SCIENTIFIC NOTEBOOK

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by

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INITIAL ENTRIES

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Title: TPA 5.0 Code Development

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

In-Process Entries

1-9-04 RISK ANALYSIS GADAMS:
File nfenv.f from tpa version 4.1k was modified to contain updated thermal equations. Hand calculations were performed on the updated code module at 0.85 m of backfill, 1.36m of backfill, and no backfill. In addition, two tests were conducted. The first test was performed for 350 realizations with 1.36m of backfill. The second test was

performed for the mean case at various percentages of the maximum backfill.

Testing was conducted on machine spock in directory: $HOME/NumericalRecipes/tpa41kanalysis

1-15-2004 RISK ANALYSIS GADAMS:
Conducted a test similar to the 350 realization test conducted under entry 1-9-04 RISK ANALYSIS GADAMS. However, in this test, the ThermalConductivityofYMRock[W/(m-K)] was changed from a uniform distribution 1.8, 2.2 to a triangular distribution 1.34, 1.59, 1.75. In addition, the output mode options were set to generate the ebsrel.ech and ebsrel.rlt files.

Testing was conducted on machine spock and test results were retrieved from directory:
$HOME/NumericalRecipes/tpa41kanalysis/tpa41kmod/test/results/backfill/test_350real1_36mbackfill_thermalcondymrocktriangular

1-30-2004 RISK ANALYSIS GADAMS:
Conducted a test similar to the mean value test conducted under entry 1-9-04 RISK ANALYSIS GADAMS. However, in this test, the ThermalConductivityofYMRock[W/(m-K)] was changed from a uniform distribution 1.8, 2.2 to a triangular distribution 1.34, 1.59, 1.75. This change resulted in the mean value for ThermalConductivityofYMRock[W/(m-K)] to equal 1.56 instead of the previous mean value of 2.0.

Testing was conducted on machine spock and test results were retrieved from directory:
$HOME/NumericalRecipes/tpa41kanalysis/tpa41kmod/test/results/backfill/test1-30-04

2-19-2004 RISK ANALYSIS GADAMS:
Within TPA Version 5.0r, evaluated waste package failure due to contact with the drip shield bulkhead. The model description and the equations used in the mechfail code are described in Scientific Notebook 410, pages 65-67.

Testing was performed on machine spock and hand calculations were performed to

check the code. A 100-realization and 350-realization base case (using tpa5.0r) and a 100-realization and 350-realization modified code test case (using the updated tpa5.0r code) were conducted. The source code was modified to account for a zero contact angle and then a third scenario 350-realization modified code test case was conducted. A comparison of the modified code 350-realization scenarios output files and gwpkdos.res files showed no change in generated output with the code modification.

Testing was conducted on machine spock and test results, hand calculations, test scenarios, and modified code were retrieved from directory: $HOME/contactangle.

2-24-2004 RISK ANALYSIS GADAMS:

Within TPA Version 5.0r, conducted a series of base case tests to use for comparison with modified code tests. All scenarios were run with 350 realizations. A description of the three base case scenarios is provided below:

Scenario 3: Base case tpa version 5.0r code, 350 realizations, base case tpa.inp file however drift degradation was turned off
(`DriftDegradationScenarioFlag(yes=1,no=0)` set to 0)

Scenario 4: Base case tpa version 5.0r code, 350 realizations, modified tpa.inp file to include sampled parameter:

```
normal
ContactAngle[degrees]
0.0, 45.0
```

In addition, mechanical failure was turned off :
(`DriftDegradationScenarioFlag(yes=1,no=0)` set to 0)
(`SeismicDisruptiveScenarioFlag(yes=1,no=0)` set to 0)

Scenario 5: Base case tpa version 5.0r code, 350 realizations, modified tpa.inp file to include sampled parameter:

```
normal
ContactAngle[degrees]
0.0, 45.0
```

Testing was conducted on machine spock and archived to:
$HOME/contactangle_02-24-2004/

2-26-2004 RISK ANALYSIS GADAMS:
Repeated the test conducted under entry 1-15-2004 RISK Analysis GADAMS except in this test, the Emplacement Backfill Thickness was set to 0.0. Generated ebsrel.ech and ebsrel.rlt files for further analysis.

Testing was conducted on machine spock and test results were retrieved from directory:

$HOME/NumericalRecipes/tpa41kanalysis/tpa41kmod/test/results/nobackfill/test 2-20-04.

