (~3.6 m) CDSP WPs: 2109

Mass of BWR in 44-BWR AP WP: ~ 8.8 MTHM
Number of 44-BWR AP WPs: 2831

Mass of PWR in 21-PWR AP WP: ~ 10 MTHM
Number of 21-PWR AP WPs: 4299

Average mass in CSNF WPs: (8.8*2831+10*4299)/(2831+4299)=9.5 MTHM

These WP types represent 94% of the total WPs by number, so the other types of
WPs ( ~ 630 WPs) may be neglected for this task.
If Short WPs are normalized by (5.2/3.6=1.44), then number of normalized CDSP
WPs: 1369+2109/1.44=2834
Average mass in normalized CDSP WP: (7000/2834=2.47 MTHM)

Total number of these normalized representative WPs:1369+1465+2831+4299=9964
Average payload for these WPs: (2.47*2834+8.8*2831+10*4299)/9964=7.5 MTHM per
normalized 5.2m long WP.

Oleg.
```

May 9, 2005   TPA stats.

The following e-mail was received from C. Scherer:

```
I ran a 430 realization run at 100,000 years with all files appended on
spock over the weekend.  It ran to completion, but it used up 7.1 G for file
space.
```

May 19, 2005   TPA 5.0.1beta at NRC

The following e-mail was received from C. Grossman:

```
I got the code to run by placing it in a directory closer to the root.  The
pathname lenght must have a limit.
```

This error was not reproducible on ALBY.

May 19, 2005   IDAHO Base Case Run

The following script can be submitted using the **qsub** command for a base case run on IDAHO.

```
date

setenv TPA_TEST ~/tpa501beta
setenv TPA_DATA ~/tpa501beta
setenv TPA_RUN coso350r6a10y

mkdir  /var/tmp/rwj
cd  /var/tmp/rwj
mkdir $TPA_RUN
cd $TPA_RUN
/bin/rm -r *

touch $TPA_RUN.out
hostname >>$TPA_RUN.out
date >>$TPA_RUN.out
pwd >>$TPA_RUN.out

cp ~/$TPA_RUN/tpa.inp tpa.inp
(time $TPA_TEST/tpa.e >tpa.out) | tee >> $TPA_RUN.out

date >>$TPA_RUN.out

/bin/rm *.e
gzip -r *
gzip -d $TPA_RUN.out.gz
cp * ~/$TPA_RUN
/bin/rm -r *
date
```

May 26, 2005   Inhalation files for SCR568.

Three output files are requested in conjunction with the implementation of the *ashremob.f* module.

1) A time history of the inhalation dose from each nuclide for each realization.
2) A time history of the total inhalation dose for each realization.
3) A log of peak total dose, including both ground water and inhalation pathways, for each realization.

Files 1 & 2 can use existing files (1 - *rgnsr.tpa*; 2 - *rgssr.tpa*) for the desired output. Even though the files were designed for use with the *dcags.f.* module, they can also be used here since the output array from the *ashremob.f* module contains only inhalation data. The files will continue to also be used with the *dcags.f* module as well, since in that case the *dcags.f* module returns the same array with both ingestion and inhalation quantities. The **dcags** and **ashremob** modes are mutually exclusive and will not have to compete for access to the same files.

File 3 will need to be designed and developed as a new file (*totpkdos.res*) and have a structure similar to the *airpkdos.res*.

May 31, 2005 Appendix B files

The following is from B. Winfrey:

```
data files for Appendix B are located at S:\bwinfrey\Appendix B


These files include the spreadsheet updates that I received as
well.  If the file did not need to be updated, I did not put it
in this directory.  It only includes new files that were turned
in. ... the only files I have not received are from P. LaPlante
and D. Farrell (dilution.dat - he did stop
by and say that there were no new changes to this file).
```

May 31, 2005   Colloid Enhancement Factors

The following was received from D. Pickett discussing the Colloid release calculations using the release factors and their relationship to the solubility limits:

```
And the solubility enhancement will be tied to the release factor itself,
e.g., if release factor is 0.9, then solubility limit (SL) is boosted 10X; if
0.85, then 6.7.  We don't need to worry about the cases where release is not
solubility-controlled.  In all cases below the "enhanced" SL, dissolved
concentration is lower than what it would be without colloids, but that's just
the way the model was conceived.  At least, with the enhancement, in the zone
where the congruent concentration is between the "real" and "enhanced" SLs,
the dissolved concentration can be as high as the "real" SL.
```

June 7, 2005   SZFT.F

The following from T. McCartin gives the fix for a poorly formatted nefiialluv.inp file:

```
Correction is to replace "0.0" in line 6439 of SZFT.f with "0"
```

June 14, 2005   TPA5.0.1betaB

Run time on SPOCK was 12 hours for 350 base case realizations.

June 17, 2005   SZFT Separate Runs vs. One for SZ

The follwoing is from T. McCartin:

```
 there is no reason to believe one solution over the other (the split is just
 a potentially more efficient way to do the calculation for some cases).  I
 would suggest that a 5-10% difference is accepatable - it would be great if
 the difference were on the order of 1-2%. One important aspect is the TPA time
 step for passing the releases could be the largest contributor to any
 difference.
```

June 21, 2005   Courant Number

TPA 5.0.1betaB with modified courant number set at 0.15, ran to completion with the base case nuclides for 350 realizations, 500k years, and 500 post compliance time steps.

July 5, 2005   MECHFAIL

The following is an e-mail from G. Adams:

```
1)      From file pkmndose.res (Note: The time column is the same for all
```

realizations. This is not correct, but I'm concerned about the dose column.),
realizations 2 and 93 show high peak mean doses. Also, from file wpsfail.res,
realizations 2 and 93 show large numbers of waste package failures due to
mechanical failure (the seismic column is indicating all mechanical failures
both from degradation and seismicity).

2)   File pkmndose.res, realization 27 shows a very low peak mean dose,
and file wpsfail.res, realization 27 shows a large number of waste package
failures due to mechanical failure. I haven't looked further into this to
understand why this is the case.

3)   I looked further at realization 2. The screen.txt file shows the
output from the single realization. Subareas 2, 3, and 6 show mechanical
failure of waste packages. For subareas 2 and 6, grid element 2 (15% of the
subarea) has the failures and for subarea 3, grid element 1(85% of the
subarea) has the failures. I show the results in the attached spreadsheet.
The value of "No" in the right-most column indicates that you would expect to
see the waste package failures, and they occur as shown in the screen output
for the times (to the nearest tpa time step) expected. From what I see, waste
package failures are occurring at low bulking factors. Currently the sample
range for bulking factors is uniform: 1.15 to 1.25 for both grid elements.
Formerly, it was 1.15 to 1.50 for grid element 1(lithophysal) and 1.35 to 1.50
for grid element 2 (nonlithophysal). Also, the fraction of the subarea that
is lithophysal was increased from 0.75 to 0.85 (I don't know that this change
has had any significant effect on the number of mechanical failures.)

4)   From what I'm seeing so far in the spreadsheet and with these
results, it appears to me that the change to smaller values for bulking factor
that we currently have in tpa.inp are contributing to higher mechanical
failures of the waste package. I was expecting a relationship to degradation
time, but it isn't apparent to me in the results for realization 2. To
understand all of this better, I'm planning to look at holding the degradation
time to its maximum of 1000 years and varying the bulking factors to see the
effect on mechanical failures. The results for realization 2 that I have so
far are for a single contact angle of 25.4 degrees. I was also going to look
at the effect of varying the contact angle but this effect has to be seen
across separate realizations instead of separate subareas.

5)   Even with the mechanical failure of the waste packages, realization
27 shows something that I need to look at further. Since a large number of
waste packages failed, but the peak mean dose was low, there is something else
outside of mechfail that is involved as well.

July 7, 2005   Drift Degradation

The following e-mail note was received from G. Adams regarding TPA 5.0.1beta:

The Max_MeanDoseAngle.xls file shows the amount that the dose (peak dose and
mean dose) changes as the contact angle is varied from 0 to 45 degrees. These
distribution parameters for contact angle haven't changed. Frank is working
on the effect of bulking factor in which the distribution values have changed

```
from what they were before.  A contact angle of 0 degrees shows only corrosion
failures, 22.5 degrees shows some mechanical failures as well, and a contact
angle of 45 degrees shows mostly mechanical failures of the wp.



The DegradationRateSensitivity.xls file shows the following (from the column
WP Mechanical Failures Occur (Y or N):

1)       At contact angles at or below 20 degrees, there will be no mechanical
wp failures regardless of the values for buckling load, bulking factor, or
degradation time (for the distributions in tpa.inp).

2)       Regardless of the contact angle, there will be no mechanical wp
failures for buckling loads at or above 125000 kg/m regardless of the bulking
factor or degradation time.

3)       No waste package failures occur at bulking factors of 1.21 or greater
regardless of the degradation time, buckling load or contact angle.



Frank is going to add the dose and wp failure sensitivity relationship to
bulking factor.



Previously, the bulking factor ranged from 1.15 to 1.50 for grid element 1 and
1.35 to 1.50 for grid element 2.  It now ranges from 1.15 to 1.25 for both
grid elements.  This input parameter change may be the greatest contributor to
the increased waste package mechanical failures.
```

July 13, 2005   SCR572   burnup.dat

This is an **excel** table that show the conversion of the *burnup.dat* values from the 7.89 MTU/package case to the 5.75 MTU/package case with the use of a 1.37217 factor. The original values <u>follow</u> the new values.

Time	bwr	pwr
1	8666.656	16007.69
2	4993.886	8725.222
3	3452.021	5661.765
5	2260.426	3331.51
10	1593.674	2124.147
15	1388.692	1796.402
20	1252.413	1597.052
25	1132.735	1432.657
30	1043.49	1310.98

61

50	755.1648	934.9177
100	408.1607	495.7845
200	225.2542	268.6157
300	173.7836	205.8824
500	125.5792	147.7668
1000	71.91241	83.00618
2000	37.62872	41.91981
5000	23.85442	26.03939
10000	17.05174	18.70736
20000	9.809821	10.87415
50000	3.492567	3.93857
100000	1.381935	1.586916
200000	0.873423	1.025695
500000	0.719687	0.84842
1000000	0.515269	0.605596
1	6316.022	11665.97
2	3639.408	6358.704
3	2515.739	4126.14
5	1647.337	2427.913
10	1161.426	1548.021
15	1012.041	1309.169
20	912.7247	1163.888
25	825.506	1044.081
30	760.4671	955.4061
50	550.3435	681.3424
100	297.4563	361.3142
200	164.1591	195.7598
300	126.6488	150.0414
500	91.51871	107.6884
1000	52.4078	60.49264
2000	27.42278	30.55001
5000	17.38445	18.97679
10000	12.42685	13.63342
20000	7.14913	7.924782
50000	2.545287	2.870322
100000	1.007116	1.156501
200000	0.636527	0.747499
500000	0.524488	0.618305
1000000	0.375514	0.441342

Note that to be consistent, changing the glass fraction in *tpa.inp* may also require a change to the values in *burnup.dat* in this manner.

July 14, 2005   Subarea Meeting

Action items from today's meeting.

My list of action items is:

1) Make sure Aug 18 presentation covers why 100% of the drift collapses in < 10K years. Also, give details of how the mechfail failure periods differ per subarea.

2) For Aug 4, explain why a detailed volcano model is used.

3) Explore the idea of putting the subarea coordinates in a data file.

4) Remove tpa.inp parameters for subareas 9 & 10.

5) Clarify the need for having multiple SFWettedFraction_SEISMO1-4_# parameters since they are independent of water contact mode (bathtub/flow through).

Bret's list is:

1) Describe the temperature effects of different subarea configurations.

2) Determine if subareas should reflect lith and non-lith abundance.

3) Schedule a climate presentation (add to flow & seepage?)

4) Cleanup tpa.inp.

5) Subdivide subarea 3.

6) Justify parameters values for new subareas (7,8,9).

July 15, 2005   TPA 5.0.1betaE Announcement

```
All,

Version 5.0.1betaE of TPA is now on the shared drive.   This version addresses
three items: 1) the implementation of the last step in converting the original
colloid release mechanism to one where the colloidal release is accounted for
by an effective increase in solubility, 2) the glass fraction and other glass
parameters were changed to the latest DOE values [this required the
reinstatement of subareas 7 & 8 to accommodate the increased number of glass
waste packages], and 3) the "direct release only" mode now copies all the
files it requires, when the ash evolution mode is set to 1.

Note that while we were changing the glass parameters we took the opportunity
to clarify the name of a related parameter.  WastePackagePayload[MTU] is meant
to mean the payload of a spent fuel package, so the name was changed to
SpentFuelWastePackagePayload[MTU].  For releaset,  all waste package failure
types are apportioned between the spent fuel and glass packages.  The glass
fraction parameter retains its meaning of 'fraction of the total MTU
inventory'.

