SOFTWARE VALIDATION REPORT
FOR
TOTAL-SYSTEM PERFORMANCE ASSESSMENT
(TPA) CODE VERSION 5.1

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Date

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Section Page

1. INTRODUCTION

1.1 Background

The Total-system Performance Assessment (TPA) Version 5.1 code is being developed as a tool to aid in the review of a potential license application for a nuclear waste repository at Yucca Mountain. The code will be used as needed by the NRC and CNWRA staffs in their independent analyses to identify those aspects of natural and engineered repository components that may significantly affect repository performance. Over the course of TPA code development, numerous changes have been made to implement modifications to the potential repository design or improvements to the conceptual understanding of natural or engineered system responses. Code development activities are guided by the CNWRA quality assurance procedures in Technical Operating Procedure (TOP)–018, Development and Control of Scientific and Engineering Software. TOP–018 requires validation testing of developed software to gain additional confidence that the software successfully implements the underlying theory and algorithms.

1.2 Purpose

The plan for conducting the validation testing of TPA Version 5.1 is documented in the March, 2007, Software Validation Plan for Total-System Performance Assessment (TPA) Version 5.1. This software validation report provides documentation of the results of the validation tests described in the plan, interpretations of those results, and identification and resolution of any problems.

1.3 Scope of Validation

As described in the Software Validation Plan for TPA Version 5.1 (Winterle, et al., 2007), validation testing will include two categories of testing: (i) process-level tests will evaluate the results of individual modules, submodules, or subroutines; (ii) system-level tests evaluate the main results of the system taken as whole. This combination of process-level and system-level testing constitutes a full validation of all of the software functions of TPA Version 5.1. Upon completion of this validation report, the accompanying Software Release Notice will indicate the validation status of TPA Version 5.1 as a “fully validated” software; that is to say, the full capability of the software will have been tested or otherwise verified.

2. SOFTWARE VERSIONS TESTED

The validation process was conducted using successive updates of the TPA version 5.1Beta code. The programs were compiled using Lahey LF95 version 7.1 (PC version) or the SUNWspro Fortran compiler version 5.0 (UNIX version). Validation testing was conducted almost entirely using the PC version of the code, which is the preferred platform. Most of the validation testing was conducted using the software version designated as TPA Version 5.1BetaT or later. A few validation tests, however, were conducted using earlier versions of the TPA 5.1Beta series (e.g., validation task P-3 used TPA Version 5.1BetaD); in these cases, it was verified through technical review that subsequent code changes did not affect the validity of the test. Because the nature of validation testing is to find and fix errors, several revisions to the software were made during the validation process (versions 5.1BetaU, 5.1BetaV, etc.). Validation tests were repeated only for those tests affected by the changes. Additionally, a subset of the system-level validation task S-4 was repeated using a penultimate version of the code (Version 5.1betaY) prior to configuration for final release. This repeated system-level testing provides confidence that changes in one software module do not introduce errors in the operation of other modules. The version of the code tested is indicated on the cover sheets for the attached reports for each of the 22 validation tasks.

3. SOFTWARE VALIDATION TEST REPORTS

As described in the Software Validation Plan for Total-System Performance Assessment (TPA) Version 5.1, the validation comprises 18 process level tasks (designated with a “P” prefix) and 4 system-level tasks (designated with a “P” prefix). Each process-level task comprises one or more tests aimed at testing particular software functionalities at the level of individual abstraction modules or subroutines. The system-level tasks are aimed at evaluating whether the software functions as a whole and that overall system results are explainable.

The testing, analysis, and interpretation of results for each of the validation tasks are documented in 22 individual software validation task reports, which follow this summary. A list of all the included validation reports is provided in Table 1. Table 1 also provides a cross reference for each of the 22 validation task reports to the applicable section of the Software Validation Test Plan (Winterle, et al., 2007) in which the test objectives are described.

Each of the attached validation task reports begins with a Software Validation Report cover sheet followed by one or more attachments that provide descriptions of the tests, test criteria, test results, and analyses of results. The cover sheet for each task contains summary information to describe the task, versions of the code used for testing, analytical methods used, locations of archived data files used in the analysis, and an overall assessment of whether the test passed or failed. Since any failed test resulted in a code fix and repeat of the test, these final validation task reports will all indicate that the tests have passed (i.e., all test criteria were met). Page numbers on each task report indicate the task identification, the attachment number, and page number of the attachment. For example, page number P11 A-2 indicates the second page of Attachment A of the Task P-11 report.

4. REFERENCE

Winterle, J., Grossman C., Janetzke, R. “Software Validation Plan for Total-system Performance Assessment (TPA) Code Version 5.1.” San Antonio, TX: Center for Nuclear Waste Regulatory Analyses. 2007.

Table 1. Summary of Process-Level and System-Level Validation Task Reports		
Task I.D.	**Software Function Tested**	**Applicable Section of Software Validation Plan (Winterle, et al., 2007)**
P-1	Executive functions: module execution and management of input/output data	6.1.1
P-2	Routine and subroutine libraries	6.1.2
P-3	Inventory control	6.1.3
P-4	Climate and subarea-averaged net infiltration	6.1.4
P-5	Near field chemical and temperature conditions	6.1.5
P-6	Drift degradation	6.1.6
P-7	Mechanical failure of drip shields and waste packages	6.1.7
P-8	Drip shield corrosion	6.1.8
P-9	Waste package corrosion	6.1.9
P-10	Releases from the engineered barrier system	6.1.10
P-11	Colloid facilitated releases from the engineered barrier system	6.1.11
P-12	Unsaturated zone flow and transport	6.1.12
P-13	Saturated zone flow and transport	6.1.13
P-14	Intrusive volcanism	6.1.14
P-15	Volcanic ash remobilization	6.1.15
P-16	Dose from direct and inhalation radiation exposure	6.1.16
P-17	Dose from groundwater radiation exposure	6.1.17
P-18	Atmospheric Transport and Deposition of Radionuclides	6.1.18
S-1	Waste Package Failure Modes	6.2.1
S-2	Radionuclide Release Rates	6.2.2
S-3	Radionuclide Dose Contributions	6.2.3
S-4	Numerical Stability	6.2.4

Software Validation Reports for TPA Version 5.1 Validation Tasks

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 06002.01.354
Software Name: TPA	Versions: 5.1betaX, 5.1betaY, and 5.1betaW
Test ID: **P-1**	Test Series Name: Executive Functions

Test Method

☐ code inspection	☒ spreadsheet
☒ output inspection	☒ graphical
☐ hand calculation	☐ comparison with external code results

Test Objective: Verify the following:
P-1.1 New routines for assigning inventory to drift segments and for assigning drift segments to subareas are working as intended.
P-1.2 Inventory is appropriately apportioned between subareas.
P-1.3 Input, output, and intermediate files are reasonably transparent and traceable.
P-1.4 Values reported in *tpamin.dat*, *tpameans.dat*, and *tpamax.dat* are correct
P-1.5 to P-1.8 Conduct additional test to enhance confidence in the performance of the code at the discretion of the analyst

Test Environment Setup

Hardware (platform, peripherals): Tests P-1.4), P-1.5), P-1.7), and P-1.8) of Test Procedures (see below) were performed on PC (Pentium 4). Tests P-1.3) and P-1.6) were performed on a SUN workstation

Software (OS, compiler, libraries, auxiliary codes or scripts): Windows XP (SP2); SOLARIS

Input Data (files, data base, mode settings): See attached test descriptions.

Assumptions, constraints, and/or scope of test: See Attachments A–F

Test Procedure: The following tests correspond to the above-stated objectives:
P-1.1) Based on review of SCRs 598 & 600, the new drift routines have been tested sufficiently.
P-1.2) Based on review of SCRs 598 & 600, the new subareas have been tested sufficiently.
P-1.3) Prepare a listing of all possible files generated by the code; generate all files with multiple runs using all of the necessary control flags; inspect all reformatted files for transparency and traceability (Attachment F)
P-1.4) Prepare a *tpa.inp* file with all distribution types represented; check each type for mean, maximum, and minimum values; submit all 3 files for execution to check for operational compatibility with the TPA code. (see Attachments A and B)
additional tests include:
P-1.5) Check *rgwsap.tpa* values for consistency between single and multiple realization runs. (Attachment C)
P-1.6) Exercise all control flags in *tpa.inp* for successful execution. (Attachment E)
P-1.7) Planned test to exercise all importance analysis flags was omitted; importance analysis is no longer supported.
P-1.8) Check LHS Monte-Carlo sample set for proper distributions. (Attachment D)

Test Results

Location: CD labeled "TPA Version 5.1 Validation Task P-1"

Test Criterion and Analysis of Results: See Attachments A–F.