2-27-2004 RISK ANALYSIS GADAMS:
An analysis was performed on the time required to perform the thermal calculations within the nfenv module. A summary of the times follows:

```
=================================================================
Stop statement added prior to thermal calculations portion of code
Optimization level O4 (standard build)

-----------------------------------------------------------------------
     subarea   1 of  10           realization    1 of    1
-----------------------------------------------------------------------
 exec: calling uzflow
 exec: calling nfenv

real        7.8
user        5.2
sys         0.8


Optimization level O1

-----------------------------------------------------------------------
     subarea   1 of  10           realization    1 of    1
-----------------------------------------------------------------------
 exec: calling uzflow
 exec: calling nfenv

real        6.4
user        5.3
sys         0.7
=================================================================
Stop statement added after the thermal calculations portion of code
```

```
Optimization level O4 (standard build)

-----------------------------------------------------------------------
     subarea   1 of  10           realization    1 of    1
-----------------------------------------------------------------------
 exec: calling uzflow
 exec: calling nfenv

real        6.5
user        5.2
sys         0.9


Optimization level O1
-----------------------------------------------------------------------
     subarea   1 of  10           realization    1 of    1
-----------------------------------------------------------------------
 exec: calling uzflow
 exec: calling nfenv

real        6.6
user        5.3
sys         0.9
=================================================================

Time to execute one realization of the tpa code for ten subareas
Optimization level O4 (standard build)

 exec:  Run Successfully Completed


real     1:12.6
user     1:00.2
sys         8.9

=================================================================
Time to execute two realizations of the tpa code for ten subareas
Optimization level O4 (standard build)

 exec:  Run Successfully Completed


real     2:26.8
user     2:04.4
sys        16.6


=================================================================
Time difference
```

```
real      1:14.2
user      1:04.2
sys          7.7

=================================================================
Time to execute one realization of the tpa code for subarea 1

 exec:  Run Successfully Completed


real        11.5
user         8.6
sys          2.3


=================================================================
Time to execute one realization of the tpa code for subareas 1 and 2

 exec:  Run Successfully Completed


real        19.3
user        14.9
sys          3.4

+++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
Per subarea time difference:
real         7.8
user         6.3
sys          1.1
```

Testing was conducted on machine SPOCK in directory:
$HOME/NumericalRecipes/tpa41kanalysis/timeanalysis

6-16-2004 RISK ANALYSIS GADAMS:
Evaluated waste package mechanical failure due to contact of the drip shield bulkhead with the waste package outer barrier. This work was previously described in entry 2-19-2004 RISK ANALYSIS GADAMS; however, the code changes were implemented in version 5.0u of the tpa code instead of version 5.0r of the tpa code. In addition, for the test analyses, 450 realizations were used. Three primary analyses were conducted: 1) The base case tpa5.0u code was executed for 450 realizations, 2) The base case tpa5.0u code was executed without mechanical failure for 450 realizations, and 3) The modified tpa5.0u code was executed. The tpa code was modified to include waste package mechanical

failure. The following files were modified: mechfail.f, seismo2.f, mechfail.def, and tpa.inp. These code modifications are included as part of SCR-481.

Testing and hand calculations to verify the code changes were performed on machine spock. Test results, hand calculations, and the modified code were retrieved from machine spock and are archived in: SPOCKHOMEcontactangle_06-16-2004.

6-17-2004 RISK ANALYSIS GADAMS:
Evaluated the effect of heat transfer through a porous natural backfill material on waste package temperature and the resulting dose. In this analysis, a 450 realization probabilistic assessment was performed for subarea 1. In addition, a sensitivity study was conducted for the mean case on subarea 1. In this study, the values for mean particle diameter, porosity, skewness, tortuosity, and coefficient of variation were varied to observe the effect on waste package temperature. The tpa code version 5.0s was used for this study.

Testing and hand calculations to verify the code changes were performed and the modified code was archived along with the test results and hand calculations in: task20_06-17-2004.zip.

7-9-2004 RISK ANALYSIS GADAMS:
Evaluated waste package mechanical failure due to contact of the drip shield bulkhead with the waste package outer barrier. This work repeats the work previously described in entry 6-16-2004 RISK ANALYSIS GADAMS; however, localized corrosion was eliminated. Localized corrosion was eliminated by setting ErpInterceptWeld[mVSHE] and OuterOverpackErpIntercept both to high values (1.0×10^{10}).

Test results were retrieved from machine spock and are archived in: SPOCKHOMEcontactangle_07-09-2004.

7-28-2004 SCR-480, SCR-481 GADAMS:
Modified tpa version 5.0v to implement changes in SCR480 and 481. SCR 480 takes the drift degradation computed in the mechanical failure modules (Seismo, Mechfail) and provides a degraded drift diameter and natural backfill diameter to

the thermal models in nfenv.f. The thermal models were also upgraded to account for the natural backfill accumulation over time. SCR 481 was included to account for mechanical failure of the waste package due to contact of the drip shield with the waste package. The following files were added/modified to incorporate these changes: ashplumo.f, driftcmn.i, ebsfail.f, ebsrel.f, exec.f, execa.i, mechfail.def, mechfail.f, nfenv.f, nrutil.f, seismo2.f, tpa.inp, zbrent.f.