It is requested that Team #8 add a test to their validation suite to check the
number of waste packages assigned to each failure type for both the spent fuel
and glass in the ebsrel.inp input file, and to add a test that checks both the
aqueous and colloidal TPA release rates relative to the raw release rates
obtained from releaset.
```

July 20, 2005   TPA Results Comparison

The following report is from Rob Rice:

(Blank to next page)

TPA 4.1j   **TPA 5.0.1betaD**

Peak Expected Dose

0.021 mrem/yr at 9,769 yr   106 mrem/yr at 9,543 yr
(basecase, 350 realizations, 10,000 yr)   (basecase, 1024 realizations, 10,000 yr)

% Peak Expected Dose

Tc-99	**51.90%**	**Pu-239**	**50.20%**
I-129	**25.43%**	**Pu-240**	**38.67%**
Np-237	**20.43%**	**Am-243**	**8.63%**
Cl-36	0.13%	Tc-99	0.99%
Se-79	0.02%	I-129	0.80%
		Cm-245	0.19%
		Am-241	0.18%
		U-234	0.10%
		Th-230	0.06%
		Np-237	0.05%
		Cm-246	0.03%
		Se-79	0.02%
		U-238	0.02%
		Cl-36	0.01%
		U-233	0.01%

Simulation Time Effect on Peak Expected Dose

10,000 yrs: 0.021 mrem/yr at 9,769 yr   available results: 10,000 yr; 100,000 yr;
100,000 yr: 9.9 mrem/yr at 100,000 yr   and 1,000,000 yr simulations give similar
                                             results (i.e., ~100 mrem/yr at ~10,000 yr)

WP failures

only initial defective WPs in 10,000 yr   initial, seismic, corrosion (localized),
(average = 0.5% of all WPs)   weld
WP corrosion failures 40,000 - 100,000 yr   **initial:** average =   0.5% of all WPs
                                             seismic: average =   12.5% of all WPs
                                                                        at 762 yrs
                                                                        (325 to 1,562 yr)
                                             corrosion: average =   5.7% of all
                                                                        WPs
                                                                        at 1,092 yrs
                                                                        (515 to 3,227 yr)
                                             weld: average =   26% of subarea
                                                                        calculations
                                                                        at 1,153 yrs
                                                                        (475 to 6,040 yrs)

65

In addition to the 5.7% corrosion failures
For 1,000,000 yr/350 realizations:
0.1% realizations (all subareas in 1
realization) have WP corrosion failure
from 47,000 to 57,000 yr; and 0.1% of
subareas (6 subareas) have WP corrosion
failure from 640,000 to 900,000 yr. There
are no corrosion failures in all other cases
for 1,000,000 yrs.

WP Failure Effect on Peak Expected Dose

no effect (only initial defective WP failures
in 10,000 yr)

basecase: 106 mrem/yr at 9,107 yr

w/o irrev*:   3.1 mrem/yr at 2,863 yr
                 (34x less)

w/o corr*:   51.2 mrem/yr at 10,000 yr
                 (52% decrease)

w/o seis*:   79.3 mrem/yr at 9,543 yr
                 (25% decrease)

w/o weld*:   91.7 mrem/yr at 8,896 yr
                 (13% decrease)

Also,
only initial*:   0.052 mrem/yr at 2,796 yr
(i.e., w/o irrev/corr/seis/weld)   (2,040x less)
Note: I129 (65%); Tc99 (33%); Cl36 (1%)
contribute to this peak. (matches TPA4.1j)

only initial/irrev*:   2.6 mrem/yr at 10,000
yr

(i.e., w/o corr/seis/weld) (50x more)

w/o irrev/corr*: same as w/o irrev

w/o seis/weld*: 63.8 mrem/yr at 9,322 yr

(* = all other settings are basecase)

Individual Realization Effect on Peak Expected Dose

1% of realizations (10/1,024) constitute 90%
of Peak Expected Dose (1 realization
contributes to 50% o Peak Expected Dose at
~50 rem/yr)

Drip Shield Failure Time

sampled parameter (lognormal distribution)   calculated with "dsfail"
mean = 7,422 yr (2,700 to 20,400 yr)   mean = 1,036 yr (658 to 1,131 yr)

Climate Data (in "climato2.dat")

100,000 yr climate cycle (symmetric)   no repeating cycles/not symmetric/varying
                                               relative maximums/minimums with varying
                                               durations during 1,000,000 yrs

Flow of Water into WP

determined from "ebsflo.dat" and   determined from "ebsflo.dat" and
multiplicative constant factors for   multiplicative time dependent factors for
Fmult, Fow, and flowfactor   Fmult and Fow; also using time varying
                                     factors for the drip shield and the weld;
                                     flowfactor is still constant (note: also
                                     applying a time varying sawet factor that is
                                     specified in "wpflow.dat")

Retardation Factors - SAV

(minimum; average; maximum)   (minimum; average; maximum)
Pu (500; 24,000; 300,000)   Pu (500; 13,0 00; 62,000)
Am (8E+04; 8E+08; 7E+10)   Am (1.7E+05; 5E+8; 8E+09)
                                   Colloid Rd Factor (1; 500; 5,000)

Volcanism - Conditional Peak Expected Dose

	(with ASHREMOB)	Previous Model
100 yr: 230,000 mrem/yr	100 yr: 2,340 mrem/yr (all ~100x less)	5,920 mrem/yr
500 yr: 110,000 mrem/yr	500 yr: 1,230 mrem/yr	2,840 mrem/yr
1,000 yr: 60,000 mrem/yr	1,000 yr: 790 mrem/yr	1,760 mrem/yr
5,000 yr: 25,000 mrem/yr	5,000 yr: 360 mrem/yr	737 mrem/yr

(note: new ASHREMOB model that assumes
inhalation pathway dominates [RARI Report]

Number of WPs in Repository/Subareas

```
==================================          =====================================
    exec: Welcome to TPA Version 4.1j           exec: Welcome to TPA Version 5.0.1betaD
    Job started: Thu Jul 14 07:22:03 2005       Job started: Wed Jul 06 16:03:12 2005
==================================          =====================================
REPOSITORY DESIGN INFORMATION               REPOSITORY DESIGN INFORMATION
Subarea  Area    Waste  Number of WP        Subarea   Area     Waste  Number of WP
  #    [m^2]     [MTU]                        #    [m^2]      [MTU]
  1   723591.3  11479.9      1455             1   224091.0   4150.1      526
  2   784763.0  12371.5      1568             2   448476.0   8379.2     1062
  3   390372.0   6114.8       775             3  2621741.5  41959.0     5318
  4   207581.3   3361.1       426             4   152357.0   2706.3      343
  5   378972.8   5996.4       760             5   318122.0   5491.4      696
  6   424872.5   6714.4       851             6   439350.0   7345.6      931
  7   163938.3   2548.5       323
  8   393468.9   6674.9       846
  9   660785.5   7708.5       977
 10   589497.1   7069.4       896
```

Total Area [acre]   =   1165.76297799608   Total Area [acre]   = 1038.828144304423
Total Buried Waste [MTU] =   70039.530000   Total Buried Waste [MTU] = 70031.6400000
Repository AML [MTU/acre] =   60.0804205674   Repository AML [MTU/acre] = 67.4140765091
                                                   Watts per MTU [W/MTU]   = 967.5799977250
                                                   Watts per linear meter of drift [W/m] = 1449.992

There are 8,877 WPs in both 4.1j and 5.0.1betaD.

% of WPs in a Subarea

Subarea	%		Subarea	%
1	16		1	6
2	18		2	12
3	9		3	60
4	5		4	4
5	9		5	8
6	10		6	10
7	4			
8	10			
9	11			
10	10			

DCFs - Ingestion of Drinking Water

These DCFs decrease by factors of 2 to 5. Average decrease is estimated to be about 50%.

WP Temperature

Mean Values   Mean Values
Subarea 2 (largest)   Subarea 3 (largest)
Time of Closure = 50 yr   Time of Closure = 100 yr
Peak Temperature = 165 deg C   Peak Temperature = 199 deg C
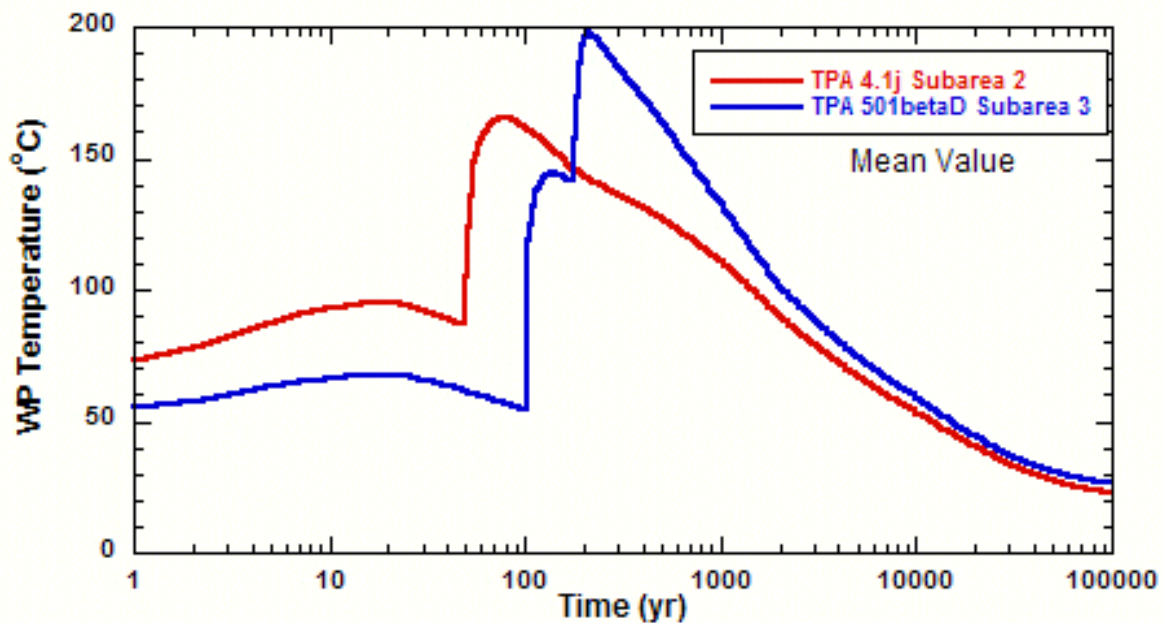Time of Peak = 81 yr   Time of Peak = 208 yr

At times past ~1000 yr to 100,000 yr, both WP temperatures are approximately equal.

At times < 100 yrs, lower WP temperatures in TPA 501betaD (ventilation effects).

In TPA 501betaD, there are rockfall effects on WP temperature.

Results from TPA 501betaE

Peak Expected Dose in mrem/yr (Time of the Peak)
364 realizations with Simulation Time = 10,000 yr

Subarea	WPs (%total)	Basecase (w/ glass)	WPs (% total)	Basecase (w/o glass)
1	526 (4%)	4.1 (5,676yr)	526 (6%) 3.7 (5,971 yr)	
2	1,062 (9%)	9.0 (7,376 yr)	1,062 (12%)	8.4 (8,101 yr)
3	6,148 (50%)	125 (10,000 yr)	5,318 (60%)	99 (10,000 yr)
4	343 (3%)	1.2 (5,696 yr)	343 (4%)	0.87 (5,970 yr)
5	696 (6%)	7.7 (8,101 yr)	696 (8%)	7.6 (7,730 yr)
6	931 (8%)	16.7 (5,063 yr)	931 (10%)	18.2 (5,307 yr)
7	723 (6%)	4.3 (9,107 yr)		
8	1,747 (14%)	194 (10,000 yr)		
Totals	**12,176**	**349 mrem/yr (10,000 yr)**	**8,876**	**124 mrem/yr (10,000 yr)**

(Subareas 3 and 8 have the shortest average and minimum GWTT in UZ and SZ)

Also, note the following.

	Peak Expected Dose in mrem/yr (Time of the Peak)
364 Realizations:	349 mrem/yr (10,000 yr)
1,024 Realizations	278 mrem/yr (10,000 yr)
Simulation Time 10,000 yrs:	278 mrem/yr (10,000 yr) for 1,024 realizations
Simulation Time 100,000 yrs:	365 mrem/yr (10,900 yr) for 1,024 realizations

GWTT UZ and SZ Minimum, Average, and Maximum Values (Basecase/364 Realizations)

	sa1uz	sa2uz	sa3uz	sa4uz	sa5uz	sa6uz	sa7uz	sa8uz	aveuz
min	2.01E+01	2.00E+01	1.50E+01	2.41E+02	4.05E+01	4.43E+01	5.85E+01	1.50E+01	9.24E+01
average	2.73E+02	1.64E+02	7.49E+01	7.43E+02	1.68E+02	3.28E+02	5.58E+02	3.83E+01	2.93E+02
max	1.48E+03	5.87E+02	4.14E+03	3.38E+03	5.44E+02	3.19E+03	3.10E+03	3.44E+03	2.35E+03

	sa1sz	sa2sz	sa3sz	sa4sz	sa5sz	sa6sz	sa7sz	sa8sz	avesz
min	1.24E+02	1.45E+02	1.40E+02	1.23E+02	1.21E+02	1.19E+02	1.20E+02	1.13E+02	1.26E+02
average	7.23E+02	8.19E+02	7.84E+02	7.13E+02	6.97E+02	6.87E+02	6.92E+02	6.83E+02	7.25E+02
max	2.31E+03	2.55E+03	2.45E+03	2.28E+03	2.24E+03	2.21E+03	2.22E+03	2.29E+03	2.32E+03

	sa1uzsz	sa2uzsz	sa3uzsz	sa4uzsz	sa5uzsz	sa6uzsz	sa7uzsz	sa8uzsz	aveuzsz
min	2.42E+02	2.16E+02	1.64E+02	5.58E+02	2.03E+02	2.79E+02	2.83E+02	1.46E+02	3.12E+02
average	9.95E+02	9.83E+02	8.59E+02	1.46E+03	8.65E+02	1.01E+03	1.25E+03	7.21E+02	1.02E+03
max	2.58E+03	2.70E+03	4.68E+03	4.03E+03	2.40E+03	3.62E+03	3.53E+03	3.86E+03	2.82E+03

Aug. 5, 2005   Ashremob

The following is from R. Benke:

```
The mass of HLW erupted in each TEPHRA realization is 10 WP * 7.89 MTU/WP =
78.9 MTU.
```

Aug. 5, 2005   Qin vs. Infil

Qin can be greater than **infil** for certain values of **WPFlowMultiplicationFactor**.

Sep. 16, 2005   Streamtube length

The following table was received from J. M. Menchaca for tpa501betaE mean value run.

Subarea	Stream Tube Length
1	20799.4
2	23149.9
3	23522.4
4	20485.3
5	20248.2
6	20075.6
7	20022.9
8	18816.4

Sep 26, 2005   Thermal Models

The following e-mail is from G. Adams:

```
The TPA code has two thermal models. The first thermal model is a linearized thermal
model that is included in the base case scenario. The model accounts for three
parallel paths: 1) the heat transfer pathway through the invert, 2) the heat transfer
pathway through the drip shield and backfill in a degraded drift, and 3) the heat
transfer pathway through the drip shield and backfill in a non-degraded drift.

The second thermal model accounts for convection and conduction through the backfill
material. Within this model, the thermal conductivity of the backfill material is
calculated using two separate particle models, whereas in the thermal model for the
```

```
base case scenario the thermal conductivity is an input parameter in the tpa.inp
file. The first particle model calculates the permeability from the median particle
diameter and a Trask sorting coefficient. The second particle model allows the user
to directly enter the coefficient of variation of the particle size distribution and
the skewness of the particle size distribution. In addition, for this
second particle model, the mean particle diameter is specified instead of
the median particle diameter.
```

Also from G. Adams:

```
The non-degraded portion of the drift is the part that is outside of the
wedge but is above the invert.  Essentially, this is the side area where
backfill initially accumulates.  Once the sides accumulate backfill out to
the rock wall, then the backfill is allowed to accumulate on top which is in
the wedge area.

Also, when a thickness for backfill is specified in tpa.inp, then this
becomes engineered backfill.  The models all allow an engineered backfill to
be used instead of a natural backfill from drift degradation.
```

Sep. 26, 2005   SEISMO Parameters

The following e-mail is from C. Grossman:

```
The seismic intervals are used for evaluating release from WPs failed
due to seismically-induced rockfall (4 intervals selected as a
reasonable compromise between efficiency and impact of variation over
time of WP failures).  The first interval  (0-2000 yrs) was selected to
capture WP failures at the hottest temperatures (note: failure time was
1000 yrs. for TPA 3.2 and 4.0).  The second interval (2000-5000 yrs) was
selected to capture WP failures at intermediate temperatures (note:
failure time was 3500 yrs for TPA 3.2).  The third interval (5000-10000
yrs) was selected to capture WP failures through the cool down phase
(note: failure time was 7500 yrs for TPA 3.2 and 4.0).  The fourth
interval (10,000 until the minimum of the end of the simulation and the
corrosion failure time for TPA 3.2 and 4.0) was selected to capture WP
failure of long-lived containers (note: failure time is the mean of the
10000 yr and the minimum of the simulation period and corrosion failure
times).   These were all based on NRC/CNWRA best estimates according to
TPA 3.2 and 4.0 user's manuals, appendix A.  I could locate little to no
information regarding these intervals in the description of consequence
modules.
```

Pertinent *tpa.inp* parameters are:

BeginningOfSEISMOWPFailureInterval*
SFWettedFraction_SEISMO*_*

Oct. 17, 2005   Near Field Chemical Environment

Logical Truth Table for the Determination of Near Field Chemical Environment
(0=False; 1=True)

Relative Humidity < Critical Relative Humidity for Aqueous Corrosion	Time < Drip Shield Failure Time	Drift Wall Seepage = 0.0 m³/yr	Relative Humidity < Rewetting Humidity	Near Field Chemical Environment
0	0	0	0	Environment III
0	0	0	1	Environment II
0	0	1	0	Environment I
0	0	1	1	Environment I
0	1	0	0	Environment I
0	1	0	1	Environment I
0	1	1	0	Environment I
0	1	1	1	Environment I
1	0	0	0	Dry
1	0	0	1	Dry
1	0	1	0	Dry
1	0	1	1	Dry
1	1	0	0	Dry
1	1	0	1	Dry
1	1	1	0	Dry
1	1	1	1	Dry

Oct. 20, 2005   Volcano Conduit Diameter

The tephra lookup table for ASHREMOB is based on an ejected MTU quantity of 7.89 to 78.9 MTU. Note that the lower end of the range is 10% of the upper end. With the addition of glass waste form, the average payload per package has been reduced. It is desired to determine the new conduit diameter range to account for the new average payload.

Fraction of repository in glass form = 0.0126
Fraction of repository in SF form = 0.9874
Total MTU in repository = 70040.0 MTU
Total MTU in glass form = 70040.0 x 0.0126 = 882.5 MTU
Total MTU in SF form = 70040.0 x 0.9874 = 69157.0 MTU

Glass package = 0.258641 MTU
SF package = 7.89 MTU
Number of glass packages = 882.5 / 0.258641 = 3412 packages
Number of SF packages = 69157.0 / 7.89 = 8765 packages

Ratio of SF to glass packages = 8765 / 3412 = 2.569

For the purposes of emplacement the packages are assumed to be placed in a linear geometric 3 1 2 1 pattern (SF SF SF GL SF SF GL). This gives a ratio of SF to glass of 5/2 = 2.5 which is close to the ratio of 2.569 based on MTU.

Package spacing = 5.265 m

A sequence of 14 cans = 10 x 7.89 + 4 x 0.258641 = 79.9356 MTU

This is close to the 78.9 MTU that the tephra lookup table is based on.

Package spacing = 5.265 m

Upper end of conduit diameter range = 14 x 5.265 = 73.71 m
Lower end of conduit diameter range = 73.71 x 0.10 = 7.371 m

Oct. 31, 2005 Scientific Notebook

* = Contributing chapters for last 6 months.

1 - Janetzke*
2 - Mohanty
3 - Rice*
4 - Scherer*
5 - Pensado
6 - Benke
7 - LaPlante
8 - Adams*
9 - Winfrey
10 - Smith
11 - Lozano*
12 - Wojcik
13 - Osidele
14 - open
15 - Menchaca*
16 - Portillo
17 - Povetko
18 - LeNeveu*
19 - Nes
20 - Stead
21 - Mancillas

Nov. 22, 2005   Run logs.

Possible content for a run log file could be:

```
    start date: Wed. 12-oct-2000
    start time: 12:34:56
    stop date : Wed. 12-oc-2000
    stop time : 12:34:56
    run label : fsv1r11a201s10y200s
    run path  : /home/janetzke
    data path :
    codes path:
    version   : 4.1a
    user name : janetzke
    host name : vulcan
    host type : SUN
    >>>> Code Compilation Data <<<<
    date : wed, 12-oct-2000
    time : 12:34:56
    host : scratchy1
    path : /home/janetzke
    user : janetzke
    f77  : SUN 5.0
```

Dec. 1, 2005   *Gnewdf.dat* ICRP72

P. LaPlante supplied references for the new data in *gnewdf.dat* file updated in SCR618.

```
Environmental Protection Agency. EPA-520/1-88-020, "Limiting Values of
Radionuclide Intakes and Air Concentration and Dose Conversion Factors
for Inhalation, Submersion, and Ingestion." Federal Guidance Report No.
11. Washington, DC: EPA. 1988.

International Commission on Radiological Protection. "Age-Dependent
Doses to Members of the Public from Intake of Radionuclides. Part 5:
Compilation of Ingestion and Inhalation Dose Coefficients". ICRP 72.
Annals of the ICRP. Tarrytown, NY: Elsevier Science Inc. 1996.

International Commission on Radiological Protection. "ICRP Database of
Dose Coefficients: Workers and Members of the Public", Version 2.01.
ICRP,  Tarrytown, NY: Elsevier Science Inc. 2001.
```

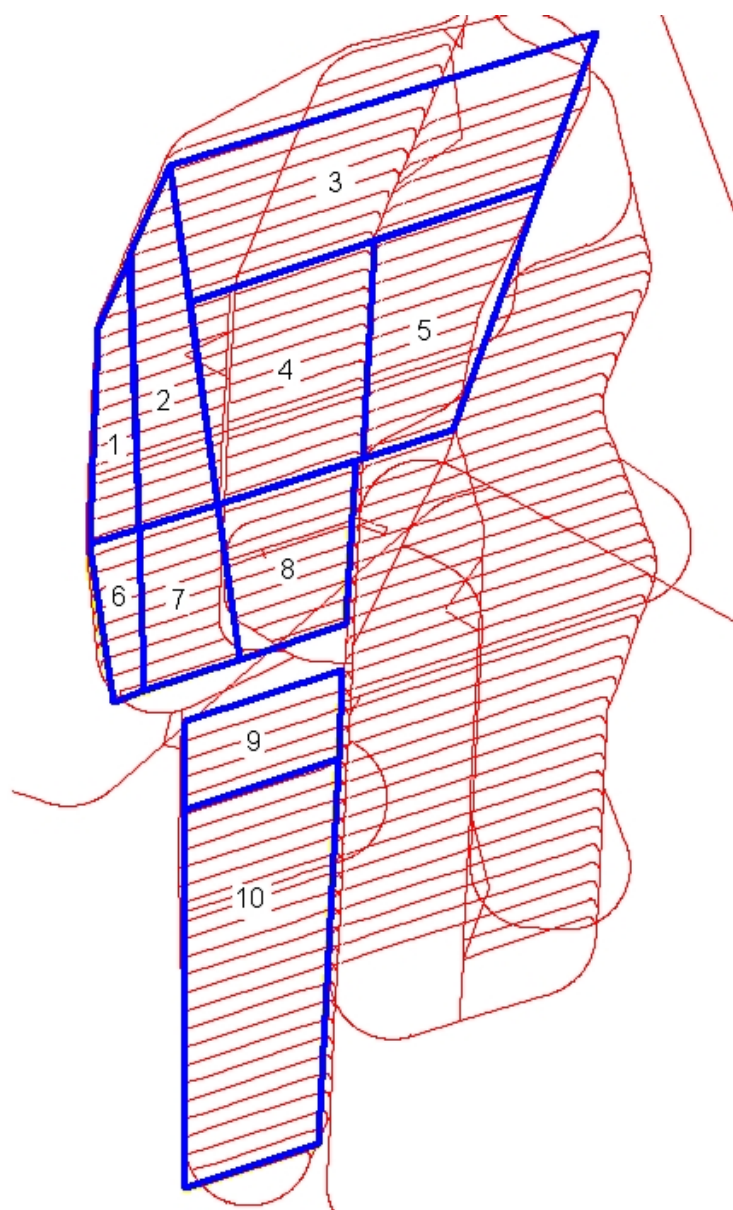Dec. 7, 2005   Winterle subareas for V5.1

The following in an e-mail from J. Winterle:

```
One of the suggested updates for TPA 5.1 was to break up what is now subarea 3
into smaller subareas.  The purpose is to improve consideration of spatial
variability and to prevent the situation of peak mean dose estimates being
dominated by a few realizations in which mechanical failure occurred in the
very large subarea 3.  The first of the attached figures shows what I propose
for new subarea delineation.  Basically, subarea 3 is divided up into 3 smaller
subareas and all others are the same, except for the renumbering.

The bases for dividing up subarea 3 are (i) the horizontal line between
subareas 4and 5 in the figure follows an access tunnel that separates
repository drifs, and separates subarea 4, which is mostly lithophysal rock
type at the repository horizon from subarea 5, which is mostly nonlithophysal
rock type; and (iii) the near horizontal line at the bottom of subarea 2
follows the strike of the drifts and goes through a kink in the access tunnel,
so it made for a logical separation point, and it also helps separate out
nonlith zone for subarea 5.  The second attached figure shows what I am saying
about the different rock types at the repository horizon.