Test Evaluation (Pass/Fail): PASS (See Attachments A–F)

Tester: R. Janetzke / C. Scherer	Date: 6-20-07

Attachment A
TPA Version 5.1 Validation Task P-1

Test P-1.4.1 Description and Results

Objectives

This test verifies the internal calculation of several statistical measures of each of the probability distribution functions (PDFs) for the sampled parameters specified in the *tpa.inp* file. These statistical measures appear in output files *tpamin.out, tpameans.out* and *tpamax.out*. The Log scale and Discrete PDFs for the *tpameans.out* file are a heuristic approximation of the mean since the solution is not a closed form solution for these cases. These files provide a convenient method of generating special purpose *tpa.inp* input files. The following PDFs will be tested:

Normal
LogNormal
Uniform
LogUniform
Triangular
LogTriangular
Beta
LogBeta
Exponential
FiniteExponential
IUniform
UserDiscreteEmpirical
UserSuppliedDiscrete
UserSuppliedPWiseCDF

The statistical measures tested are <u>minimum</u>, <u>mean</u>, and <u>maximum</u>.

Assumptions

It is assumed that all of the internal statistical calculations are presented in the output files before the first realization is started.

The extraneous values used in specifying the 'iuniform' distribution in this test are not processed by the TPA code and do not affect this validation test.

Test Procedure

The reference case *tpa.inp* file is used as the template for constructing the input file for the test case. The PDFs of several of the first sampled parameters (mostly in the UZFLOW section) were
modified to use the set of PDFs listed above. No consideration is given to the non-physical nature that some of the numerical ranges for a given parameter used in this test. The success of this test does not depend on the proper operation of any of the modules, and for computational efficiency reasons, the test is designed to halt upon entering the first realization.

The parameters listed below were modified to select each of the PDFs with arbitrary ranges supplied.

```
**
normal
uzflow_ReferenceMATAtStart[degC]
0.001, 9.999
**
lognormal
uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
0.27, 126
**
uniform
uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum
1.8, 2.3
**
loguniform
uzflow_MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC]
0.7, 0.9
**
triangular
uzflow_HydraulicPropertyUncertaintyDeviation[N(0,1)]
-3.0902, 0.0, 3.0902
**
logtriangular
uzflow_LongTermAverageOnsetTime[yr]
0.1, 0.2, 3.0902
**
beta
uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
0.0, 10.0, 0.5, 2.0
**
logbeta
uzflow_TimeStep[yr]
0.1, 100., 0.5, 2.0
**
exponential
uzflow_StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr]
100.0
**
finiteexponential
uzflow_StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]
0.0, 100, 0.1
**
iuniform
uzflow_CorrelationBetweenMAPAndMATPerturbations
-10, -1, 0 , 1, 10
**
** Note: ClimatePerturbationSet should be greater than zero
**
userdiscreteempirical
uzflow_ClimatePerturbationSet
5
-2
 -1
 0
 10
 20
**
**          ***>>> NFENV  <<<***
**
** Thermal Model used to calculate indrift temperatures.
** Model 1 is a linearized model and Model 2 is an iterative model.
**
```

```
usersupplieddiscrete
SelectThermalModel(1,2)
5
10., 0.1
11., 0.2
20., 0.3
50., 0.3
51., 0.1
**
** FractionAllowedToDegrade is only used in thermal model 1
**
usersuppliedpwisecdf
FractionAllowedToDegrade[]
5
10., 0.0
11., 0.3
20., 0.6
50., 0.9
51., 1.0
```

The test run is executed, and the output saved in the P-1(4) folder. The file containing the full sampled set of parameters to be analyzed is *lhs.out*. This file is imported into a spreadsheet (*P-1(4).xls*) that calculates the minimum, mean, and maximum of each of the first fourteen parameters.

<u>Criteria</u>

Three files are checked for appropriate values.

tpamin.out - values for the fourteen parameters listed above should equal the minimum values specified in the *tpa.inp* file for each respective parameter, except for the exponential PDF which has no minimum value specification. In this case the minimum value should equal

-ln(0.9999) / l

where ☆ is the value specified in the *tpa.inp* file.

tpameans.out - values for the fourteen parameters listed above should be the same as the indicated average values from the spreadsheet, except the Log scale and Discrete PDFs where the heuristic mean should be within the parameter range.

tpamax.out - values for the fourteen parameters listed above should equal the maximum values specified in the *tpa.inp* file for each respective parameter, except for the exponential PDF which has no maximum value specification. In this case the maximum value should equal

-ln(0.0001) / l

where ☆ is the value specified in the *tpa.inp* file.

Test Results

tpamin.out

Minimum value display from *tpamin.out*.

```
**
constant
uzflow_ReferenceMATAtStart[degC]
 1.000000000000000E-03
**
constant
uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
 0.2700000000000000
**
constant
uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum
 1.800000000000000
**
constant
uzflow_MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC]
 0.7000000000000000
**
constant
uzflow_HydraulicPropertyUncertaintyDeviation[N(0,1)]
 -3.090200000000000
**
constant
uzflow_LongTermAverageOnsetTime[yr]
 0.1000000000000000
**
constant
uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
 0.000000000000000E+00
**
constant
uzflow_TimeStep[yr]
 0.1000000000000000
**
constant
uzflow_StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr]
 1.000050003333473E-06
**
constant
uzflow_StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]
 0.000000000000000E+00
**
iconstant
uzflow_CorrelationBetweenMAPAndMATPerturbations
 -10
**
**
** Note: ClimatePerturbationSet should be greater than zero
**
constant
uzflow_ClimatePerturbationSet
 -2.000000000000000
**
**          ***>>> NFENV  <<<***
**
** Thermal Model used to calculate indrift temperatures.
** Model 1 is a linearized model and Model 2 is an iterative model.
**
```

```
constant
SelectThermalModel(1,2)
 10.00000000000000
**
** FractionAllowedToDegrade is only used in thermal model 1
**
constant
FractionAllowedToDegrade[]
 10.00000000000000
**
```

All values for *tpamin.out* satisfy the test criteria.

tpameans.out

Spreadsheet output:

	Normal	LogNormal	Uniform	LogUniform	Triangular	LogTriangular	Beta	LogBeta	Exponential	FiniteExponential	IUniform	UserDiscreteEmpirical	UserSuppliedDiscrete	UserSuppliedPWiseCDF
Minimum	1.00E-03	2.70E-01	1.80E+00	7.00E-01	-2.98E+00	1.07E-01	7.82E-06	1.00E-01	5.21E-06	1.41E-02	-1.00E+01	-2.00E+00	1.00E+01	1.00E+01
Average	5.00E+00	9.56E+00	2.05E+00	7.96E-01	-2.41E-04	5.32E-01	1.99E+00	1.92E+00	9.98E-03	9.98E+00	-5.50E+00	5.40E+00	2.93E+01	2.33E+01
Maximum	9.90E+00	1.26E+02	2.30E+00	9.00E-01	2.92E+00	2.98E+00	9.73E+00	6.49E+01	6.29E-02	6.36E+01	-1.00E+00	2.00E+01	5.10E+01	5.10E+01

Mean value display from *tpameans.out*.

```
**
constant
uzflow_ReferenceMATAtStart[degC]
 5.000000000000000
**
constant
uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
 5.832666628567075
**
constant
uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum
 2.050000000000000
**
constant
uzflow_MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC]
 0.7937253933193772
**
constant
uzflow_HydraulicPropertyUncertaintyDeviation[N(0,1)]
 0.000000000000000E+00
**
constant
uzflow_LongTermAverageOnsetTime[yr]
 0.3953716525552601
**
constant
uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
 2.000000000000000
**
constant
uzflow_TimeStep[yr]
 0.3981071705534973
**
constant
uzflow_StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr]
 1.000000000000000E-02
```

```
**
constant
uzflow_StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]
 9.995459800899031
**
iconstant
uzflow_CorrelationBetweenMAPAndMATPerturbations
 -5
**
** Note: ClimatePerturbationSet should be greater than zero
**
constant
uzflow_ClimatePerturbationSet
 10.00000000000000
**
**          ***>>> NFENV  <<<***
**
** Thermal Model used to calculate indrift temperatures.
** Model 1 is a linearized model and Model 2 is an iterative model.
**
constant
SelectThermalModel(1,2)
 20.00000000000000
**
** FractionAllowedToDegrade is only used in thermal model 1
**
constant
FractionAllowedToDegrade[]
 23.35000000000000
**
```

The values match the spreadsheet values except the Log scale and Discrete PDFs. These do however occur within the parameter ranges, and satisfy the test criteria.

tpamax.out

Maximum value display from *tpamax.out*.

```
**
constant
uzflow_ReferenceMATAtStart[degC]
 9.999000000000001
**
constant
uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
 126.0000000000000
**
constant
uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum
 2.300000000000000
**
constant
uzflow_MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC]
 0.9000000000000000
**
constant
uzflow_HydraulicPropertyUncertaintyDeviation[N(0,1)]
 3.090200000000000
**
constant
uzflow_LongTermAverageOnsetTime[yr]
 3.090200000000000
**
constant
```

```
uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
 10.00000000000000
**
constant
uzflow_TimeStep[yr]
 100.0000000000000
**
constant
uzflow_StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr]
 9.210340371976183E-02
**
constant
uzflow_StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]
 100.0000000000000
**
iconstant
uzflow_CorrelationBetweenMAPAndMATPerturbations
 -1
**
** Note: ClimatePerturbationSet should be greater than zero
**
constant
uzflow_ClimatePerturbationSet
 20.00000000000000
**
**           ***>>> NFENV  <<<***
**
** Thermal Model used to calculate indrift temperatures.
** Model 1 is a linearized model and Model 2 is an iterative model.
**
constant
SelectThermalModel(1,2)
 51.00000000000000
**
** FractionAllowedToDegrade is only used in thermal model 1
**
constant
FractionAllowedToDegrade[]
 51.00000000000000
**
```

All values for *tpamax.out* satisfy the test criteria.