Hand calculations, the modified files, and test results are included in archive: SCR480_481_7-28-04.zip.

11-15-2004 SCR 521GADAMS:
Performed testing on SCR 521 for version tpa41jpdls_beta of the tpa code. This version of the code is used for long simulation periods. Five system level tests were conducted and are as follows:
SL-1: Temperature and Reflux Comparison, compare temperature, relative humidity, and flows between the base version (tpa4.1jpd1k) and the long simulation version of the code.
SL-2: Seismic Analysis, generate comparable output (time and magnitude of seismic events) between the base version and the long simulation version.
SL-3: Cladding/Gap Fraction Effect on Release, verify changes in cladding and gap fraction will affect the release in a similar manner between the base case and the long simulation versions of the code.
SL-4: Matrix Diffusion Calculations, as diffusion rate was decreased to zero, the delta time (between release from the UZ and SZ) for the peak release rates for Np237 and I129 decreased.
SL-5: Thermal Perturbation Period Restriction Removed, verifies that the flow hitting the waste package is reduced when the 10,000 year reflux restriction is removed.

The test plan and test results are included in archive: SCR521.zip.

11-15-2004 SCR 520 GADAMS:
Performed modifications to version tpa5.0.0d of the tpa code to incorporate the following changes:
1) Consistent drip shield failure time: Modified exec.f to move the mechanical failure calculations to before the call to nfenv. This change provides a consistent

drip shield failure time for the concentration calculations in nfenv. Also, modified ebsrel.f such that if there is no failure during the simulation period, then the time of drip shield failure is set to a time later than the simulation period.
2) Relative humidity calculation: Added a smoothing algorithm to nfenv.f to the relative humidity calculations such that the relative humidity for the period immediately after closure is weighted to use the preclosure relative humidity.
3) Vapor pressure calculation: Modifications were made within nfenv.f to limit the temperature range for the vapor pressure calculation. The calculations for the vapor pressure at temperatures above 374.3C were limited to the vapor pressure at 374.3C.

The modified source code files are included in archive: SCR520.zip.

12/15/2004 TPA Validation GADAMS:
Performed tpa 5.0.1 validation testing of the NFENV module using version tpa500e of the tpa code. Performed seven validation tests that are described as follows:
1) SVTR-NFENV1: Performed testing of permeability calculations within the iterative thermal module.
2) SVTR-NFENV2: Performed testing of thermal calculations within the iterative thermal module.
3) SVTR-NFENV3: Performed testing of thermal calculations within the linear thermal module for the wedge subcase.
4) SVTR-NFENV4: Performed testing of thermal calculations within the linear thermal module for the no-wedge subcase.
5) SVTR-NFENV5: Performed testing of the distributions generated for pH, nitrate, and chloride chemistries.
6) SVTR-NFENV6: Performed testing of the algorithm used to select the chemistry values.
7) SVTR-NFENV7: Performed verification that the reflux model could generate the same output results as in version tpa5.0o of the tpa code.

Tests 1 and 2 did not pass since the equations did not match the documented information. Tests 3-7 passed.

Output and test results are included in archive: tpa5.0.1validation.zip.

2/11/2005 SCR553 GADAMS:

Implemented changes to TPA code version 5.0.0f for SCR553. The following code modules were changed: nfenv.f, seismo2.f, condxyzt.f, cond3dxyzt.h, exec.f, mechfail.f, nrutil.f; and the following data files were changed: tpa.inp and mechfail.def. The following outlines the changes made to the tpa code:

Used the following reference to establish thermal properties for air in tpa.inp: Incropera, Frank P. and David P. Dewitt. 1981. Fundamentals of Heat Transfer. New York, New York: John Wiley & Sons.

Parameters are based on a peak waste package temperature in a no-backfill condition of 165 °C or 438 K.

1) Changed parameter:
constant
KinematicViscosity[m^2/s]
32.39e-6

to

constant
KinematicViscosityOfAir[m^2/s]
30.95e-6

based on Table A.4 of the reference:
400K: 26.41e-6 m^2/s
450K: 32.39e-6 m^2/s
linear interpolation to 438K: 30.95e-6 m^2/s

2) Changed parameter:
constant
VolumeOfThermalExpansion[1/K]
2.85e-3

to

constant
VolumeOfThermalExpansionOfAir[1/K]
2.28e-3

based on:
Assumption of an ideal gas and using equation 9.10 from the above reference:
$\beta = 1 / T = 1/438K = 2.28e-3$

3) Added parameter:
constant
DensityOfAir[kg/m^3]
0.797

based on Table A.4 of the reference:

400K: 0.8711 kg/m^3
450K: 0.7740 kg/m^3
linear interpolation to 438K: 0.797 kg/m^3

4) Added parameter:
constant
SpecificHeatOfAir[kJ/kg-K]
1.019

based on Table A.4 of the reference:
400K: 1.014 kJ/kg-K
450K: 1.021 kJ/kg-K
linear interpolation to 438K: 1.019 kJ/kg-K

5) Added parameter:
constant
PrandtlNumberForAir[]
0.687

based on Table A.4 of the reference:
400K: 0.690
450K: 0.686
linear interpolation to 438K: 0.687

6) Removed parameter:
constant
ThermalDiffusivity[m^2/s]
3.417e-4

Replaced with the following calculation within nfenv.f:
Thermal Diffusivity of Backfill = conductivity of backfill / (density of air * specific heat of air)

7) Modified the calculation for standard deviation of a particle size distribution to agree with equation 11-5 of the RARI report.

8) Added parameter TimeOfRepositoryClosure[yr] and updated nfenv.f, exec.f, seismo2.f, cond3dxyzt.f, and mechfail.f to use this parameter in place of TimeOfBackfillEmplaced[yr].
constant
TimeOfRepositoryClosure[yr]
50.0

Removed parameter:
constant
TimeOfBackfillEmplaced[yr]
10000.0

9) Changed parameter
constant
ThermalConductivityOfAir[W/(m-C)]
37.3e-3

to

constant
ThermalConductivityOfAir[W/(m-C)]
36.5e-3

based on Table A.4 of the reference:
400K: 33.8e-3 W/(m-K)
450K: 37.3e-3 W/(m-K)
linear interpolation to 438K: 36.5e-3 W/(m-K)

Files which were changed for SCR553 are archived in SCR553.zip.

4/8/2005 TPA Parameters - Particle Size GADAMS:

A set of 5000 particle sizes generated from Monte Carlo sampling was used to generate values for the mean, median, skewness, and standard deviation of backfill particles. The following parameter changes in tpa.inp were identified:

For the Section of tpa.inp under NFENV

** For particle model 1, the BackfillParticleDiameter is the median
constant
BackfillParticleDiameter[m]
0.1549
**
** For particle model 2, the BackfillParticleDiameter is the mean
constant
BackfillParticleDiameter[m]
0.2044

constant
SkewnessOfDistribution[]
0.623

We also have a standard deviation for the particle size distribution which together with the BackfillParticleDiameter will replace the CoefficientOfVariation

constant
BackfillParticleStandardDeviation[m]
0.1838

The files used to generate the distribution and obtain the resulting parameters are included in archive particlesize.zip.

4/22/2005 SCR562 GADAMS:

TPA code version 5.0.0m was modified to implement the following changes:

```
1)Removed the parameters TiCorrosionRateVsFluorideSlope[],
MinimumFluoride[mol/L], MaximumFluoride[mol/L], and
UseFluorideEnhancingFactor(0=no,1=yes)from tpa.inp.
2) Modified dsfail.f to allow the user to change the name for the fluoride
data file.
3) Changed ThermalConductivityOfBackfill[W/(m-C)] to
ThermalConductivityOfBackfillModelOne[W/(m-C)] and added parameter
ThermalConductivityOfBackfillModelTwo[W/(m-C)]. Also, placed these parameters
near the parameter, SelectThermalModel(1,2) within tpa.inp.
4) Corrected the spelling error in exec.f (changed shiled to shield).
5) Added a note in tpa.inp section Disruptive Scenario Flags to indicate that
both SeismicDisruptiveScenarioFlag(yes=1,no=0) and
DriftDegradationScenarioFlag(yes=1,no=0) must be set to no(0) in order to turn
off natural backfill accumulation.
```

The following files were changed to implement this SCR: setupCommons.h, buildInputFiles.h, dsfail.f, exec.f, nfenv.f, dsfailt.def, and tpa.inp.

The files that changed as well as some hand calculation check files are included in archive: SCR562.zip.

6/15/2005 TPA Parameters GADAMS:

Entry 2/11/2005 SCR553 GADAMS includes parameter values based on information in Incropera, Frank P. and David P. DeWitt. 1981. Fundamentals of Heat Transfer. New York, New York: John Wiley & Sons. Data was rechecked in a newer version of the reference. The following updated reference was used: Incropera, Frank P. and David P. DeWitt. 2002. Fundamentals of Heat and Mass Transfer, 5th edition. John Wiley & Sons. Table A.4 of the updated reference was used along with equation 9.9 in this reference.

7/1/2005 TPA Validation GADAMS:

Conducted validation testing under task 6 for the tpa software version 5.0.1Beta. This testing involved the linear thermal model included in nfenv.f for cases with and without backfill. For this testing, spreadsheet calculated thermal parameters agreed to within 0.5% with those generated from the tpa execution and displayed within the thermal.dat files.