Unless there are strong objections to this approach, I will begin implementing
the change to the tpa.inp file.  The change will include specifying the new
subarea coordinates; and adding new subarea dependent parameters, such as CHnv
thickness, drift degradation time, etc.
```
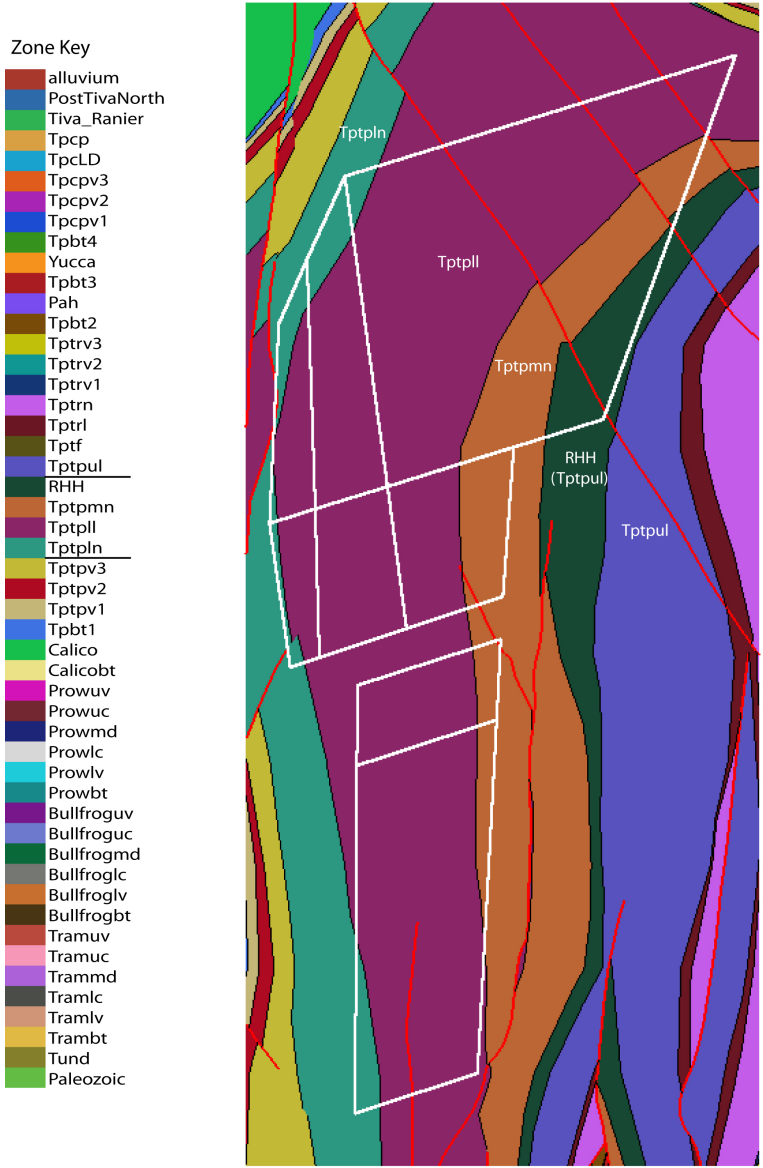
(Blank to next figure.)

(Blank to next figure.)

Zone Key

- alluvium
- PostTivaNorth
- Tiva_Ranier
- Tpcp
- TpcLD
- Tpcpv3
- Tpcpv2
- Tpcpv1
- Tpbt4
- Yucca
- Tpbt3
- Pah
- Tpbt2
- Tptrv3
- Tptrv2
- Tptrv1
- Tptrn
- Tptrl
- Tptf
- Tptpul
- RHH
- Tptpmn
- Tptpll
- Tptpln
- Tptpv3
- Tptpv2
- Tptpv1
- Tpbt1
- Calico
- Calicobt
- Prowuv
- Prowuc
- Prowmd
- Prowlc
- Prowlv
- Prowbt
- Bullfroguv
- Bullfroguc
- Bullfrogmd
- Bullfroglc
- Bullfroglv
- Bullfrogbt
- Tramuv
- Tramuc
- Trammd
- Tramlc
- Tramlv
- Trambt
- Tund
- Paleozoic

(Blank to next page.)

Dec. 8, 2005   Run Times for Reduced Nuclides.

Results from R. Rice:

Comparison of TPA Results
TPA Version 5.0.2
362 Realizations

		Maximum Simulation Time		
	PMD = Peak Expected Dose TPMD = Time of PMD PMD in mrem/yr (TPMD in yr)	10,000 years	100,000 years	1,000,000 years*
Scenario				
Basecase Radionuclides (22 aqueousnuclides - 4 chains w/ 2, 2, 4, & 5 members) (11 colloidalnuclides - 4 chains w/ 2, 2, 3, & 3 members)	PMD in mrem/yr (TPMD in yr) Run Time on TPA/GOLDSIM	84 (9,323) 2h 36 m	89 (9,769) 5h 56m	88 (9,769)* 67h 16m
Tim's List of 9 Aqueousnuclides w/ No Chains (Np237, U238, Pu239, Th230, Pu240, I129, Tc99, Cs135, & Pu242) (colloidalnuclides are Jp239, Jp240, & Jp242)	PMD (TPMD) Run Time on TPA/GOLDSIM	78 (9,323) 2h 6m	82 (9,543) 3h 55m	81 (9,543)* ** 41h 16m ***
	Change in Performance (i.e., % decrease in run time achieved by reducing number of radionuclides and no chains)	-19%	-34%	-39%

* = UZ Courant number set equal to 0.15
** = note that PMD and TPMD are the same w/ UZ Courant Number of 1.50 for the Reduced List
*** = note that runtime decreases 3% (i.e., 1h 15m in a 42h 31m run) when UZ Courant Number changes from 1.50 to 0.15

Dec. 14, 2005   Volcanic Conduit

A message from B. Hill indicates that an MTU line load of 1.1MTU/m could be used for the geometric model of the TPA code.

2006---

Feb. 3, 2006   ASHREMOB Ejected MTU

Roland submitted a run with the payload of each WP adjusted to be the same while maintaining the same overall amount of buried waste, and noticed that the results did not change. My response follows:

```
I think the results you described are correct, since the the number of WPs
ejected is not divided into SF or glass partitions.  Consideration is only
given to MTU ejected.  For this an average can inventory is used instead of the
can payload per type.  The average can MTU is based on the fraction of total
buried MTUs in glass form, and not on the payload for a given can type.
```


Mar. 10, 2006   New Hazard Curve for Seismic Events.

A new hazard curve for seismic events was added to *sampler.f* . This hazard curve can only be invoked when the name of the hazard curve *tpa.inp* input parameter is **SeismicHazardCurveforSEISMO**. This permits the old hazard curve to operate as usual, while accommodating the new seismic hazard curve for the new DRIFTFAIL and MECHFAIL modules. The new hazard curve uses Mean Annual Probability of Exceedance (MAPE) to indicate the type of seismic event and frequency to indicate the recurrence period for each event type.

Luis Ibarra provided the distribution and data tables in the following paragraphs.

The MAPE is specified as an index rather than the actual MAPE value, according to the following table:

Index	MAPE
4	10^{-4}
5	10^{-5}
6	10^{-6}
7	10^{-7}
8	10^{-8}

So Index = $-\log_{10}$(MAPE).

The hazard curve parameter type provides both a list of event times and event types. The hazard curve handler in *sampler.f* was changed to use the MAPE index for the seismic hazard curve rather than the seismic magnitude. The difference is more in the method than in the scale used. The new method interpolates between MAPE values based on the random number from **ran1seis()**.

The period values are sampled as before using the **raneseis()** function to find times between events based on the frequency data provided. An array of event times is returned to the calling routine.

The original hazard curve handler returned discrete values from the input table in the *tpa.inp* file. The new handler returns continuously interpolated values from an exponential distribution that constrains the number of events between the MAPE index values of 4 and 5 to be 90% of the total number of events. The following is the empirical equation derived to approximate these conditions.

$$type = \frac{-\ln(e^{-\lambda B} + r(e^{-\lambda A} - e^{-\lambda B}))}{\lambda}$$

where:
A = 4
B = 8
λ = 2.3
r = random number in the range (0,1].

82

Finite Exponential Equation

$$f(t) = \lambda e^{-\lambda t}$$

Finite Exponential Integral (find N)

$$N \int_A^B \lambda e^{-\lambda t} dt = 1$$

$$N\lambda \int_A^B e^{-\lambda t} dt = 1$$

$$N\lambda \left(\frac{e^{-\lambda t}}{-\lambda} \right) \Big|_A^B = 1$$

$$-Ne^{-\lambda t} \Big|_A^B = 1$$

$$N\left(e^{-\lambda A} - e^{-\lambda B} \right) = 1$$

$$N = \frac{1}{\left(e^{-\lambda A} - e^{-\lambda B} \right)}$$

For the case where the cumulative probability of events from MAPE indices 4 to 5 is 90% then

$$N\int_A^x \lambda e^{-\lambda t}\, dt = 0.9$$

where
A=4
x=5

Finite Exponential Integral (solve for *x*)

$$N\int_A^x \lambda e^{-\lambda t}\, dt = 0.9$$

$$x = \frac{-\ln\!\left[e^{-\lambda A} - 0.9\!\left(e^{-\lambda A} - e^{-\lambda B}\right)\right]}{\lambda}$$

Find λ that satisfies:
A=4
B=8
x=5

The value of 2.3 for λ to be used in the *type* equation was obtained via trial and error.

In general the "area" for the case where both bounds (α, β) are internal to the [4,8] range use:

$$Area = \frac{e^{-\lambda\alpha} - e^{-\lambda\beta}}{e^{-\lambda A} - e^{-\lambda B}}$$

The Peak Ground Velocity (PGV) values associated with the MAPE index is:

Index	PGV (m/s)
4	0.47
5	1.07
6	2.44
7	5.35
<7	5.35

The Peak Ground Acceleration (PGA) values are sampled from a lognormal distribution that has its control parameters (mean and standard deviation) interpolated from the following table:

Index	Mean (g)	Standard Deviation
4	0.47	0.64
5	2.27	0.64
6	4.75	0.53
7	12.7	0.53
<7	12.7	0.53

The lognormal distribution used is:

```
pga  =  exp( FINVNOR( r ) * ln(SD)  + ln(Mean)  )
```

where:
r = uniform random number
FINVNOR = normal distribution subroutine from the SNLLHS code.

The same uniform random number *r* used to sample the PGA distribution is used to interpolate the rubble compaction factor (CF) tables. This tends to enhance the correlation between the PGA and CF parameters. Two quantities are specified in the table. CF1 is the base value for each index and CF2 is a sampled positive delta applied using the form

```
CF  =  CF1 + r * CF2
```

Index	CF1	CF2
4	0.1	0.1
5	0.2	0.2
6	0.3	0.3
7	0.4	0.2
<7	0.4	0.2

The **PeakSeismicVandA()** routine is intended to be called after each call to **samplehazardcurve()** in the executive module using the array of event types (MAPE index) returned from the **samplehazardcurve()** routine. It returns to the executive the MAPE, PGV, PGA, and CF arrays for use in the **driftdriver()** routine. The **PeakSeismicVandA()** and the **FINVNOR()** routines reside in the *sampler.f* file.

March 28, 2006   TPA V5.0.2o Results

The following was received from R. Rice:

```
Basecase
10,000 yr and 460 realizations
Peak mean dose = 12.9 mrem/yr
Time of peak mean dose = 8,293 yr

MECH failed WPs
65/4600 or 1.4% of subarea calculations
failure times 996 - 7,380 yr (using seismic intervals)
# WPs failed = 65,085/56,014,200 = 0.1% of all WPs

CORR failed WPs
```

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```
348/4600 or 7.6% of subarea calculations
failure times 591 - 2,600 yr
# WPs failed = 436,040/56,014,200 = 0.8% of all WPs
```

April 13, 2006   TPA 5.0.2u Results

The following e-mail was received from J. M. Menchaca:

```
------------------------- tpa502u results -------------------------

Basecase:
Peak Mean Dose is 3.30171E-02 rem/yr at   10000.0 yr, based on   445
realizations.

no_colloids:
Peak Mean Dose is 1.32068E-02 rem/yr at    3634.7 yr, based on   445
realizations.

no_colloids_no_drift_degrad_no_loc_corrosion:
Peak Mean Dose is 4.21954E-04 rem/yr at    3996.8 yr, based on   445
realizations.

no_drift_deg:
Peak Mean Dose is 4.94505E-03 rem/yr at    3722.1 yr, based on   445
realizations.
```

April 13, 2006   Importance Analysis

The following technique can be used to neutralize localized corrosion.

```
"To eliminate localized corrosion, we can set the critical chloride
concentration to a high value (a value of 100.0 is high enough).  We
need to do this for the weld and the waste package."
```

From O. Pensado.