Test P-1.4.1 Status: **PASS**

Attachment B
TPA Version 5.1 Validation Task P-1

Test P-1.4.2 Description and Results

Objectives

This test verifies that the *tpamin.out, tpameans.out* and *tpamax.out* files are generated in a format that is compatible with the TPA READER module and can be used as an input file successfully.

Assumptions

It is assumed that all of the TPA code fully processes the *tpa.inp* file before the first realization is started.

Test Procedure

Each of the three files that are the subject of this test are moved to an empty folder (*P-1(4.1), P-1(4.2),* and *P-1(4.3)*) and renamed to *tpa.inp*. The TPA code is then invoked in this folder and the screen output captured in the *tpa.out* file.

Criteria

The screen capture file for each run should indicate that analysis of realization 1 has started.

Test Results

tpamin.out

Screen capture for run using *tpamin.out* as input file.

```
======================================================================
         exec: Welcome to TPA Version 5.1betaW
       Job started: Tue Apr 24 18:42:00 2007
======================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
   #      [m^2]     [MTU]
   1    224091.0     3025.5        526
   2    448476.0     6108.4       1062
   3   1241313.5    16703.3       2904
   4    775953.1    10313.0       1793
   5    605892.0     8351.7       1452
   6    152357.0     1972.9        343
   7    318122.0     4003.3        696
   8    439350.0     5355.0        931
   9    305880.0     4158.6        723
  10    747165.5    10048.4       1747

Total Area [acre]         =  1299.382289078371
Total Buried Waste [MTU]  =  70040.00000000000
Repository AML [MTU/acre] =  53.90253552684494
Watts per MTU [W/MTU]     =  1327.684245650000
Watts per linear meter of drift [W/m] =  1450.448314791551

Specified Global Parameters:

               Compliance Period =  10000.0 (yr)
         Maximum Simulation Time =  10000.0 (yr)
          Number Of Realizations =    500
```

```
              Number Of Subareas =     10
              Volcanism scenario =      0 (yes=1, no=0)
               Faulting scenario =      0 (yes=1, no=0)
     Mechanical failure scenarios:
                      Seismicity =      1 (yes=1, no=0)
               Drift Degradation =      1 (yes=1, no=0)
      Distance to Receptor Group =     18.0 (km)

**>>> CAUTION: CHECKING OF NUCLIDES AND CHAINS IS DISABLED <<<**
**>>> You may not be using the standard chains specified   <<<**
**>>> in the invent module.                                <<<**
**>>> (see "CheckNuclidesAndChains(yes=1,no=0)" in tpa.inp)<<<**

The specified path for data  = d:\ronj-\tpa51betaW\
The specified path for codes = d:\ronj-\tpa51betaW\

**To modify global parameters or the path, stop code execution using control-C**
-----------------------------------------------------------------------
    subarea   1 of  10           realization    1 of  500
-----------------------------------------------------------------------

 ***>>> Error in valuesp <<<***
 called valuesp for integer sp
 need to call ivaluesp
 ipdf =  42
 itype =  10
 name = uzflow_CorrelationBetweenMAPAndMATPerturbations
```

This test output satisfies the test criteria.

tpameans.out

Screen capture for run using *tpameans.out* as input file.

```
=======================================================================
         exec: Welcome to TPA Version 5.1betaW
       Job started: Tue Apr 24 18:42:17 2007
=======================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
   #     [m^2]      [MTU]
   1    224091.0     3025.5         526
   2    448476.0     6108.4        1062
   3   1241313.5    16703.3        2904
   4    775953.1    10313.0        1793
   5    605892.0     8351.7        1452
   6    152357.0     1972.9         343
   7    318122.0     4003.3         696
   8    439350.0     5355.0         931
   9    305880.0     4158.6         723
  10    747165.5    10048.4        1747

Total Area [acre]         =  1299.382289078371
Total Buried Waste [MTU]  =  70040.00000000000
Repository AML [MTU/acre] =  53.90253552684494
Watts per MTU [W/MTU]     =  1327.684245650000
Watts per linear meter of drift [W/m] =  1450.448314791551

Specified Global Parameters:

               Compliance Period =  10000.0 (yr)
         Maximum Simulation Time =  10000.0 (yr)
          Number Of Realizations =    500
              Number Of Subareas =     10
              Volcanism scenario =      0 (yes=1, no=0)
               Faulting scenario =      0 (yes=1, no=0)
     Mechanical failure scenarios:
                      Seismicity =      1 (yes=1, no=0)
               Drift Degradation =      1 (yes=1, no=0)
      Distance to Receptor Group =     18.0 (km)

**>>> CAUTION: CHECKING OF NUCLIDES AND CHAINS IS DISABLED <<<**
**>>> You may not be using the standard chains specified   <<<**
**>>> in the invent module.                                <<<**
**>>> (see "CheckNuclidesAndChains(yes=1,no=0)" in tpa.inp)<<<**
```

```
The specified path for data  = d:\ronj-\tpa51betaW\
The specified path for codes = d:\ronj-\tpa51betaW\

**To modify global parameters or the path, stop code execution using control-C**
-----------------------------------------------------------------------
    subarea   1 of  10           realization    1 of  500
-----------------------------------------------------------------------

 ***>>> Error in valuesp <<<***
 called valuesp for integer sp
 need to call ivaluesp
 ipdf =  42
 itype =  10
 name = uzflow_CorrelationBetweenMAPAndMATPerturbations
```

This test output satisfies the test criteria.

tpamax.out

Screen capture for run using *tpamax.out* as input file.

```
=======================================================================
         exec: Welcome to TPA Version 5.1betaW
       Job started: Tue Apr 24 18:42:31 2007
=======================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
   #     [m^2]      [MTU]
   1    224091.0     3025.5         526
   2    448476.0     6108.4        1062
   3   1241313.5    16703.3        2904
   4    775953.1    10313.0        1793
   5    605892.0     8351.7        1452
   6    152357.0     1972.9         343
   7    318122.0     4003.3         696
   8    439350.0     5355.0         931
   9    305880.0     4158.6         723
  10    747165.5    10048.4        1747

Total Area [acre]         =  1299.382289078371
Total Buried Waste [MTU]  =  70040.00000000000
Repository AML [MTU/acre] =  53.90253552684494
Watts per MTU [W/MTU]     =  1327.684245650000
Watts per linear meter of drift [W/m] =  1450.448314791551

Specified Global Parameters:

               Compliance Period =  10000.0 (yr)
         Maximum Simulation Time =  10000.0 (yr)
          Number Of Realizations =    500
              Number Of Subareas =     10
              Volcanism scenario =      0 (yes=1, no=0)
               Faulting scenario =      0 (yes=1, no=0)
     Mechanical failure scenarios:
                      Seismicity =      1 (yes=1, no=0)
               Drift Degradation =      1 (yes=1, no=0)
      Distance to Receptor Group =     18.0 (km)

**>>> CAUTION: CHECKING OF NUCLIDES AND CHAINS IS DISABLED <<<**
**>>> You may not be using the standard chains specified   <<<**
**>>> in the invent module.                                <<<**
**>>> (see "CheckNuclidesAndChains(yes=1,no=0)" in tpa.inp)<<<**

The specified path for data  = d:\ronj-\tpa51betaW\
The specified path for codes = d:\ronj-\tpa51betaW\

**To modify global parameters or the path, stop code execution using control-C**
-----------------------------------------------------------------------
    subarea   1 of  10           realization    1 of  500
-----------------------------------------------------------------------

 ***>>> Error in valuesp <<<***
 called valuesp for integer sp
 need to call ivaluesp
 ipdf =  42
 itype =  10
```

```
name = uzflow_CorrelationBetweenMAPAndMATPerturbations
```

This test output satisfies the test criteria.

Test P-1.4.2 Results: **PASS**

Attachment C
TPA Version 5.1 Validation Task P-1

Additional Test P-1.5 Description and Results

Objectives

This test verifies the generation of the data presented in the *rgwsap.tpa* file. This file contains the dose due to groundwater for each of six pathways, summed over all nuclides, and averaged over all realizations.

Assumptions

It is assumed that the groundwater dose from each of the first two realizations is significantly different than the average dose over both realizations. It is sufficient to check just two realizations since this test is a verification of the averaging algorithm rather than the fully analyzed parameter distributions for the calculation of the final dose statistics.

It is sufficient to check the averaging mechanism of one pathway, since all use a common algorithm.

Test Procedure

The TPA version5.1betaY code was modified to include the scaling change for *rgwsap.tpa* file that is part of SCR694.

The reference case *tpa.inp* file is used as the template for constructing the input file for the test cases. Three runs are prepared, the first to generate a two realization simulation, the second to generate a one realization simulation of the first realization only, and the third to generate one realization simulation of the second realization only.