Supporting files are included in archive validation_task_6-2.zip.

7/29/2005 SCR589 GADAMS:

For the thermal calculations, the degraded drift diameter that was being used was the diameter for the time step after backfill reached 5.5 m in the degraded portion of the drift. Instead of using this value, the nfenv.f code was modified to interpolate between the times for which the backfill reaches 5.5 m. Modifications were made to version 5.0.1BetaE of the tpa code.

Supporting files to include the modified nfenv.f file and test results are included in archive SCR589.zip.

11/8/2005 SCR594 GADAMS:
The file, dsfail.res, does not provide consistent, cumulative failures for mechanical and corrosive drip shield failures. File exec.f in tpa version 5.0.1BetaH was modified to allow the code to recognize when no mechanical drip shield failures occurred prior to corrosion failure for all time steps in addition to the initial time step.

Supporting files to include the modified exec.f file and test results are included in archive SCR594.zip.

12/7/2005 SCR586 GADAMS:
Performed acceptance testing for SCR586 using versions tpa5.0.1BetaG and tpa5.0.1BetaH. Performed two process level tests and two system level tests. The process level tests were used to compare the thermal calculation outputs to spreadsheet calculations for the cases of no backfill and natural backfill. The system level tests were used to compare the output from the iterative model to both previous results and to results from the linear thermal model.

Supporting test result files are included in archive SCR586.zip.

12/27/2005 SCR604 GADAMS:
Made code modification changes for SCR604 to add passive ventilation during the preclosure period. TPA code version 5.02C was used for these changes and the following files were modified: tpa.inp, nfenv.f, condxyzt.f, driftcmn.i, and cond3dxyzt.h. The tpa.inp file was modified to include factors for ventilation heat loss during both active and passive periods. Thermal calculation algorithms were modified to use the active and passive heat loss factors, and the mountain scale

conduction model routine was modified to consider these two preclosure ventilation periods.

Testing results showed that with 20 Gauss Legendre weights compared to 100 Gauss Legendre weights, an integration error of about 2 degrees C occurred during the passive ventilation period and an integration error of about 3 degrees C occurred during the postclosure period.

Test results and modified code files are included in archive SCR604.zip.

12/28/2005 HT_Convection GADAMS:
Performed an analysis of rock size distribution for which alpha varies between 0.1 and 0.35 as one alternative and between 0.1 and 0.6 as a second alternative. Both alternatives had a maximum fragment size of 700 mm. For the first alternative, the mean rubble diameter is 0.13m with a standard deviation of 0.18m and skewness of 1.5. For the second alternative, the mean rubble diameter is 0.18m with a standard deviation of 0.20m and skewness of 1.0.

Performed calculations for the Rayleigh number as a function of permeability and porosity for the first alternative with porosity varied between 0.1 and 0.6, the temperature difference varied between 10 °C and 40 °C, and the thickness of the porous medium varied between 0.26 m and 1.36m. The following values were held constant:

Symbol	Parameter	Value
β	Volume of thermal expansion	0.00228 1/K
ν	Kinematic viscosity	3.1×10^{-5} m^2/s
g	Acceleration caused by gravity	9.81 m/s^2
τ	Tortuosity of the medium	2.125
r_i	Inner radius of annulus	1.39 m

α_m	Thermal diffusivity	3.32×10^{-4} m²/s

Spreadsheet calculations, a plot of the Rayleigh number versus permeability and porosity, and the alternative 1 and alternative 2 rubble size distribution results are included in archive: HT_Convection.zip.

1/26/2006 SCR603 GADAMS:
Performed acceptance testing for SCR603 using version 5.0.2e of the tpa code. Performed one process level test and four system level tests. The process level test was used to verify the screen output shows the actual path of the system environment variables. The system level tests were used to verify the correct number of waste packages are being tabulated in wpsfail.res and that these tabulated values reflect the number of waste packages used in the release module.

Supporting files for test results are included in archive SCR603.zip.

2/9/2006 SCR605 GADAMS:
The drythick.dat file was updated to include data for a degraded and nondegraded drift and a time for the end of the thermal pulse. Also, ebsrel.f was modified to copy ebsrel.inp to ebsrelsf.inp before running the glass waste form. The following files were modified in version 5.0.2f of the tpa code: nfenv.f, exec.f, seismo2.f, ebsrel.f, and drythick.dat.