April 13, 2006   TPA 5.0.2u Results

Final results from Marty and Rob:

```
Basecase:
Peak Mean Dose is 3.30171E-02 rem/yr at   10000.0 yr, based on   445
realizations.

no_colloids:
Peak Mean Dose is 1.32068E-02 rem/yr at    3634.7 yr, based on   445
realizations.

no_colloids_no_drift_degrad_no_loc_corrosion:
Peak Mean Dose is 4.21954E-04 rem/yr at    3996.8 yr, based on   445
realizations.

no_drift_deg:
Peak Mean Dose is 4.94505E-03 rem/yr at    3722.1 yr, based on   445
realizations.

no_loc_corrosion:
Peak Mean Dose is 1.17754E-03 rem/yr at    3226.8 yr, based on   445
realizations.

no_loc_corrosion_no_drift_degrad:
Peak Mean Dose is 6.56119E-04 rem/yr at   10000.0 yr, based on   445
realizations.

no_seismic:
Peak Mean Dose is 3.28384E-02 rem/yr at   10000.0 yr, based on   445
realizations.

no_seismic_no_drift_degrad:
Peak Mean Dose is 1.77663E-03 rem/yr at    2539.8 yr, based on   445
realizations.
```

April 13, 2006   TPA 5.1beta

TPA 5.1beta was delivered via CD containing both UNIX and PC versions.

April 19, 2006   Scientific Notebook Contributions

* = Contributing chapters for last 6 months.

1 - Janetzke*
2 - Mohanty

3 - Rice*
4 - Scherer
5 - Pensado
6 - Benke
7 - LaPlante
8 - Adams*
9 - Winfrey
10 - Smith
11 - Lozano
12 - Wojcik
13 - Osidele
14 - open
15 - Menchaca
16 - Portillo
17 - Povetko
18 - LeNeveu
19 - Nes
20 - Stead*
21 - Mancillas*
22 - Epps

June 7, 2006   Distribution for SF Dissolution Rate Pre-exponential

The following is an e-mail from R. Rice:

```
444 realizations

TPA Version 51betaB (with the fix, so that releases are not zeroed out if there is no WP failure)
10,000 yr and 100,000 yr simulation times.

(the following results are peak mean dose in mrem/yr and time of that peak mean dose in yr)

                                                10,000 yr                100,000 yr
                                                ************             ***********
Basecase                                        32.8 @ 3,004             28.8 @ 66,700
logbeta distribution equivalent to lognormal 20.5 @ 3,004                27.0 @ 66,700
New Distribution (lognormal)                    19.2 @ 3,304             27.3 @ 66,700
```

June 30, 2006   WP & Drift wall temperature

The 5.1betaC version was used with a mean value run, but sampling the ventilation time from 0 to 100 years using the **userdiscreteempirical** PDF to select 11 integers in the range, with increments of 10 years. The following is the realization order:

Realization Ventilation_Time
1   80
2   0
3   20
4   100
5   60
6   70
7   30
8   40
9   90
10   10
11   50

The following plots are generated from the data in *nfenv.rlt:*

Drift Wall and WP Temperatures
for Ventilation Time = 0 years

Drift Wall and WP Temperatures
for Ventilation Time = 100 years

Subarea 1 Drift Wall Temperatures
with Selected Ventilation Times

Subarea 4 Drift Wall Temperatures
with Selected Ventilation Times
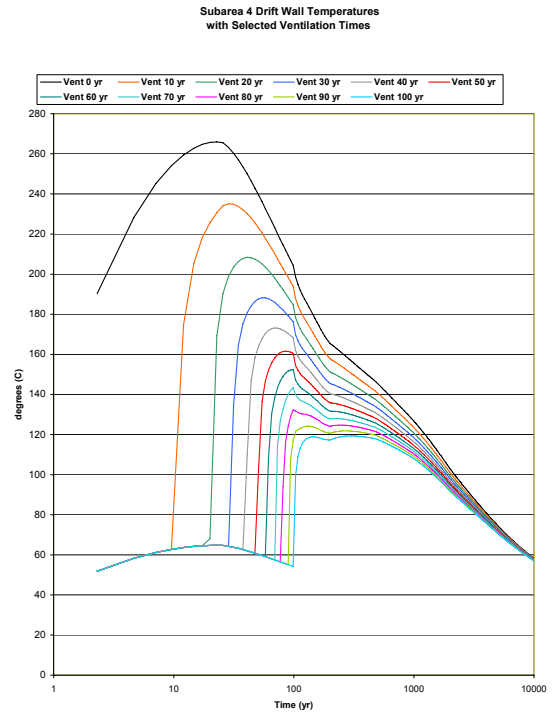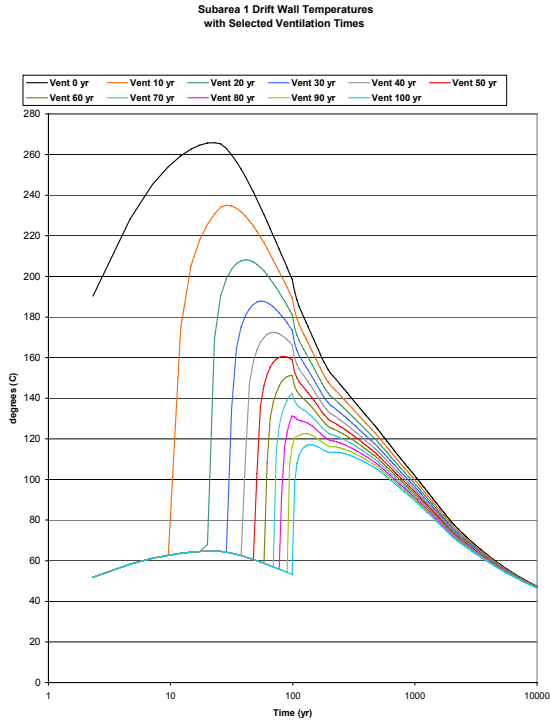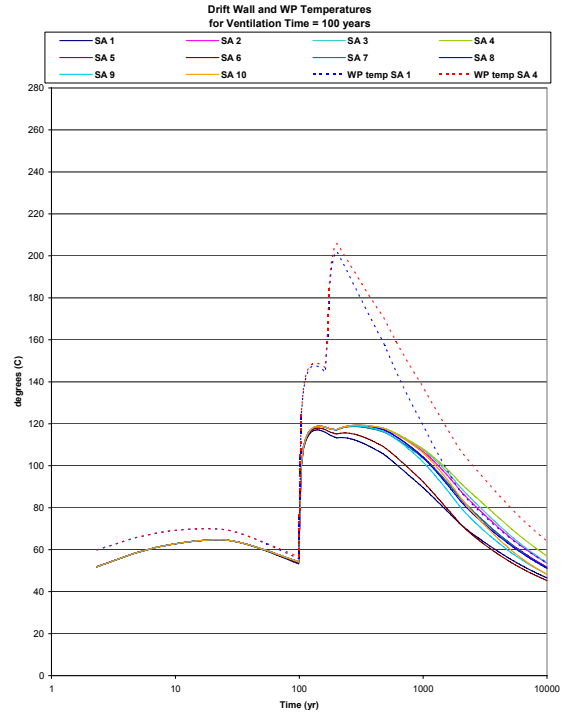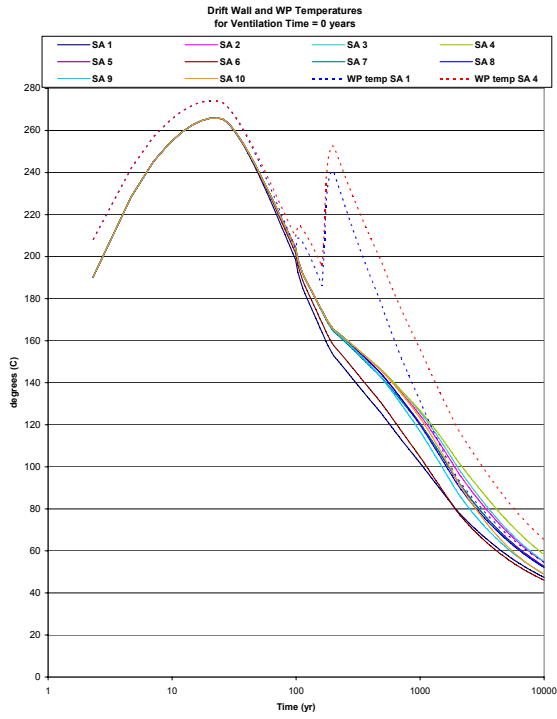
Aug. 29, 2006   Weldfail and *corrfail.f*

A note from G. Adams about *weldfail.f*:

```
The module is corrfail.f.  This module used to be weldfail.f  Weldfail.f was
originally written to be a standalone like failt; however, it was combined
with failt.  So now ebsfail invokes failt and failt calls subroutines within
corrfail.f.
```

Aug. 30, 2006   Inventory from *nuclides.dat* to *ebsrel.f*

Inventory data is read from the *nuclides.dat* file and transferred to the *invent.f* routine and subsequently to the *ebsrel.f* routine. Glass waste data and spent fuel data follow the same path, but are stored in different arrays.

The data from *nuclides.dat* has units of Ci/MTU and is converted to mole/MTU in the *invent.f* module with the aid of the activity (Ci/mole) values and stored in amolepermtuat10yr().

The calendar year of emplacement is used to find the time which represents T0, and a delta T can then be used in the aging of the fuel. The aged fuel values are first stored in a two dimensional array and then transferred to the amolepermtuatemplace() array.

These values are then stored in the ammtu() array in *ebsrel.f*, and combined with the payload and activity data to arrive at Ci/WP values written to *ebspac.nuc*. The following is a units check of the equation:

$$\frac{mole}{MTU} \cdot \frac{MTU}{WP} \cdot \frac{Ci}{mole} = \frac{Ci}{WP}$$

Sept 14, 2006   Unix Fortran Compilers

The following SUN compilers are associated with the path names listed:

```
f77 V4.2 = /solapps/SUNWspro.4.2/bin/f77
f77 V5.0 = /solapps/SUNWspro/bin/bin/f77
f77 V5.3 = /solapps/SUNWspro6/bin/f77
```

Default is set in `~/.cshrc`

Sept. 15, 2006   Chapter 22

Chapter 22 of this notebook is closed but considered incomplete, because the author terminated employment before completion. As a result some staff members do not agree with some of the conclusions presented.

Sep. 21, 2006   Scientific Notebook Contributions

* = Contributing chapters for last 6 months.

1 - Janetzke* {ALBY\\D:\ronj-\wp\sn612e.wpd}
2 - Mohanty - not used
3 - Rice* {ALBY\\D:\RonJ-\rob\SN612E*}
4 - Scherer {Guardian\\d:\docs\ScientificNotebooks\SN612-4E}
5 - Pensado - not used
6 - Benke* {PHOENIX\\D:\Shared\Sci Notebook 612-6e}
7 - LaPlante {FROGGY\\D:\TPA\sci.notebk.612-7e.wpd}
8 - Adams* {PITOR\\D:\scientific notebook\Notebook612-8E\SN612-8E.wpd}
9 - Winfrey - closed
10 - Smith - not used
11 - Lozano - closed
12 - Wojcik - closed
13 - Osidele - not used
14 - unassigned
15 - Menchaca* {stu2560\\D:\jmenchaca\ScientificNotebook\SN612e.wpd}
16 - Portillo - closed
17 - Povetko* {Paladin\\ D:\ScientificNotebooks\SN612_section17E_TPApovetko.wpd
18 - LeNeveu {ALBY\\D:\RonJ-\leneveu\SCIENTIFIC NOTEBOOKoct5.doc}

19 - Nes - mot used
20 - Stead {\\Adriana\Data\DStead\TPAstuff\Sci_NB\SN612e_DStead.wpd}
21 - Mancillas {Manta\\D:\Notebooks\SN612-21.wpd}
22 - Epps* - closed

Sept. 28, 2006 TPA V5.1betaG output files

A table of TPA V5.1betaG output files has been prepared to list the conditions under which a given file is created. Not all files are created in each TPA run. The input flags in the *tpa.inp* file can control the creation of some of the files for a particular run. Below is a list of *tpa.inp* flags considered as controlling flags, followed by the table of file names. An 'X' in a box indicates that the file is not created when this flag is set to 0. Some flags require the setting of other flags to enable their operation. It is assumed that the TPA code is run with all the necessary flags set to enable the operation of the flag in question.