The pathway selected for this test is the drinking water pathway. The source data for checking the *rgwsap.tpa* file is the *rgwnapdw.tpa* file. This file is captured for each of the three simulations and the time history of the pathway dose is summed over all nuclides. The average dose of the two single realization runs are plotted against time and compared to the data of the *rgwnapdw.tpa* and *rgwsap.tpa* files.

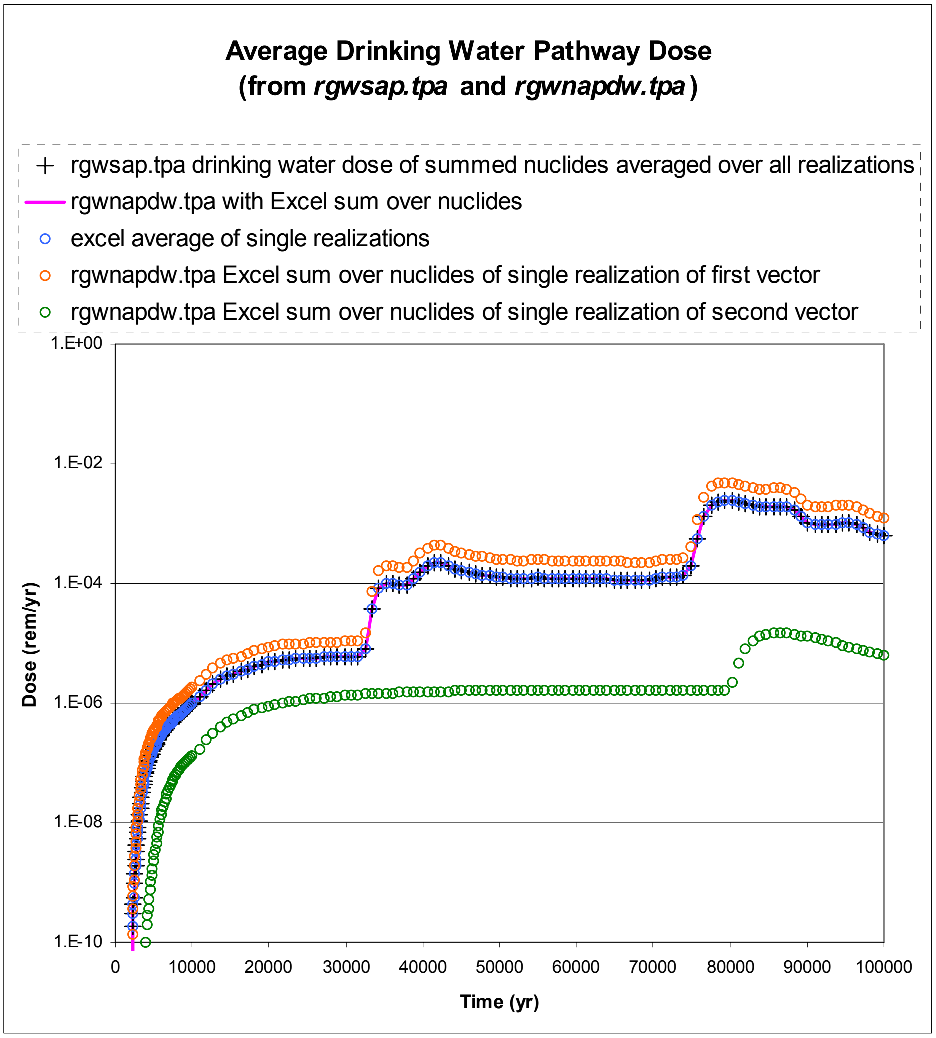
The output from the two realization run is archived in *P-1(5)* folder, and the spreadsheet containing the *rgwsap.tpa* data is stored in *dw.xls*. The spreadsheet containing the data from the *rgwnapdw.tpa* files in stored in *rgwnapdw.xls*. The single realization run of the first realization output is in *P-1(5.1)* and that of the second realization is in *P-1(5.2)*.

Criteria

The average dose listed for drinking water in the *rgwsap.tpa* file should be consistent with the calculated averages from the *rgwnapdw.tpa* file from the same run as well as the calculated averages from the single realization runs where the two realizations are run independently .

Test Results

The Excel plots show that the *rgwsap.tpa* file is consistent with the *rgwnapdw.tpa* file from the same run and with the Excel average of the *rgwnapdw.tpa* information from the two independent runs.



Test P-1.5 Status: **PASS**

Attachment D
TPA Version 5.1 Validation Task P-1

Additional Test P-1.8 Description and Results

Objectives

This test verifies the statistical distributions of parameters that were sampled using the Monte Carlo option of the SNLLHS standalone code. Each of the probability distribution functions (PDFs) for the sampled parameters specified in the *tpa.inp* file are represented. The following PDFs will be tested:

Normal
LogNormal
Uniform
Triangular
LogTriangular
Beta
LogBeta
Exponential
FiniteExponential
IUniform
UserDiscreteEmpirical
UserSuppliedDiscrete
UserSuppliedPWiseCDF

Assumptions

It is assumed that a proper distribution of sampled values can be determined graphically by visual inspection of plots using a histogram of 20 bins and a sample size of 500 realizations.

Test Procedure

The reference case *tpa.inp* file is used as the template for constructing the input file for the test case. The PDFs of several of the first sampled parameters (mostly in the UZFLOW section) were
modified to use the set of PDFs listed above. No consideration is given to the non-physical nature that some of the numerical ranges for a given parameter used in this test. The success of this test does not depend on the proper operation of any of the modules, and for computational efficiency reasons, the test is designed to halt upon entering the first realization. Each distribution is rated on a three point subjective scale of Good, Poor, and Failed through visual inspection. A successful test is one were none of the distributions are rated as Failed.

The parameters listed below were modified to select each of the PDFs with arbitrary ranges supplied.

```
**
normal
uzflow_ReferenceMATAtStart[degC]
0.001, 9.999
**
lognormal
uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
0.27, 126
**
uniform
uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum
1.8, 2.3
**
loguniform
uzflow_MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC]
0.7, 0.9
**
triangular
uzflow_HydraulicPropertyUncertaintyDeviation[N(0,1)]
-3.0902, 0.0, 3.0902
**
logtriangular
uzflow_LongTermAverageOnsetTime[yr]
0.1, 0.2, 3.0902
**
beta
uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
0.0, 10.0, 0.5, 2.0
**
logbeta
uzflow_TimeStep[yr]
0.1, 100., 0.5, 2.0
**
exponential
uzflow_StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr]
100.0
**
finiteexponential
uzflow_StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]
0.0, 100, 0.1
**
iuniform
uzflow_CorrelationBetweenMAPAndMATPerturbations
-10, -1, 0 , 1, 10
**
** Note: ClimatePerturbationSet should be greater than zero
**
userdiscreteempirical
uzflow_ClimatePerturbationSet
5
-2
 -1
 0
 10
 20
**
**          ***>>> NFENV  <<<***
**
** Thermal Model used to calculate indrift temperatures.
** Model 1 is a linearized model and Model 2 is an iterative model.
**
usersupplieddiscrete
SelectThermalModel(1,2)
5
```

```
10., 0.1
11., 0.2
20., 0.3
50., 0.3
51., 0.1
**
** FractionAllowedToDegrade is only used in thermal model 1
**
usersuppliedpwisecdf
FractionAllowedToDegrade[]
5
10., 0.0
11., 0.3
20., 0.6
50., 0.9
51., 1.0
```

A single run is executed with 500 realizations and the LatinHypercubeSampling flag is set to zero. The resulting *lhs.out* file is imported into a spreadsheet and a histogram of the samples from the first fourteen parameters is calculated and plotted.

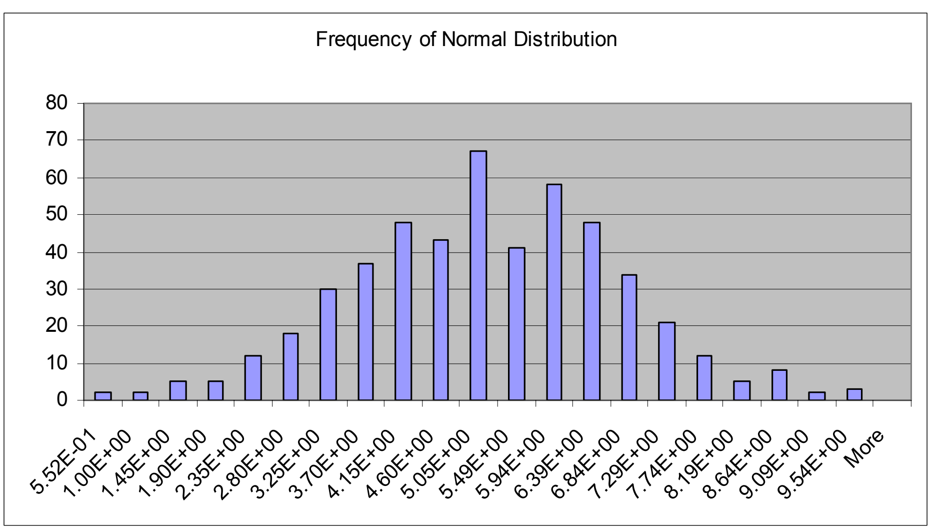
The test run is executed, and the output saved in the *P-1(8)* folder. The file containing the full sampled set of parameters to be analyzed is *lhs.out*. This file is imported into a spreadsheet (*P-1(8).xls*) that calculates the minimum, mean, and maximum of each of the first fourteen parameters.