In order to generate data for the degraded case which could be used in drythick.dat, a mean case tpa 5.0.2f test run was conducted with the following changes to tpa.inp:

```
beta
BulkingFactorRockTypeOneSubarea_1[]
1.0,2.0,23.175,92.699

beta
BulkingFactorRockTypeTwoSubarea_1[]
1.0,2.0,23.175,92.699

lognormal
DegradationTimeRockTypeOneSubarea_1[yr]
369.32, 1523.05
```

```
lognormal
DegradationTimeRockTypeTwoSubarea_1[yr]
369.32, 1523.05
```

Modified files and support files for the mean case test run are included in archive: SCR605.zip.

2/24/2006 SCR605 GADAMS:
Changed the logic in file nfenv.f to use the time of degradation that is the time of first full drift degradation (either rock type 1 drifts or rock type 2 drifts). Previously, the time of degradation used was just the time for rock type 1 drifts to reach full drift degradation.
The modified nfenv.f file is included in archive: SCR605_extended.zip.

3/22/2006 SCR609 GADAMS:
Replaced the existing mechanical failure abstraction in version 502h of the tpa code with a new mechanical failure abstraction. Drift failure was separated out and included in a DRIFTFAIL module and implemented under SCR610. Mechanical failure of the drip shield and waste package were implemented in the new MECHFAIL module implemented under this SCR.

The following files were affected by this change: ashplumo.f, cumfail.h, ebsfail.def, ebsfail.f, ebsfail.h, ebsrel.f, exec.f, execa.i, failt.f, fileunit.f, fileutil.f, getdsfailure.h (removed), getdsfailure.t (removed), mechadj.i (removed), mechdrive.f (added), mechfail.f, putfailwp.h, releaset.f, sampler.f, seismo2.f (removed), tpa.inp, wpsfail.res, seisadj.i, mechfail_ds.def (added), and mechfail_wp.def (added).

The mechanical failure module is a standalone module contained in file mechfail.f. The mechanical failure driver is included in file mechdrive.f. The mechanical failure module is invoked twice per subarea by the tpa executive. When the module is first invoked, it is used to generate the fraction of drip shields that fail versus time. When it is invoked the second time, it is used to generate the fraction of waste packages that fail versus time.

As part of the changes for the MECHFAIL module, the waste package corrosion failure module (EBSFAIL/FAILT) had to be moved and modified. The waste

package corrosion module was modified to generate waste package outer layer thickness versus time. This module was moved to execute prior to the second call to MECHFAIL so that waste package outer layer thickness could be supplied to the MECHFAIL module.

A partial list showing the tpa code module execution order is as follows:
DRIFTFAIL (SCR610) –> NFENVFL –> DSFAIL –> MECHFAIL (Drip Shield) –> NFENV –> EBSFAIL –> MECHFAIL (Waste Package)

The modified files are included in archive: SCR609.zip.

4/10/2006 SCR610 GADAMS:
Tested a modified version of tpa 5.0.2q on Windows machine, "tpa" and UNIX machine, "spock." Version 5.0.2 q was used with updated driftdrive.f and driftfail.f files. All process level and system level tests successfully passed.

Developed eight process level and two system level tests. The process level tests were designed to compare the DRIFTFAIL module outputs against spreadsheet calculations. The system level tests were designed to check drift degradation time and vertical pressure outputs over multiple realizations.

In the process level tests, drift heights, vertical pressures, and equivalent diameters were checked against spreadsheet calculations. For tests pl-1 through pl-6, version tpa5.0.2qmod1 was used. Tests pl-1 and pl-2 were degradation-only scenarios; tests pl-3 and pl-4 were degradation and seismic scenarios; and tests pl-5 and pl-6 were degradation and seismic scenarios with an early seismic event. For tests pl-7 and pl-8, version tpa5.0.2qmod2 was used. Tests pl-7 and pl-8 were seismic-only scenarios.

For the process level tests, the "drift height above the invert" percentage errors between the tpa generated results and the spreadsheet calculations were consistently greater than the percentage errors between other spreadsheet and tpa generated values. There was a difference in the technique for averaging and calculating the resulting drift heights between the code and the spreadsheets. This larger percentage error occurs during the early period of drift degradation.

In the first system level test, the drift degradation times generated from multiple realizations were compared to the target input distribution. The first test case was a degradation-only scenario, and the second test case involved both degradation and seismicity. In the second system level test, the vertical pressures for the chimney and trapezoid drift degradation mechanisms were compared over multiple realizations.

After completing the process level and system level tests on Windows machine "tpa" the tests were repeated on UNIX machine "spock." The output files from the UNIX execution were compared to those from the Windows execution. All testing on machine "spock" was done with version tpa5.0.2qmod2.

The modified files used in versions 5.0.2qmod1 and 5.0.2qmod2 and test results are included in archive: SCR610.zip.