Case ID	Parameter Name	Clear Value	Set Value
0	Base Case (all values cleared)	-	-
1a	GenerateRestartFiles(yes=1,no=0) {Run permitted to complete normally}	0	1
1b	GenerateRestartFiles(yes=1,no=0) {Run interrupted after the first realization is completed but before any following realizations are completed}	0	1
2	VolcanismDisruptiveScenarioFlag(yes=1,no=0)	0	1
3	FaultingDisruptiveScenarioFlag(yes=1,no=0)	0	1
4	SeismicDisruptiveScenarioFlag(yes=1,no=0)	0	1
5	DriftDegradationScenarioFlag(yes=1,no=0)	0	1

Case ID	Parameter Name	Clear Value	Set Value
6	DirectReleaseOnlyFlag(yes=1,no=0)	0	1
7	SelectAppendFiles	0	1
8	SelectAppendFiles	0	2
9	SelectAppendFiles	0	3
10	SelectAppendFiles	0	4
11	SelectAppendFiles	0	5
12	SelectAppendFiles	0	6
13	SelectAppendFiles	0	7
14	SelectAppendFiles	0	8
15	SelectAppendFiles	0	9
16	SelectAppendFiles	0	10
17	SelectAppendFiles	0	11
18	SelectAppendFiles	0	12
19	SelectAppendFiles	0	13
20	SelectAppendFiles	0	14
21	SelectAppendFiles	0	15
22	SelectAppendFiles	0	16
23	SelectAppendFiles	0	17
24	SelectAppendFiles	0	18
25	SelectAppendFiles	0	19
26	SelectAppendFiles	0	20

Case ID	Parameter Name	Clear Value	Set Value
27	SelectAppendFiles	0	21
28	SelectAppendFiles	0	22
29	GroundwaterProtectionCalc(yes=1,no=0)	0	1
30	TabularTemperatureRHFlag(yes=1,no=0)	0	1
31	InvertBypass(0=ebsfilt,1=bypass-ebsfilt)	1	0
32	UZVelocity(0=average,1=time-dependent)	0	1
33	SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)	0	1
34	ExtrusiveEventFlag(extrusive=1,intrusive=0)	0	1
35	LatinHypercubeSampling(yes=1,no=0)	0	1
36	OneTemperatureCellPerWP(yes=1,no=0)	0	1
37	IrreversibleColloidModel[0=no,1=yes]	0	1
38	ReceptorGroup(1=Farming,2=Residential)	1	2
39	PlumeCaptureModel(1=UserDefined,2=Calculated)	1	2
40	VolcanoModel(1=Geometric,2=Distribution)	1	2
41	AshEvolutionMode[0=no_ashremob,1=ashremob]	0	1

Table of TPA file creation status per Case ID.

	0	1a	1b	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
airpkdos.res																																	
arpkds_c.res																																	
ashcmd.out	⊠	⊠				⊠		⊠		⊠				⊠				⊠			⊠				⊠			⊠			⊠		⊠
ashout.res																																	
ashplume.exe	⊠	⊠				⊠		⊠		⊠				⊠				⊠			⊠				⊠			⊠			⊠		⊠
ashplume.in	⊠	⊠				⊠		⊠		⊠				⊠				⊠			⊠				⊠			⊠			⊠		⊠
ashplume.out	⊠	⊠				⊠		⊠		⊠				⊠				⊠			⊠				⊠			⊠			⊠		⊠
burnup.dat																																	
check.pnt	⊠	⊠				⊠		⊠		⊠				⊠				⊠			⊠				⊠			⊠			⊠		⊠
chlrdmf.dat																																	
climato1.dat																																	
climato2.dat																																	
coefkdeg.dat				⊠																													

Column headers: 0, 1a, 1b, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41

Row labels:
- corrode.out
- cp.tpa
- cumrel.res
- cumrelse.out
- cumrel_c.res
- dcagw.ech
- dcagw.rlt
- dcfgw.cum
- deltaec.inp
- diagnose.out
- dilution.dat
- driftfail.dat
- driftfail.ech
- driftfail.exe
- driftfail.inp
- driftfail.out
- driftfail.rlt
- drifts.dat
- drythick.dat
- dsfail.ech
- dsfail.res
- dsfail.rlt
- dsfailt.dat
- dsfailt.def
- dsfailt.exe
- dsfailt.inp
- dsfailt.out
- ebscld.out
- ebsfail.def
- ebsfail.ech
- ebsfail.inp
- ebsfail.rlt
- ebsfilt.def
- ebsfilt.exe
- ebsfilt.inp
- ebsfilt.out
- ebsflo.dat
- ebsglass.dat
- ebsnef.dat

Column headers: 0, 1a, 1b, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41

Row labels:

- ebsnef.out
- ebsnef2.dat
- ebspac.nuc
- ebspacglass.nuc
- ebspacsf.nuc
- ebsrel.cum
- ebsrel.def
- ebsrel.ech
- ebsrel.inp
- ebsrel.rlt
- ebsrelglass.inp
- ebsrelsf.inp
- ebssf.dat
- ebstrh.dat
- ebstrhc.inp
- echofail.dat
- echofilt.dat
- env.exe
- envin.exe
- epa_ave.out
- epapktim.out
- failt.cum
- failt.exe
- failt.out
- FILENAME.DAT
- fluoride.dat
- frac_rel.out
- gbioac1.dat
- gdefauls.def
- gdefault.def
- gdefault.inp
- gdosinc2.dat
- gencorrfail.out
- gentoo.out
- genv.cum
- genv.in
- genv.out
- gftrans.def
- gftrans.inp

	0	1a	1b	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41
gftranss.def																																											
ggamen.dat																																											
ggenii.cum																																											
ggenii.def																																											
ggenii.inp																																											
ggenii.out																																											
ggeniis.def																																											
ggrdf.dat																																											
gmedia.out																																											
gnewdf.dat																																											
grmdlib.dat																																											
gs_cb_ad.dat																																											
gs_cb_ci.dat																																											
gs_pb_ad.dat																																											
gs_pb_ci.dat																																											
gsccdf.res																																											
gsccdf_c.res																																											
gwccdf.res																																											
gwccdf_c.res																																											
gwork.buf																																											
gwpkdos.res																																											
gwpkds_c.res																																											
gwttuzsz.res																																											
gw_cb_ad.dat																																											
gw_cb_ci.dat																																											
gw_pb_ad.dat																																											
gw_pb_ci.dat																																											
infile.ash																																											
infilper.res																																											
inv1000.out																																											
lhs.csv																																											
lhs.inp																																											
lhs.out																																											
lhse.out																																											
maxrel.dat																																											
maydtbl.dat																																											
mechfail.ech																																											
mechfail.exe																																											
mechfail.inp																																											

	0	1a	1b	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41
mechfail.rlt																																											
mechfail_ds.dat																																											
mechfail_ds.def																																											
mechfail_ds.inp																																											
mechfail_ds.out																																											
mechfail_ds.res																																											
mechfail_wp.dat																																											
mechfail_wp.def																																											
mechfail_wp.inp																																											
mechfail_wp.out																																											
mechfail_wp.res																																											
mv.tpa																																											
nearfld.res																																											
nefii.dis																																											
nefii.inp																																											
nefii.out																																											
nefii.rel																																											
NEFII.VEL																																											
nefiisz.dis																																											
nefiisz.inp																																											
nefiisz.out																																											
nefiisz.src																																											
nefiisz.vel																																											
nefiiuz.dis																																											
nefiiuz.inp																																											
nefiiuz.out																																											
nefiiuz.src																																											
nefiiuz.vel																																											
nefmks.exe																																											
nfenv.ech																																											
nfenv.rlt																																											
npkdoset.res																																											
npkdst_c.res																																											
nuclides.dat																																											
organdf.dat																																											
pkmndose.res																																											
pkreltim.res																																											
pkrltm_c.res																																											
relccdf.res																																											

Column headers: 0, 1a, 1b, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41

Row labels:

- relcum.out
- relcumglass.out
- relcumsf.out
- releaset.cum
- releaset.exe
- releaset.out
- relfrac.out
- relgwgs.res
- rel_flow.out
- repdes.dat
- rgsna.tpa
- rgsnr.tpa
- rgssa.tpa
- rgssr.tpa
- rgwgssa.tpa
- rgwna.tpa
- rgwnapani.tpa
- rgwnapdw.tpa
- rgwnapext.tpa
- rgwnapinh.tpa
- rgwnapmlk.tpa
- rgwnappla.tpa
- rgwnr.tpa
- rgwsa.tpa
- rgwsap.tpa
- rgwsr.tpa
- rlccdf_c.res
- rlgwgs_c.res
- samplpar.abb
- samplpar.hdr
- samplpar.res
- smaydtbl.dat
- snllhs.exe
- sotnef.dat
- sp.tpa
- spquery.tpa
- strmtube.dat
- sz_kdrd.out
- sz_revers.out

	0	1a	1b	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41
szft.ech	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
szft.rlt	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
tefkti.inp	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
thermal.dat																																×											
totdose.res																																											
totdos_c.res																																											
tpa.inp																																											
tpa.inp~																																											
tpa.out																																											
tpamax.out																																											
tpameans.out																																											
tpamin.out																																											
tpanames.dbs																																											
tpasys.tmp																																											
tpa_include.inp																																											
trelease.out							×																																				
uz_kdrd.out																																											
uz_revers.out																																											
uzflow.ech	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
uzflow.rlt	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
uzft.ech	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
uzft.rlt	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×	×
weldfail.out							×																																				
wpfillstats.out																																											
wpflow.dat							×																																				
wpflow.def							×																																				
wpsfail.res																																											

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Oct. 5, 2006   Reformat of *tpa.inp*

The following e-mail was sent to respondents of the *tpa.inp* reformat questionnaire:

Thanks to everyone for their excellent and timely responses. The responses included several good comments. The results below, from 8 respondents, indicate that only questions #2 & #4 have significant spread in opinion. For #2, assuming those who selected c) could probably be convinced to switch to a) if comments were added to the tpa.inp file which indicate that a given parameter is used in more than one place (with pointers to the other places). So a) would be the suggestion here. Question #4 is more difficult, unless one considers that b) & c) are nearly the same in implementation and usage, then there is a clear majority. A decision will be made between b) & c) after the rest of the file is reformatted to see if a logical path emerges for this case.

Thanks again to everyone.
 - - - - - - - - - - - - - - - - - -

Select one response per question.

1) Should the parameters be grouped by module, by physical quantity (e.g. thickness; KD, etc.), or alphabetically?
    __7__   a) by module
    _____   b) physical quantity
    _____   c) alphabetically
    _____   d) seek NRC guidance
    __1__   e) don't care
    COMMENT:__An alphabetical cross reference was suggested for the User's Guide_____

For the remainder of the questionnaire assume that parameters are sorted by module

2) Where should a parameter that is used by more than one module be placed (it may only appear once in the tpa.inp input file)?
    __3__   a) with the module that calls it first
    _____   b) with the module that uses it the most number of times
    __4__   c) in a separate section dedicated to multiply used parameters
    _____   d) in the exec section
    _____   e) seek NRC guidance
    __1__   f) don't care
    COMMENT 1:___If a), add comments referencing the usage in other modules. _____
    COMMENT 2:___It should be associated with the module that most closely matches the subject matter of the parameter.

3) In what order should the module groups appear in the tpa.inp input file?
    __7__   a) the order in which they are invoked by the executive
    _____   b) alphabetically
    _____   c) in increasing order of the number of parameters used by the module
    __1__   d) in the order they appear in the User's Guide
    _____   e) seek NRC guidance
    _____   f) don't care
    COMMENT:__If a), separate the base case modules from the disruptive scenario modules. __

4) Where should the control flags for things like disruptive scenario switches be placed?
    __2__   a) in their respective module section

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__3__   b) in the exec section
__3__   c) in a separate section dedicated to control flags
_____   d) seek NRC guidance
_____   e) don't care
COMMENT:___If c), put control flags at the top of the tpa.inp file._____

5) Should a separate section be developed to contain the repository design and site characteristics data, even though this would mean separating parameters from the module grouping in which they would normally appear?
__1__   a) YES
__6__   b) NO
__1__   c) seek NRC guidance
_____   d) don't care
COMMENT:___If these parameters are not sampled, they should be removed from tpa.inp.__

6) Should a separate section be developed to contain seismic data, even though this would mean separating parameters from the module grouping in which they would normally appear?
_____   a) YES
__6__   b) NO
__1__   c) seek NRC guidance
__1__   d) don't care
COMMENT:_____

7) Should the included parameters (those that reside in tpa_include.inp) be maintained in one file in the same way as the tpa.inp file is organized, or divided such that included parameters for a module are in a separate 'module specific' include file?
__5__   a) one include file
__1__   b) multiple 'module specific' include files
_____   c) seek NRC guidance
__2__   d) don't care
COMMENT 1:___If a), measures should be taken to keep it small. _____
COMMENT 2:___Add a column to Appendix A of the User's Guide to indicate the modules that use the parameter. ___

GENERAL COMMENT Additional sort criteria should be applied to parameters within a module section:
Criterion 1: Sort from most to least likely to be changed.
Criterion 2: Sort by the order in which the parameters are used within the module.