<u>Criteria</u>

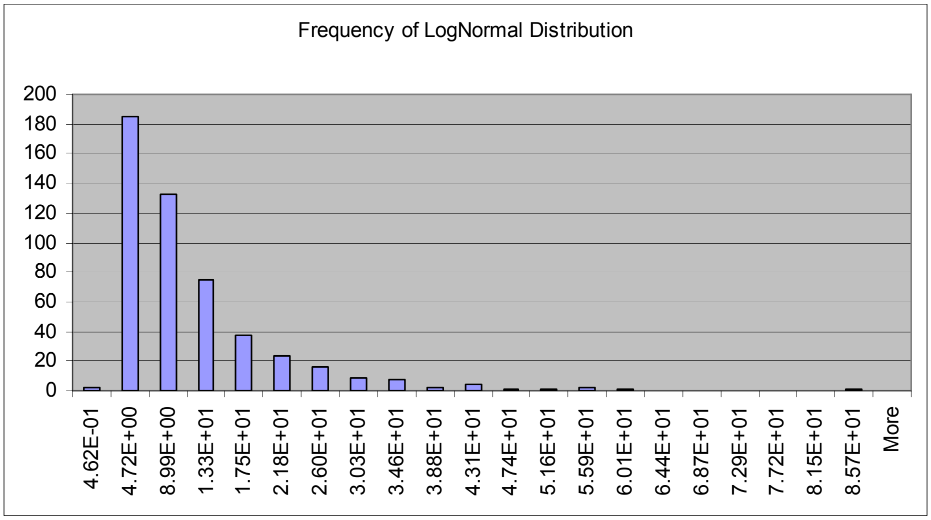
Visual inspection of the parameter distribution histograms should confirm the proper distribution of sampled values.

<u>Test Results</u>

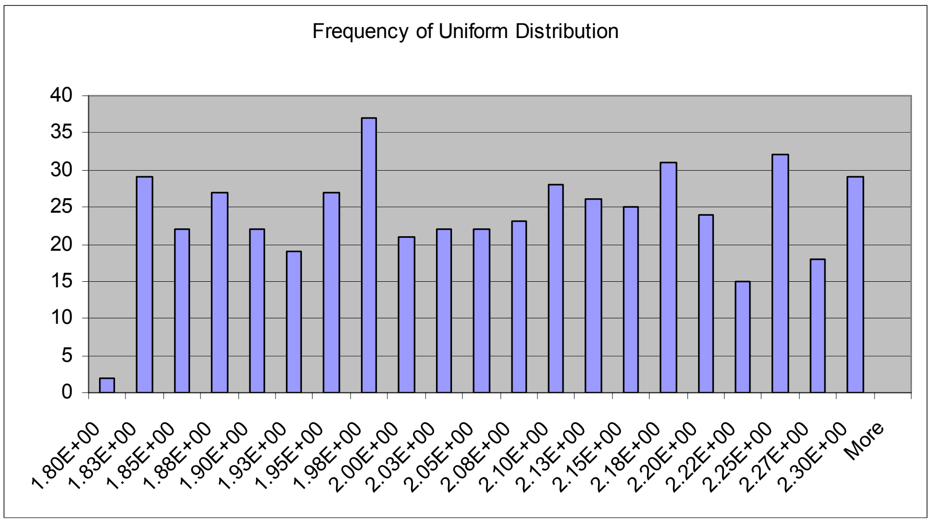
These are the Excel plots of the fourteen parameter distribution types under test. Each test is rated with a degree of agreement with expected curve shapes. The final test status corresponds to the lowest rating of the fourteen distributions.



Good

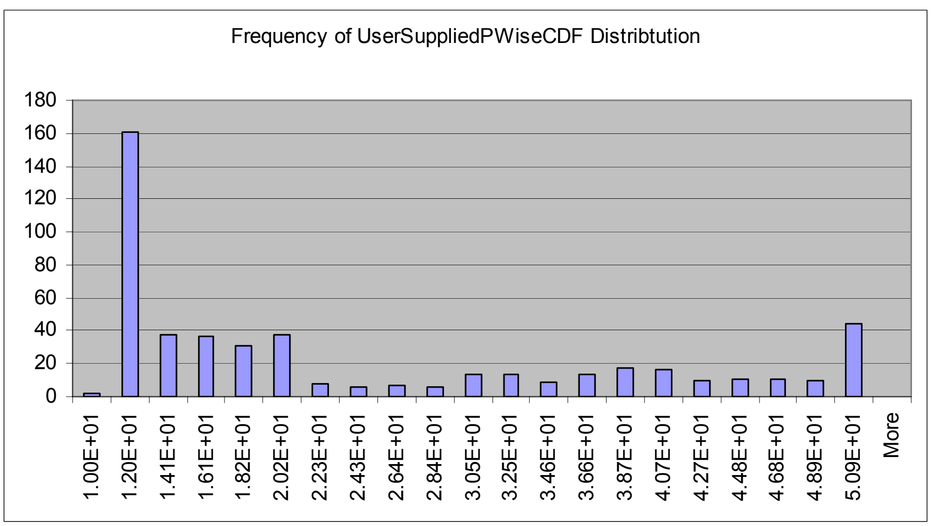


Good

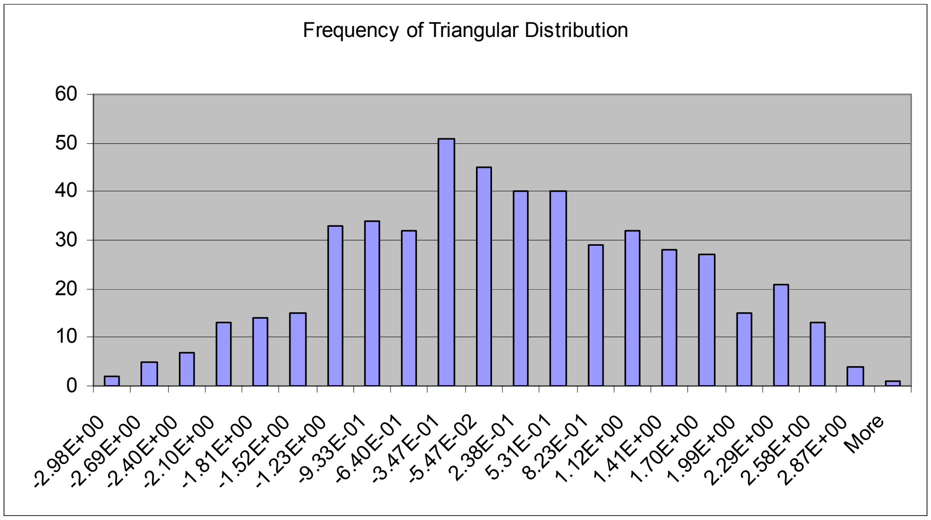


Poor*

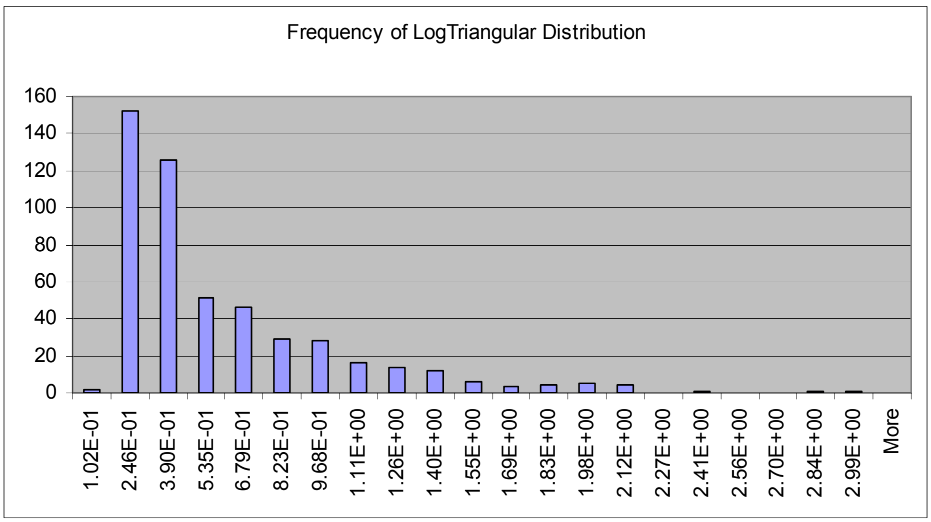
* an increased number of realizations would make a better visual agreement with expected shape of a uniform distribution.