5/30/2006 TPA Validation GADAMS:
Conducted Task-8 validation using version 5.1BetaB of the tpa code. This validation was for the nrutil module of the tpa code. In this task, equations were compared against references 1 through 3 below. In addition parameter values were compared against values identified in SCR553 and references 4 and 5 below. Validation passed for these comparison checks. The following references were identified for this task:

1. Mohanty, S., et. al. "Risk Analysis for Risk Insights Progress Report," Center for Nuclear Waste Regulatory Analyses. San Antonio, TX. May 2005.

2. Fedors, R.W., et. al. "Thermal Conductivity, Edge Cooling, and Drift Degradation - Abstracted Model Sensitivity Analyses for Yucca Mountain," CNWRA Report, San Antonio, Texas: Center for Nuclear Waste Regulatory Analyses. 2003.

3. Panda, M. and Larry Lake. "Estimation of Single-Phase Permeability from Parameters of Particle-Size Distribution," AAPG Bulletin. Vol. 78, No. 7. American Association of Petroleum Geologist. July 1994.

4. DOE. "Ventilation Model and Analysis Report," ANL-EBS-MD-000030 Rev 03. Las Vegas, Nevada: DOE. 2003

5. DOE. "Multiscale Thermohydrologic Model," ANL-EBS-MD-000049 Rev00 ICN 01. Las

Vegas, Nevada: DOE. 2000.

8/17/2006 TPA Validation GADAMS:
Conducted Task-5 validation testing of the DRIFTFAIL module using version 5.1BetaD of the tpa code. In this task, the drift degradation vertical pressures generated from TPA runs were compared against those documented in Scientific Notebook 782E.

There were two test cases. In the first test case, vertical pressures for the tpa trapezoidal degradation mechanism were compared against the vertical pressures from the Terzaghi mechanism. In the second test case, vertical pressures for the chimney mechanism were generated along with vertical pressures for the trapezoidal mechanism. The vertical pressures for the chimney mechanism were compared against the vertical pressures for the piping mechanism. The validation testing passed for both of these test cases.

Supporting files are archived in: validation_task_5.zip.

9/25/2006 SCR660 GADAMS:
The changes in SCR660 primarily affected the MECHFAIL module of the TPA code. For this SCR, two result files were added for the MECHFAIL module. To track mechanical waste package failures, mechfail_wp.res was added. To track mechanical drip shield failures, mechfail_ds.res was added. Modifications were also made to send the waste package outer layer thickness from general corrosion to the MECHFAIL module. In addition, the array dimension for variable, BF, was increased in file sizes.inc to allow analyses to take place for long simulation periods.

Modifications were made to version 5.1BetaD of the TPA code. The following files were modified for this SCR: exec.f, mechdrive.f, mechfail.f, ebsfail.f, driftdrive.f, sizes.inc. The modified files are archived in: SCR660.zip.

12/20/2006 SCR669 GADAMS:
Reformatted the mechanical failure module (MECHFAIL) default input files mechfail_wp.def and mechfail_ds.def. Added subroutines to fileutil.f to retrieve the input in the updated format. Modified mechdrive.f and mechfail.f to use the

new subroutines in fileutil.f.

Modifications were made to version 5.1BetaG of the TPA code. The following files were modified for this SCR: fileutil.f, findrecord.f (new), mechdrive.f, mechfail.f, mechfail_wp.def, mechfail_ds.def. The modified files are archived in: SCR669.zip.

1/26/2007 SCR677 GADAMS:
This SCR involved the reformatting of output files. Altogether, 10 output files were affected: failt.cum, nearfld.res, mechfail.ech, mechfail.rlt, mechfail_ds.res, and mechfail_wp.res.

On the following files, the extension was changed to ".dbg:" echofail.dat to echofail.dbg, mechfail_ds.out to mechfail_ds.dbg, and mechfail_wp.out to mechfail_wp.dbg.

Removed the file, "corrode.out."

Modifications were made to TPA version 5.1BetaJ. The following files were modified: mechdrive.f, exec.f, ebsfail.f, codes/failt.f, data/ebsfail.def, codes/corrfail.f, and codes/corrosn.f. The modified files are archived in: SCR677.zip.

2/15/2007 SCR680 GADAMS:
This SCR involved the reformatting of output files. Altogether 4 output files were affected: nfenv.ech, nfenv.rlt, chlrdmf.dat, and thermal.dat. Files nfenv.ech, nfenv.rlt, and chlrdmf.dat were reformatted, and the file extension was changed for thermal.dat to thermal.dbg.

Modifications were made to TPA version 5.1BetaK. The following files were modified: exec.f, nfenv.f, ebsfail.f, and codes/failt.f. The modified files are archived in: SCR680.zip.

3/9/2007 SCR659 GADAMS:
This SCR involved minor edits to the MECHFAIL module to remove hardcoded values from the code and to change the bulking factor distribution from a uniform

distribution to a beta distribution. In addition, an interpolation table was added to mechfail_ds.def to remove hardcoded values for the drip shield temperature multiplier calculation.