Oct. 5, 2006 *tpa.inp* Parameter Usage

The following template was used to find the modules that use each parameter:

```
echo PARM=ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]
grep -l "ArealAverageMeanAnnualInfiltrationAtStart\[mm/yr\]" \
        array.f      \
        ashplumo.f  \
        ashrmovo.f  \
        ashremob.f  \
        dcagw.f      \
```

```
        dcags.f        \
        driftdrive.f \
        dsfail.f       \
        ebsfail.f      \
        ebsrel.f       \
        exec.f         \
        faulto.f       \
        invent.f       \
        mechdrive.f \
        mv.f           \
        nfenv.f        \
        nrutil.f       \
        szft.f         \
        reader.f       \
        iareader.f     \
        vt_util0.f     \
        sampler.f      \
        subarea.f      \
        uzflow.f       \
        uzft.f         \
        volcano.f      \
        ran.f          \
        numrecip.f     \
        condxyzt.f     \
        peakfind.f     \
        fileunit.f     \
        fileutil.f     \
        vt_file_utilities.f   \
        vt_print_utilities.f   \
    zportunx.f
```

The parameter names were extracted from files *sp.tpa* and *cp.tpa* and the template was repeated in a UNIX script for each parameter. Some parameter names were shortened, since their full name does not appear in the source code.

Oct. 30, 2006   *Tpa.inp*

Proposed rules for parameter placement in *tpa.inp*.

1) Parameters should be grouped by module. The module order should reflect the order in which the modules are invoked by the executive. An alphabetical cross reference may be created from Femi's spreadsheet for the user's guide.

2) Within a module's section, parameters should be sorted in the order they are used by the module.

3) If a parameter is used by more than one module, it should appear with the module that first uses the parameter. Comments that list the other modules that share a given parameter, should be added to the sections of all modules that share a parameter.

4) Module control flags should be placed in their appropriate module section, not the executive section.

5) Seismic parameters should be put in the DRIFTFAIL section.

6) Consider moving all seldom modified constants to *tpa_include.inp*.

7) Rules 1-5 should be applied to *tpa_include.inp* also.

Nov. 27, 2006   GENTPA

Re-linking the GENTPA code with the SUN/f90 compiler using an f77 *ritqa.o* file causes spurious form feed(FF) controls on output. This is only a cosmetic issue since it just controls pagination of the standard output.

Dec 13, 2006   Files used by O. Pensado:

driftfail.rlt
ebsrel.rlt (consider removing **xnoloss** column)
infilper.res
mechfail.rlt
nefii.dis
nfenv.rlt
rgwnr.tpa
samplpar.res
sotnef.dat
szft.rlt
totdose.res
uzft.rlt

Jan. 18, 2007   Reformatted files.

The following e-mail was received from G. Adams in response to some questions about the reformatted files:

```
1) failt.cum; Is the outer layer temperature column valid if the outer layer thickness is 0?
Does it eventually (in time) apply to the Inner layer?
```

```
It is calculated without regard to corrosion failure of the waste package.  It is the temperature
that would be at the surface of the outer layer without degradation of the outer layer.  It is
part of the corrosion rate calculations for general corrosion of the outer layer.  The
temperature at the inner layer is not computed separately but would not be much different than
this value due to the high conductivity of the metal.
```

```
Will modify the file description from:
```

```
! Outer Layer Temperature ; surface temperature of the waste
```

```
!                          package outer layer
```

```
To:
```

```
! Outer Layer Temperature ; surface temperature of the waste
```

```
!                          package outer layer prior to corrosion
```

```
2) failt.cum; If the critical potential and corrosion potential is for the current layer
indicated in column two, this should be spelled out in the header descriptions.
```

```
It looks like from the code that the ecrit and ecorr values would apply to either layer 1 or
layer 2.
```

```
Will modify the headers from:
```

```
 Critical     Corrosion
```

```
Potential     Potential
```

```
To:
```

```
Critical     Corrosion
```

```
Potential     Potential

for Layer     for Layer
```

And descriptions from:

```
! Critical Potential      ; critical potential for localized

!                           corrosion initiation

! Corrosion Potential     ; corrosion potential
```

To:

```
! Critical Potential for Layer      ; critical potential for localized

!                                     corrosion initiation for this layer

! Corrosion Potential for Layer     ; corrosion potential for this layer
```

3) failt.cum; If the outer layer thickness is 0, and layer 2 is processed, will the column heading change to Inner layer thickness?

The column heading will not change for different layers.

4) failt.cum; The mode abbreviations and what they mean should be put in the header description area.

Will modify the description from:

```
! Mode                 ; mode of corrosion
```

To:

```
! Mode                 ; mode of corrosion

                       ; dry oxd: dry air oxidation

                       ; hmd oxd: humid air oxidation

                       ; local:   aqueous localized corrosion

                       ; general: aqueous general corrosion
```

5) failt.cum; In section 5 item 1, the header should indicate whether the wetting time is a duration or a start time?

Will modify the description from:

! Item 1: wetting time - waste package wetting time

To:

! Item 1: wetting time – time of transition to aqueous corrosion

6) nearfld.res; The Avg WP Chloride column has different values at the end of the file. Is this due to increased precision on input?

These values are the subarea averaged values where the subarea values are displayed in file chlrdmf.dat. The variation occurs for the environment II values because they are sampled from a user specified piecewise distribution for each subarea. I'm not seeing a problem with the result values from a run that I did. I checked the lhs.out values with the values displayed in chlrdmf.dat, and they are the same.

7) failt.out; See comments 1-5 for failt.cum.

Will make corresponding changes

8) mechfail.rlt; If the DS Total is the sum of corrosion , static, and dynamic, that would be a good point to mention in the header description of DS Total. The same would apply to WP Total.

Will modify the description from:

!! DS Total   ; total drip shield failure fraction

!! WP Total   ; total waste package failure fraction

To:

!! DS Total   ; total drip shield failure fraction

                  ; sum of corrosion, static, and dynamic

                  ; drip shield failure fractions

!! WP Total   ; total waste package failure fraction

                  ; sum of static and dynamic waste

                  ; package failure fractions

9) mechfail.rlt; The reference for the fractions should be mentioned in the header (fraction of drip shields in Subarea?). It would be nice to find a way to put the term fraction in the column header also, or maybe even in place of the units.

Will modify the description from

```
!! SECTION 2 ; TIME VARYING DATA

!!

!! This section displays failure fractions

!! for each tpa time step


To:


!! SECTION 2 ; TIME VARYING DATA FOR SUBAREA

!!

!! This section displays failure fractions

!! for each tpa time step for the subarea

!! identified in SECTION 1
```

Will modify the header from:

```
  Step      TPA Time      DS Total  DS Corrosion    DS Static    DS Dynamic      WP Total      WP
Static    WP Dynamic

            (year)


To:


  Step      TPA Time      DS Total  DS Corrosion    DS Static    DS Dynamic      WP Total      WP
Static    WP Dynamic

                          Fraction      Fraction      Fraction      Fraction      Fraction
Fraction       Fraction

            (year)    (unitless)    (unitless)    (unitless)    (unitless)    (unitless)
(unitless)    (unitless)
```

10) mechfail.ech; Change the description for Event to "seismic event number".

Will modify:


```
!! Event          ; seismic event
```

To:

110

```
!! Event          ; seismic event number
```

11) mechfail.ech; Although it is OK to repeat the Section 2 for each subarea, it may not be necessary to do so.

It's repeated because the vertical pressures change for each subarea. I missed that in the original coding.

12) mechfail_wp.res; If there is a way to indicate that the mechanism in the Failure Mechanism column is a drift mechanism and not a WP failure, that would be helpful.

Will modify:

```
!! Failure Mechanism ; drift degradation mechanism

!!                   (0=trapezoid, 1=chimney)
```

To:

```
!! Caving Mechanism ;  caving failure mechanism for the drift

!!                   (0=trapezoid, 1=chimney)
```

And for the header, from:

Failure

Mechanism

To:

Caving

Mechanism

13) mechfail_wp.res; What kind of grid is used for the grid elements?

The grid corresponds to one grid element for each rock type in the subarea. In the original coding, you could have multiple grid elements in each subarea and a certain number of grid elements would be assigned to each rock type in a subarea based on the fraction of rock type 1 and rock type 2 in the subarea. For example, if you had 10 grid elements and rock type 1 was 70%, then 7 would be assigned to rock type 1 and 3 to rock type 2. The processing in mechfail is done for each grid element, so you would have, in this case, 7 failure calculations over all time steps for rock type 1 and 3 for rock type 2 for that subarea. However, now there are only two grid elements and the grid element results are weighted by the fraction of rock type one and rock

```
type two.
```

```
14) mechfail_ds.res;  What does "exceedance" refer to in the MAFE description?  What is being
exceeded?
```

```
It is described in the MECHFAIL Report, Ibarra, et. al., June 2006 in Section 5.2.4.2.  For a
Poisson process (c^x) (e^-c) / x!, and in this case when estimating the occurrence of seismic
events, c = MAFE {mean rate of occurrence of the event} * t {time in which the event can take
place}
```

```
15) mechfail_ds.res;  Does "Creep threshold" have units?
```

```
It has no units.  It is used to develop the creep multiplier and is described in Section 5.1.5 of
Ibarra, et. al., June 2006.  It also corresponds to the tpa.inp sample parameter:
```

```
uniform
```

```
DripShieldCreepThreshold[]
```

```
0.9, 1.2
```

Jan 22, 2007   Input Parameter Control

A possible input parameter control syntax for future versions could be:
Global
SynchronousAdvance (one realization per sample set)
DifferentialAdvance   (one realization per differential value times number of differential parameters; requires next four lines)
DifferentialReference   (requires next line)
'MIN' or 'MAX' or 'MEAN' or 'MINMAXAVG' or 'SPECIAL'
DeltaSet or RangeSet (-+%) (See descriptions below)
-1, +1, -10, +10, etc.
Parameter
ParameterName
lhs or min or mean or max or minmaxavg or special or differential
uniform or loguniform or beta or constant etc (ignored for point samples)
-1, 1   (range used for both LHS and POINT samples except SPECIAL)
1.0   (SPECIAL value independent of range but may be altered by DeltaSet or RangeSet operations; if value is not specified use MEAN as default)

[*DeltaSet   (-+%) (ignored for synchronous advance runs, relative to MIN, MEAN, MAX or SPECIAL only) or RangeSet (-+%) (ignored for synchronous advance runs, relative to MAX - MIN)*]

Feb 16, 2007   Disk Space

The following e-mail was sent to D. Pickett:

The PC and UNIX platforms give about the same results for space requirements. There are 4 major
modes in which the code can be run. With and without a post-compliance period, and with an
without the 'append' files. The numbers can be scaled up linearly for the number of realizations
for any of the modes.   The user does not usually need to run with the append files, but most
likely will always ask for the Post-Compliance Period option. Most runs will be about 500
realizations.

Space Per Realization

```
With Append Files           Without Append Files
100MB                             15MB                Without Post-Compliance Period
200MB                             30MB                With Post-Compliance Period
```

Feb 19, 2007   TPA validation

The following e-mail was received from J. Winterle:

```
 NRC no longer wants us to maintain a Unix version of the TPA code.
Please make sure any testing that is done gets done on a PC platform.
If we still want to have a Unix version for our own use, we can finish
compiling and validating that after the June 22 deadline for delivering
the PC version.
--Jim
```

Mar 1, 2007 LHS Correlations

The following e-mail was received from S. Stothoff:

```
I looked into the software end of the SNL LHS sample because of the issue
with incorrect correlations.

The original software was obtained sometime in the 1980's, with the first
modification by NRC in August 1989 by Codell.  The original software was
documented in SAND83-2365 (early 1980's).

A google search popped up with
http://www.cs.sandia.gov/DAKOTA/papers/LhsManual2004.pdf, which describes an
updated version for Unix/Linux from 2004.  This version is apparently very
similar to a windows version from 1998 documented in SAND98-0210.
Apparently substantial revision occurred in the mid-1990's, with more than
25 new distributions and porting to fortran 90.

In reading the new documentation, it became clear that we were
underspecifying the correlations.  It is not sufficient to specify 2 pairs
out of 3 variables, especially if they are highly correlated.  All three
pairwise correlations are needed.  The SNL LHS routines in the TPA code
appears to work correctly if all correlations are defined with valid values.
So we need to come up with some additional correlations if the infiltration
```

and seepage values are to be implemented properly.

I suggest that we take a look at the revised version of the LHS for future incorporation into the TPA code. There are some useful new distributions, such as truncated normal and truncated lognormal distributions, that would be very handy.

I also suggest that we invest in some off-line checking that all correlations are reasonable (all eigenvalues are nonnegative) in the TPA input. The new version of the LHS code prints out warnings if the input is inconsistent, but the older version does not.

March 13, 2007   Scientific Notebook Contributions

* = Contributing chapters for last 6 months.