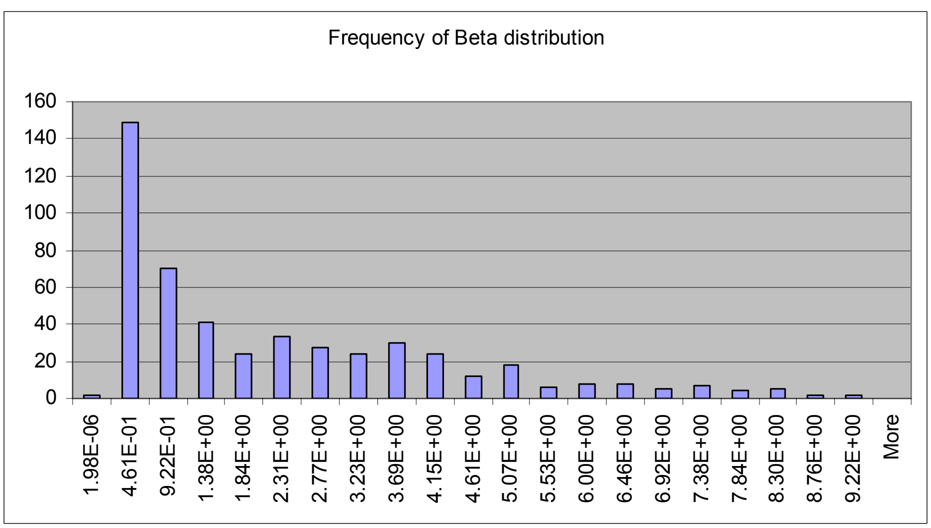
Good



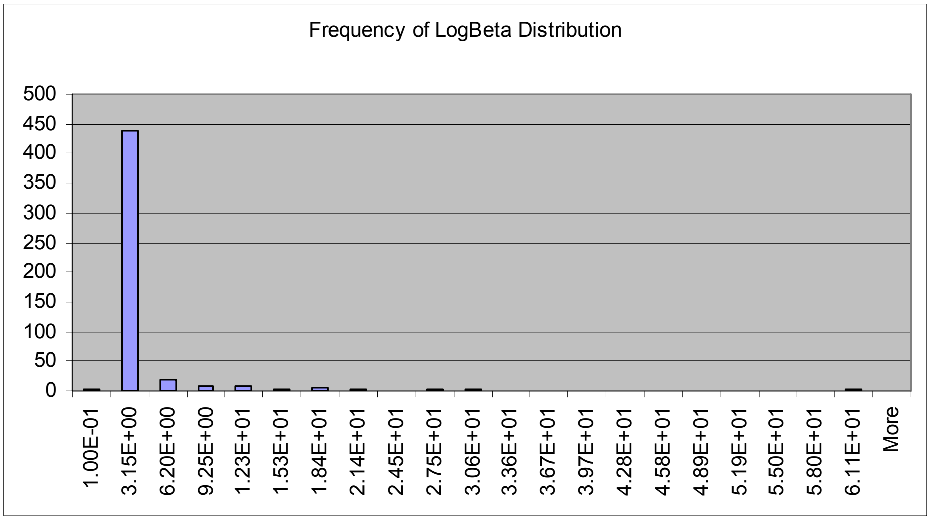
Good



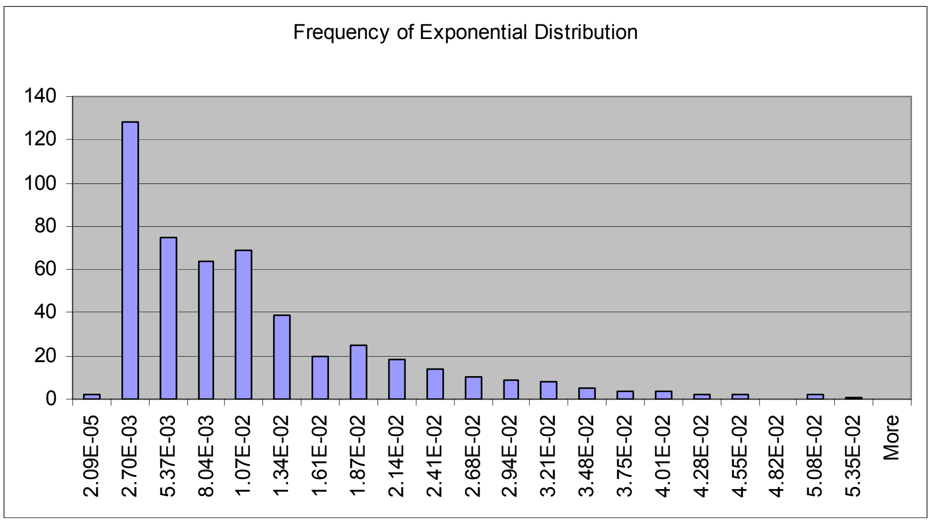
Good



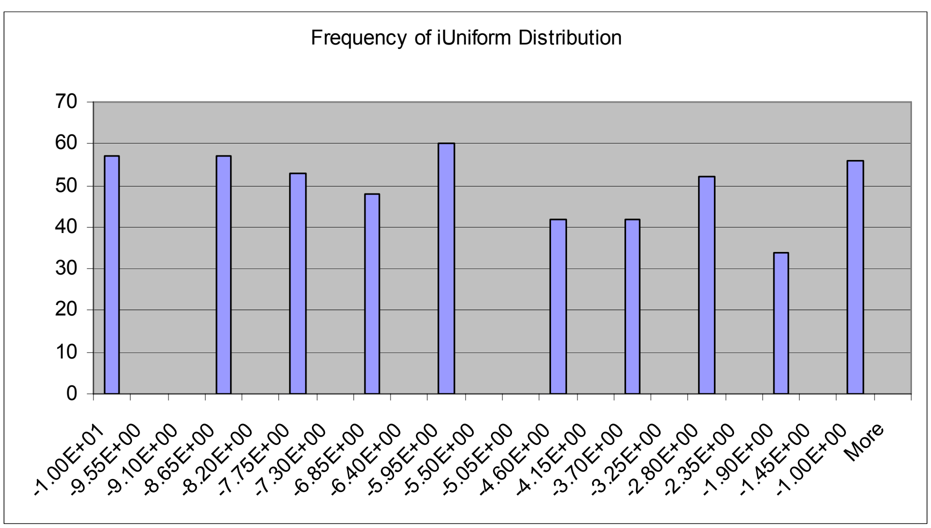
Good



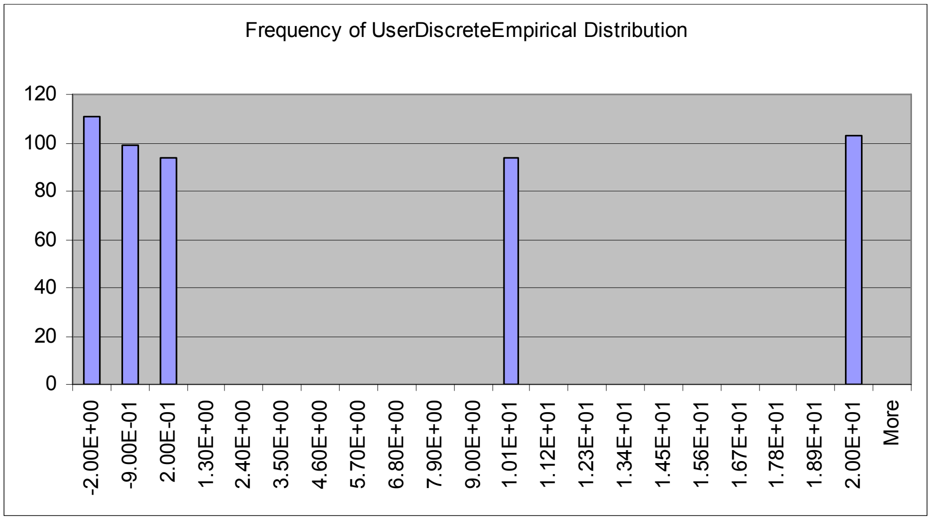
Good



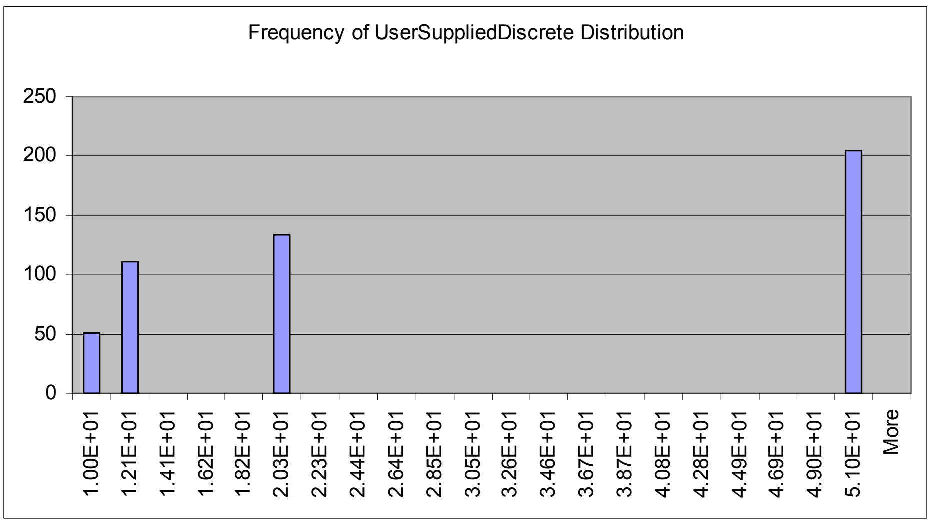
Good



Good



Good



Good

Test P-1.8 Status: **PASS**

Attachment E
TPA Version 5.1 Validation Task P-1

Additional Test P-1.6 Description and Results

Objectives

This test verifies the functionality of the code when the default values of control flags and parameters are modified.