Modifications were made to TPA version 5.1 BetaM. The following files were modified: tpa.inp, mechfail_ds.def, codes/mechfail.f, and mechdrive.f. The modified files are archived in: SCR659.zip.

3/9/2007 SCR664 GADAMS:
This SCR was a minor change to exec.f to remove the display of seismic event information from driftfail.ech and driftfail.rlt when the SeismicDisruptiveScenarioFlag(yes=1,no=0) is set to 0.
The testing was performed on version 5.1BetaQ and the test results are archived in: SCR664.zip.

3/9/2007 SCR681 GADAMS
This change involved removing hardcoded values for seismic evaluation by replacing the parameter SeismicHazardCurveforSEISMO with Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_].

The testing was performed on version 5.1BetaQ and the test results are archived in: SCR681.zip.

5/7/2007 SCR685 GADAMS:
This work involved the testing of certain components of the SCR change. Testing was done for change 1: RockMassDensityForRockTypeOne changed to 2068 kg/m^3 and RockMassDensityForRockTypeTwo change to 2245 kg/m^3 and change 8: drip shield thickness decreases before drip shield emplacement.

For change 1, version 5.1BetaW was tested on Machine GOLDSIM. and files tpa.inp and driftfail.inp were reviewed for the correct rock mass density values.

For change 8, three cases were run using version 5.1BetaW on Machine GOLDSIM. The drip shield thickness was evaluated at an initial thickness of 0.0 m, 0.13 m, and the base case value of 0.015 m. Files dsfail.rlt, mechfail_ds.inp, and mechfail_wp.inp were examined for drip shield thickness versus time. The

drip shield thickness remained at the initial thickness value for the period prior to repository closure in all three cases.

This SCR passed for the tests on changes 1 and 8; however, the parameter for MassDensityofYMRock had a value of 2540. Recommended this parameter be considered for consisitency with the mass density values being used in the MECHFAIL module. The test result files are archived in: SCR685.zip.

Subsequent to this SCR and testing, the following change and justification was developed for the TPA parameters concerning rock mass density:

Justification for Values of TPA Parameters

Parameters: RockMassDensityForRockTypeOne (bulk density of lower lithophysal unit)
RockMassDensityForRockTypeTwo (bulk density of middle nonlithophysal unit)
MassDensityofYMRock (average site-scale bulk density)

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Date: April 3, 2007
Revised: April 25, 2007

Bechtel SAIC Company, LLC. (2003, table 8-7, p. 8-20) provides values of dry bulk density ($\rho_{b\text{-}dry}$) for Topopah Spring Tuff units, including

$\rho_{b\text{-}dry}$ = 1979 kg/m3 for Tptpll (lower lithophysal unit)
$\rho_{b\text{-}dry}$ = 2148 kg/m3 for Tptpmn (middle nonlithophysal unit)
$\rho_{b\text{-}dry}$ = 2211 kg/m3 for Tptpln (lower nonlithophysal unit)

Values of moist bulk density are not provided but an average saturated bulk density ($\rho_{b\text{-}sat}$) of 2411 kg/m^3 is given for the Tptpln unit (Bechtel SAIC Company, LLC., 2003, table 8-8, p. 8-21).

To estimate the moist bulk density for Tptpll and Tptpmn units using this data, it is assumed the bulk density (ρ_b) at a given saturation (s)[range: 0.0, 1.0] can be represented using the equation

$\rho_b = \rho_{b\text{-}dry} + s(\rho_{b\text{-}sat} - \rho_{b\text{-}dry})$ and $\rho_{b\text{-}sat} - \rho_{b\text{-}dry} = \alpha\rho_{b\text{-}dry}$

The data for Tptpln gives α=0.09 and s is set to 0.9 to obtain an estimate for average moist conditions. Therefore, the above equations give

$\rho_b = 1.081(\rho_{b\text{-}dry})$

which gives

ρ_b = 2,139 for Tptpll and ρ_b = 2,322 for Tptpmn. The average site-scale bulk density $\rho_{b\text{-sitescale}}$ is estimated as a weighted average assuming Tptpll and Tptpmn occupy 85% and 15%, respectively, of the site.

$\rho_{b\text{-sitescale}} = 0.85(2139) + 0.15(2322) = 2166$

Therefore,

RockMassDensityForRockTypeOne = 2,139 kg/m3
RockMassDensityForRockTypeTwo = 2,322 kg/m3
MassDensityofYMRock = 2,166 kg/m3

References

Bechtel SAIC Company, LLC. "Subsurface Geotechnical Parameters Report" 800-K0C-WIS0-00400-000-00A. Las Vegas, Nevada: Bechtel SAIC Company, LLC. 2003.

No Further entries JRW 2/11/2010