1 - Janetzke* {ALBY\\D:\ronj-\wp\sn612e.wpd}
2 - Mohanty - not used
3 - Rice {ALBY\\D:\RonJ-\rob\SN612E*}
4 - Scherer {Guardian\\d:\docs\ScientificNotebooks\SN612-4E}
5 - Pensado - not used
6 - Benke {PHOENIX\\D:\Shared\Sci Notebook 612-6e}
7 - LaPlante {FROGGY\\D:\TPA\sci.notebk.612-7e.wpd}
8 - Adams* {PITOR\\D:\scientific notebook\Notebook612-8E\SN612-8E.wpd}
9 - Winfrey - closed
10 - Smith - not used
11 - Lozano - closed
12 - Wojcik - closed
13 - Osidele - not used
14 - unassigned
15 - Menchaca* {stu2560\\D:\jmenchaca\ScientificNotebook\SN612e.wpd}
16 - Portillo - closed
17 - Povetko {Paladin\\ D:\ScientificNotebooks\SN612_section17E_TPApovetko.wpd
18 - LeNeveu {ALBY\\D:\RonJ-\leneveu\SCIENTIFIC NOTEBOOKoct5.doc}
19 - Nes - not used
20 - Stead {\\Adriana\Data\DStead\TPAstuff\Sci_NB\SN612e_DStead.wpd}
21 - Mancillas* {Manta\\D:\Notebooks\SN612-21.wpd}
22 - Epps - closed

March 19, 2007   Reformatted Files List

In UNIX use:

```
>grep -c '! ' * | grep -v ':0' > grep.out
```

March 26, 2007   5000 Time Steps

A 500 realization run with 5001 time steps in 10k years, processing only the 10th subarea was manually halted at realization 255 due diminishing disk space. No errors were found.

March 27, 2007   5000 Time Steps

A 500 realization run with 5001 time steps in 10k years, processing all subareas, with NFENVFL and all modules after MECHFAIL omitted, halted in debug mode at realization 203 due to diminishing disk space. No errors were found.

March 29, 2007   Lahey Memory Leak Error

The following demonstration code for the Lahey memory leak error was prepared for Lahey support staff.

```
C Memory Leak
C March 29, 2007
        Program Memory_Leak
        character*80 c1
        character*80 c2
        character*80 c3
        character*80 c4

        c1 =' 1'
        c2 ='i10'
        c3 =' , '
        c4 ='(1i10 , 1i10)'
        open (11,'ml.out',status='UNKNOWN')
```

```
        do i=1,20000000
            write (6,fmt=c4) i, i*2

C Using the following line in V7.10.02 will cause
C a run time error when virtual memory size exceeds 2GB.
C (jwe0911i-u)
C Similar constructions using a READ do not cause the error.
            write (11,fmt='('//c1//c2//c3//c1//c2//')') i, i*2

        end do

        stop

        end
```

The lines in *fileutil.f* that exhibit the memory leak are 347, 416, 713, 719, 788, 794, 835, 900, and 977.

The suggested work around for the error at line 977 is:

FROM:

```
     WRITE(format_string(1:40), FMT = '(I5, A15, I5, A15)')
    &  numRealCols, '(2x, 1pe12.5),', numIntCols, '(13x, I1)'

c     Write the new line of text to the output file
     WRITE(ioutFile, FMT = '(1X, I5,' // format_string // ')')
    &    irow, (drealValues(index1), index1 = 1, numRealCols),
    &    (intValues(index2), index2 = 1, numIntCols)
```

TO:

```
     WRITE(format_string(1:50), FMT = '(A7, I5, A15, I5, A15,A2)')
    & '(1x,i5,',
    &  numRealCols, '(2x, 1pe12.5),', numIntCols, '(13x, I1)'
    & ,' )'

c     Write the new line of text to the output file
     WRITE(ioutFile, FMT = format_string)
    &    irow, (drealValues(index1), index1 = 1, numRealCols),
    &    (intValues(index2), index2 = 1, numIntCols)
```

Similar modifications can be made to the other lines to avoid concatenation

operations in the FORMAT string.

March 30, 2007   Lahey Response to Memory Leak Problem

```
Hi,
    I can see that there is a problem here - I have reproduced the error
on this machine with the same error messages. However, there are no
further patches planned for the Windows v7.1 compiler, and so all I can
suggest is that you find a way to work around the problem.

I'm sorry that I can't help any more.


--
Rob Appleyard            Lahey.Support@polyhedron.com
Lahey Compiler Support Team - Polyhedron Software Ltd.
Programs for Programmers - QA, Compilers, Graphics, Consultancy
********* Visit our Web site on http://www.polyhedron.com/ *********

Registered Office: Linden House, 93 High St,
Standlake, Witney, OX29 7RH, United Kingdom.
Registered in England No.2541693. Vat Reg No. GB 537 3214 57
```

May 5, 2007   Releaset variables

The following email attachment was received from R. Rice:

RELEASET variables

The following are variables contained in the *cumrel.out* file and also the *ebsrel.rlt* file.

xnoloss [Ci] – for a radionuclide, the number of Curies present in a WP; calculated based in the initial inventory available for release; accounting only for decay/ingrowth; and assuming no EBS release

amwp [Ci] – for a radionuclide, at a time corresponding to the maximum TPA code simulation time, the number of Curies that have accumulated in a WP from SF dissolution, but have not been released from the EBS; (note that this inventory may accumulate because of solubility limits)

xmass [Ci] – for a radionuclide, at a time corresponding to the maximum TPA code simulation time, the cumulative number of Curies that have been released from the EBS; this value may be found be integrating the releases in *ebsnef.dat* (a RELEASET output file that the TPA code reads) over the entire TPA code simulation time

<u>**Others**</u>

claddingcorfact – a *tpa*.inp file parameter (constant equal to 1); this factor has a proportionate affect on **amwp**, but no impact on **xnoloss** and a small impact on **xmass** (less than 0.5%); That is, if the factor is decreased from 1.0 to 0.5, **amwp** decreases by 50%. This value is included in the RELEASET input file *ebsrel.inp*.

sawetfrac – a *tpa*.inp file parameter (uniform from 0 to 1); this factor used to scale the calculated RELEASET values to reflect the inventory available for release; any change in this parameter results in a proportionate change in the three variables described above for the *relcum.out* file. This value is included in the RELEASET input file *ebsrel.inp*.

May 8, 2007   3 digit exponent format for *ashremob.out*

To handle 3 digit exponents for *ashremob.out* values the following format is suggested:

1pe13.4e3

May 17, 2007   Importance Analysis Parameters

The following text was removed from the User Guide at the request of NRC:

4.6   Importance Analysis Parameters

Some methods for revealing the degree of importance for a parameter require the direct manipulation of the sample parameter set. Specifically, it may be desired to assign a fixed value to a sampled parameter over all realizations, while keeping the values of all other sampled parameters unaltered from the reference case sampled data set. This method of analysis can be selected with the ImportanceAnalysisFlag(yes=1,no=0) flag usually located in the *tpa_include.inp* file.

The paradigm used is a four-tier hierarchical system of identifiers (subsystem, barrier, component, and parameter). The concept is such that the subsystem is at the highest level and may have one or more barriers associated with it. The barrier is one level below the subsystem and may have one or more components associated with it. The component level must have at least one parameter associated with it in such a way that all identifiers regardless of their level are associated with at least one parameter at some level at or below it in the hierarchy. There may be up to 3 subsystems, 11 barriers, 99 components, and 999 parameters total, defined in the four tier system.

This analysis scheme is implemented in a two part declaration. First the hierarchy is declared in the *ia.dat* auxiliary file, then all or selected pieces of the hierarchy can be invoked in the importance analysis flag section of *tpa_include.inp* file.

The declaration of the hierarchy is contained in the *ia.dat* file and requires the use of five keywords (SUBSYSTEM, BARRIER, COMPONENT, PARAMETER, and VALUE). Each of the first four keywords must be followed by an equal sign (=) and a quoted identifier string. The highest level keyword must appear first followed by succeeding levels such that all lower level declarations are associated with the higher level preceding it until another identifier at the higher level is declared. The identifier strings are arbitrary, but must be unique. In addition the PARAMETER keyword identifier string must be a valid sampled parameter name declared elsewhere in the *tpa.inp* file. The VALUE keyword must be followed by an equal sign (=) and either an integer or real numeric value. This constant value is assigned to the parameter for each realization when enabled.

The top three levels of identifiers declared in the hierarchy are invoked respecting their level and any subordinate identifiers and parameters. That is, if a SUBSYSTEM identifier is enabled for analysis, then all of the subordinate levels and parameters are invoked automatically.

The second part of the analysis scheme requires setting the enabling flags in the *tpa_include.inp* file. The unique identifiers are used as parameter names of 'iflag' type, such that a flag value of 1implies that the associated parameters are to be set to the respective constant value for all realizations. A flag value of 0 disables the parameters participation in the analysis method. There is no need to remove a parameter's declaration from the *ia.dat* file to disable the parameters participation in this case.

The use of this scheme to set one or more parameters to a constant value does not relax the restriction that the number of realizations specified must be greater than the number of sampled parameters in order to maintain correlated values in the sampled data set. The parameters are considered sampled relative to this restriction. In addition, if the parameter is also a correlated parameter, the values of the correlated parameter not declared in the four tier scheme are not affected compared to the reference case sampled data set. That is because SAMPLER generates the complete sampled set before the four-tier system is processed. The reassignment of the values for a given participating parameter is performed after the normal sample data set is generated.

May 30, 2007   Time of Next Event Reset Messages

Text prepared for e-mail distribution:

```
Just a summary regarding one of the points raised at today's meeting.  Use the
following abbreviations for this message:

VOL = volcano
FAU = faulting
TNE = time of next event

For both VOL and FAU, if the TNE is a constant it may be any positive value.
If the TNE is a constant  and negative, a message is printed to the screen
notifying the user that it is being reset to 0.0 and  the run continues.
```

```
For VOL and FAU,  if the TNE is a sampled parameter, the minimum time must be
greater than 0.0, if it is not, a message is printed to the screen  notifying
the user that it is being reset to 0.0 and the run continues.

For VOL only, if the TNE is sampled and the maximum time of next event is
greater than the simulation end time, a message is printed to the screen
notifying the user that it is being reset to the simulation end time, and the
run continues.

For FAU only, if the TNE is sampled and the maximum time of next event is
anything other than the simulation end time, a message is printed to the
screen  notifying the user that it is being reset to the simulation end time,
and the run continues.
```

June 21, 2007   TPA 5.1

The TPA 5.1 (validated) was delivered to the NRC.

June 26, 2007   Pslist command

On TPA server machine use:

```
>pslist /?
```

or

```
>pslist tpa
```

for process status.

June 21, 2007   TPA 5.1

TPA Version 5.1 was delivered to the NRC shared drive.

July 9, 2007   TPA 5.1

Received notification of acceptance of the TPA Version 5.1 code by the NRC.

Aug. 28, 2007   Localized Corrosion

Localized corrosion can be forced to occur before weld corrosion with the following inputs:

simulation time = 1,000,000 years
post compliance period time steps = 4800
number of realizations = 500
start realizations =1
stop realization =1
start subarea =7
stop subarea =7
outer WP thickness = .005
critical RH for aqueous corrosion = 2%
humid air corrosion = 1%

Sep 17, 2007 Scientific Notebook Contributions

* = Contributing chapters for last 6 months.

1 - Janetzke* {ALBY\\D:\ronj-\wp\sn612e.wpd}
2 - Mohanty - not used
3 - Rice {ALBY\\D:\RonJ-\rob\SN612E}
4 - Scherer {Guardian\\d:\docs\ScientificNotebooks\SN612-4E}
5 - Pensado - not used
6 - Benke * {PHOENIX\\D:\Shared\Sci Notebook 612-6e}
7 - LaPlante {FROGGY\\D:\pa\TPA\sci.notebk.612-7e.wpd}
8 - Adams {PITOR\\D:\scientific notebook\Notebook612-8E\SN612-8E.wpd}
9 - Winfrey - closed
10 - Smith - not used
11 - Lozano - closed
12 - Wojcik - closed
13 - Osidele - not used
14 - unassigned
15 - Menchaca {stu2560\\D:\jmenchaca\ScientificNotebook\SN612e.wpd}
16 - Portillo - closed
17 - Povetko * {Paladin\\ D:\ScientificNotebooks\SN612_section17E_TPApovetko.wpd
18 - LeNeveu {ALBY\\D:\RonJ-\leneveu\SCIENTIFIC NOTEBOOKoct5.doc}
19 - Nes - not used
20 - Stead {\\Constantine\D:\DStead\TPAstuff\Sci_NB\SN612e_DStead.wpd}
21 - Mancillas {Manta\\D:\Notebooks\SN612-21.wpd}
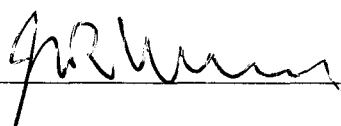22 - Epps - closed

Nov. 9, 2007   File System Errors

The following was sent to C. Grossman in response to his query on file access and I/O type errors.

```
Chris,

We have found that errors of this type are not repeatable and may indicate a
degraded file system from a Windows point of view.  These have a history of
appearing after certain operations, such as trying to access the same file
from two processes over a busy network, using a disk that needs
defragmentation, etc.  So you may be correct in assuming  that attempted
access to the screen file during a run may cause the error.  Some success has
been found by first copying the live screen output file to a temporary file
and then open the temporary file instead.

If this is a frequent error, you may want to defrag the disk and reboot the
machines on a regular basis.
```

I have reviewed this scientific notebook and find it in compliance with QAP-001.
There is sufficient information regarding methods used for conducting tests,
acquiring and analyzing data so that another qualified individual could repeat the
activity.

_____   _1/21/10_