Assumptions

It is sufficient to show that the code runs with different values for the control flags and parameters without analyzing the output data.

Test Procedure

The parameters (of type iflag and iconstant) in tpa.inp which control the flow of execution of the TPA code were identified. A series of tests were set up to run TPA with the control flags and parameters set to all possible valid values. In most cases, multiple control flags and parameters were modified in each run. Starting with the default version of the tpa.inp file, a new tpa.inp file was created for each test run by modified the control flags and parameters, according to the matrix in Table E-1. TPA was run for each of the identified test runs and the results stored in its own subdirectory (see attached CD). The output file set was checked for all output being present and for the valid termination of the code.

Criteria

If a test run of the TPA code ran to completion without aborting and generated the expected code termination mode, the run was considered a success.

Test Results

All of the test runs successfully ran to completion.

Test P-1.6 Status: **PASS**

Table E-1. TPA Control Flags and Parameters

iconstant or iflag name	Default Value	Flag Test 1	Flag Test 2	Flag Test 3	Flag Test 4	Flag Test 5	Flag Test 6	Flag Test 7	Flag Test 8	Flag Test 9	Flag Test 10	Flag Test 11
AshEvolutionMode[0=no_ashremob,1=ashremob]	1		0		0							
CalculateCreepMultiplierFlag(yes=1,no=0)	1	0										
CalculateTemperatureMultiplierFlag(yes=1,no=0)	1	0										
CheckNuclidesAndChains(yes=1,no=0)	0									1		
DirectReleaseOnlyFlag(yes=1,no=0)	0			1								
DriftDegradationScenarioFlag(yes=1,no=0)	1	0										
ExtrusiveEventFlag(extrusive=1,intrusive=0)	1	0			0							
FaultingDisruptiveScenarioFlag(yes=1,no=0)	0	1										
FlagPartialProtectionFromSeepageByInitialDefWP[1=yes,0=no]	1	0										
FlagPartialProtectionFromSeepageByMechFailedDS[1=yes,0=no]	1	0										
FlagPartialProtectionFromSeepageByMechFailedWP[1=yes,0=no]	1	0										
FlagSeepageThreshold[]	1	0										
GenerateRestartFiles(yes=1,no=0)	0					1						
GroundwaterProtectionCalc(yes=1,no=0)	1							0				
IModel	2	1	3	4								
ImportanceAnalysisFlag(yes=1,no=0)	0							1				
InvertBypass(0=ebsfilt,1=bypass-ebsfilt)	1	0*	0									
IrreversibleColloidModel[0=no,1=yes]	1											0
LatinHypercubeSampling(yes=1,no=0)	1	0										
NsetLatinHypercubeSampling	1											
nsetUsedToPickTempRHDataSet	1	2	3	4								
OneTemperatureCellPerWP(yes=1,no=0)	0										1	
OutputMode(0=None,1=All,2=UserDefined)	0	1	1	1	1	2	1	1	1	1	1	1
PlumeCaptureModel(1=UserDefined,2=Calculated)	1	2										
PresentDayDilutionModel(0,1,2,3,4)	1	0	2	3	4							
ReceptorGroup(1=Farming,2=Residential)	1	2										
SeismicDisruptiveScenarioFlag(yes=1,no=0)	1	0										
SelectAppendFiles	0											
SelectParticleModel(1,2)	2	1										
SelectThermalModel(1,2)	1	2										
SeparateNEFMKSRunsForSTFFandSAV(0=no,1=yes)	0							1				
TabularTemperatureRHFlag(yes=1,no=0)	0	1	1	1	1							
TemperatureReferencePoint(1=SubareaCentroid,2=UserDefined)[]	1	2										
UserDefinedLowerRealizationAppended	1					2**						
UserDefinedUpperRealizationAppended	1					4**						
uzflow_ClimatePerturbationSet	1	4										
uzflow_SampleMode	1	2	3									
UZVelocity(0=average,1=time-dependent)	1	0										
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	0	1	1	1	1							
VolcanoModel(1=Geometric,2=Distribution)	1		2	2								
WaterContactMode_Corrosion(0=BathTub,1=FlowThrough)	1				0							
WaterContactMode_Faulting(0=BathTub,1=FlowThrough)	1				0							
WaterContactMode_Initial(0=BathTub,1=FlowThrough)	1				0							
WaterContactMode_LocCorr(0=BathTub,1=FlowThrough)	1				0							
WaterContactMode_Mechanical1(0=BathTub,1=FlowThrough)	1				0							
WaterContactMode_Mechanical2(0=BathTub,1=FlowThrough)	1				0							
WaterContactMode_Volcanic(0=BathTub,1=FlowThrough)	1				0							
YearsOfIrrigationPriorToIntakePeriod[yr]	15								0			
* reset InvertMatrixPermeability to 7.0												
** run for 5 realizations												

Attachment F
TPA Version 5.1 Validation Task P-1

Test P-1.3 Description and Results

Objectives

This test verifies that all expected files are created from TPA runs using all of the control flags and parameters. Files that were recently reformatted were modified to increase transparency and readability. A list of all files generated by multiple TPA runs was compiled (see Table F-1), with the reformatted files indicated.

Assumptions

Test P-1.6 is run before this one.

Test Procedure

See Test P-1.6. Each test is run in a clean directory. After a run was completed, a list of files was generated and compared to the list of files expected. A composite list of all files generated was made and compared to a list of all files expected to be generated by the code.

Criteria

If all expected files are present in at least one run, and if all reformatted files have improved transparency and readability, the test passes.

Test Results

The test passed.

Test P-1.3 Status: **PASS**

Table F-1

#	Filename	#	Filename	#	Filename	#	Filename
1	^airpkdos.res	76	*failt.out	151	nefiialluv.src	226	sz_revers.out
2	^arpkds_c.res	77	^faulto.ech	152	nefiialluv.vel	227	tefkti.inp
3	ashcmd.out	78	^faulto.rlt	153	nefii.dis	228	thermal.dbg
4	ashout.res	79	FILENAME.DAT	154	nefii.inp	229	*totdos_c.res
5	ashplume.cum	80	fluoride.dat	155	nefii.out	230	*totdose.res
6	ashplume.in	81	frac_rel.out	156	nefii.rel	231	tpa_include.inp
7	ashplume.out	82	gdefauls.def	157	nefiisz.cum	232	tpamax.out
8	^ashplumo.ech	83	gdefault.def	158	nefiisz.dis	233	tpameans.out
9	^ashplumo.rlt	84	gdefault.inp	159	nefiisz.inp	234	tpamin.out
10	ashremob.out	85	gencorrfail.out	160	nefiisz.out	235	*tpanames.dat
11	^ashrmovo.ech	86	gdosinc2.dat	161	nefiisz.src	236	tpasys.tmp
12	^ashrmovo.rlt	87	gentoo.out	162	nefiisz.vel	237	trelease.out
13	*burnup.dat	88	genv.cum	163	nefiituff.cum	238	*uzflow.ech

#	Filename	#	Filename	#	Filename	#	Filename
14	burnup_glass.dat	89	genv.in	164	nefiituff.dis	239	*uzflow.rlt
15	burnup_sf.dat	90	genv.out	165	nefiituff.inp	240	*uzft.ech
16	*chlrdmf.dat	91	gftrans.def	166	nefiituff.out	241	*uzft.rlt
17	*cp.tpa	92	gftrans.inp	167	nefiituff.src	242	uz_kdrd.out
18	*climato1.dat	93	gftranss.def	168	nefiituff.vel	243	uz_revers.out
19	*climato2.dat	94	ggamen.dat	169	nefiiuz.cum	244	^volcano.ech
20	*coefkdeq.dat	95	ggenii.cum	170	nefiiuz.dis	245	^volcano.rlt
21	^cumrel_c.res	96	ggenii.def	171	nefiiuz.inp	246	weldfail.out
22	^cumrel.res	97	ggenii.inp	172	nefiiuz.out	247	wpfillstats.out
23	cumrelse.out	98	ggenii.out	173	nefiiuz.src	248	wpflow.dat
24	^dcags.ech	99	ggeniis.def	174	nefiiuz.vel	249	*wpsfail.dbg
25	^dcags.rlt	100	ggrdf.dat	175	NEFII.VEL	250	*wpsfail.res
26	^dcagw.ech	101	gmedia.out	176	nefmks.log	251	wpflow.def
27	^dcagw.rlt	102	gnewdf.dat	177	*nfenv.ech		
28	dcfgs.cum	103	grmdlib.dat	178	*nfenv.rlt		
29	dcfgw.cum	104	gs_cb_ad.dat	179	^npkdoset.res		
30	deltaec.inp	105	gs_cb_ci.dat	180	^npkdst_c.res		
31	diagnose.out	106	^gsccdf_c.res	181	*nuclides.dat		
32	dilution.dat	107	^gsccdf.res	182	*organdf.dat		
33	driftfail.dat	108	gs_pb_ad.dat	183	*pkmndose.res		
34	driftfail.dbg	109	gs_pb_ci.dat	184	^pkreltim.res		
35	*driftfail.ech	110	gw_cb_ad.dat	185	^pkrltm_c.res		
36	*driftfail.inp	111	gw_cb_ci.dat	186	relccdf.res		
37	*driftfail.rlt	112	^gwccdf_c.res	187	relcumglass.out		
38	drifts.dat	113	^gwccdf.res	188	relcum.out		
39	*drythick.dat	114	gwork.buf	189	relcumsf.out		
40	*dsfail.ech	115	*gwp_ave.res	190	releaset.cum		
41	*dsfail.res	116	gw_pb_ad.dat	191	releaset.out		
42	*dsfail.rlt	117	gw_pb_ci.dat	192	rel_flow.out		
43	dsfailt.dat	118	^gwpkdos.res	193	relfrac.out		
44	dsfailt.dbg	119	^gwpkds_c.res	194	*relgwgs.res		
45	*dsfailt.def	120	*gwppktim.res	195	remob_lut.dat		
46	*dsfailt.inp	121	^gwttuzsz.res	196	*repdes.dat		
47	ebscld.out	122	ia.dat	197	*rgsna.tpa		
48	*ebsfail.def	123	infile.ash	198	*rgsnr.tpa		
49	^ebsfail.ech	124	*infilper.cum	199	*rgssa.tpa		
50	*ebsfail.inp	125	*infilper.res	200	*rgssr.tpa		
51	^ebsfail.rlt	126	*inv1000.out	201	*rgwgssa.tpa		
52	ebsfilt.dbg	127	lhs.csv	202	*rgwnapani.tpa		
53	*ebsfilt.def	128	lhse.out	203	*rgwnapdw.tpa		
54	*ebsfilt.inp	129	lhs.inp	204	*rgwnapext.tpa		
55	ebsfilt.out	130	lhs.out	205	*rgwnapinh.tpa		
56	ebsflo.dat	131	^maidtbl.dat	206	*rgwnapmlk.tpa		
57	ebsglass.dat	132	mechfail_ds.dat	207	*rgwnappla.tpa		
58	ebsnef2.dat	133	mechfail_ds.dbg	208	*rgwna.tpa		
59	ebsnef.dat	134	*mechfail_ds.def	209	*rgwnr.tpa		
60	ebsnef.out	135	*mechfail_ds.inp	210	*rgwsap.tpa		
61	ebspacglass.nuc	136	*mechfail_ds.res	211	*rgwsa.tpa		
62	ebspac.nuc	137	*mechfail.ech	212	*rgwsr.tpa		
63	ebspacsf.nuc	138	*mechfail.inp	213	^rlccdf_c.res		
64	ebsrel.cum	139	*mechfail.rlt	214	^rlgwgs_c.res		
65	^ebsrel.ech	140	mechfail_wp.dat	215	*samplpar.abb		
66	*ebsrel.def	141	mechfail_wp.dbg	216	*samplpar.hdr		
67	*ebsrel.inp	142	*mechfail_wp.def	217	*samplpar.res		

#	Filename	#	Filename	#	Filename	#	Filename
68	*ebsrelglass.inp	143	*mechfail_wp.inp	218	smaidtbl.dat		
69	^ebsrel.rlt	144	*mechfail_wp.res	219	sotnef.dat		
70	*ebsrelsf.inp	145	*mv.tpa	220	^spquery.tpa		
71	ebssf.dat	146	*nearfld.res	221	*sp.tpa		
72	ebstrhc.inp	147	nefiialluv.cum	222	*strmtube.dat	^ = EXEC header only reformatted	
73	ebstrh.dat	148	nefiialluv.dis	223	^szft.ech	* = EXEC and file header reformatted	
74	echofail.dbg	149	nefiialluv.inp	224	^szft.rlt		
75	*failt.cum	150	nefiialluv.out	225	sz_kdrd.out		

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 06002.01.354
Software Name: TPA	Version: 5.1BetaT
Test ID: **P-2**	Test Series Name: Subroutine Libraries

Test Method

- ■ code inspection
- □ output inspection
- □ hand calculation
- □ spreadsheet
- □ graphical
- □ comparison with external code results

Test Objective: Verify the following:

1. New routines FindRootRanges(), FindRootRanges1(), RootFind(), and RootFind1() in *numrecip.f,* as described in Software Change Report 586, are correctly implemented.
2. New routines in *nrutil.f* to calculate drip shield outer surface and waste package temperatures, as described in Software Change Report 553, are correctly implemented.

Test Environment Setup

Hardware (platform, peripherals):

Software (OS, compiler, libraries, auxiliary codes or scripts):

Input Data (files, data base, mode settings):

Assumptions, constraints, and/or scope of test: Validation limited to portions of the code that have been revised or updated. It is assumed that testing documented in software change reports remains valid if no subsequent changes have been made to those portions of the code tested.

Test Procedure: Review of Software Change Reports 553 and 586 to confirm whether the above-stated objectives have been tested sufficiently. Review subsequent software changes to ensure testing remains valid. Note also that more detailed testing documented in TPA 5.1 Validation Tasks P-5 and P-7 verifies that the *nfenv.f* and *mechfail.f* modules that utilize these utility functions are working properly.

Test Results

Location: Testing documented in Software Change Reports 553 and 586.

Test Criterion and Analysis of Results: Above stated Test Objectives are met by software change testing.

Test Evaluation (Pass/Fail): **PASS**

Notes:

Tester: Ron Janetzke	Date: 4/30/2007

SOFTWARE VALIDATION REPORT (SVR)

SVTR#:	Project#: 20.06002.01.354
Software Name: TPA	Version: 5.1betaD
Test ID: P-3	Test Series Name: Inventory Module, INVENT

Test Method

x code inspection
☐ output inspection
☐ hand calculation

x spreadsheet
x graphical
☐ comparison with external code results

Test Objective: Verify implementation of new data in *burnup.dat* and consistency in using the year for emplacement in *burnup.dat* and *tpa.inp* files.

Test Environment Setup

Hardware (platform, peripherals): P-IV Toshiba Laptop

Software (OS, compiler, libraries, auxiliary codes or scripts): XP Professional, LF95 FORTRAN

Input Data (files, data base, mode settings): Execute the basecase TPA Version 5.1betaD code for a single subarea and one realization; the time for waste emplacement in *burnup.dat* and *tpa.inp* will be modified to values that are anticipated to yield expected results for the initial inventory used in release calculations; and waste package temperatures will be examined for consistency with information in the updated *burnup.dat* file.

Assumptions, constraints, and/or scope of test: See Attachment A.

Test Procedure: See Attachment A.

Test Results

Location: See the attached CD labeled "TPA 5.1 Validation Task P-3".

Test Criterion and Analysis of Results: See Attachment A.

Test Evaluation (Pass/Fail): Pass

Notes: Note that this test was already completed with TPA Version 5.1betaD when validation testing was halted to make several software revisions not related to the INVENT module. Following code changes, validation testing resumed with TPA Version 5.1betaT. Calculation checks performed during the technical review of this SVR confirm results with TPA Version 5.1betaW.

Tester: R.Rice / O. Povetko	Date: 8/9/06

Attachment A
TPA Version 5.1 Validation Task P-3
Test Procedure

Task Title: "invent" - Verify implementation of new data in *burnup.dat* and consistency in using the year for emplacement in *burnup.dat* and *tpa.inp* files.

Note that this test was already completed with TPA Version 5.1betaD when validation testing was halted to make several software revisions not related to the INVENT module. Following those code changes, validation testing resumed with TPA Version 5.1betaT. Calculation checks performed during the technical review of this SVR confirm results with TPA Version 5.1betaW.

Point of Contact: R. Rice

Other team member(s): O. Povetko

Reviewer: R. Nes

Test Suite: See below

Files to be modified: *burnup.dat*, *tpa.inp*

Output files: *ebstrh.dat* (FAILT output file/RELEASET input file containing waste package temperature); *ebspacsf.nuc* (RELEASET input file containing initial radionuclide inventories); and *rgwgsnr.tpa* (TPA code output files with the groundwater [GW] and ground surface [GS] doses)

Test methodology: **TPA CODE EXECUTION**

TEST 1: BURNUP

– Execute the TPA Version 5.1betaD code using the basecase *tpa.inp* file for one realization and subarea 1 with maximum simulation times of 10kyr, 100kyr, and 1000kyr. Use the TPA Version 5.1betD code updated *burnup.dat* file and the TPA Version 4.1jpdls_beta4 code *burnup.dat* file. For these simulations, the values for all parameters and data used in calculations will be the same, except for the data in the *burnup.dat* file characterizing temporal behavior of PWR and BWR CSNF heat output levels.

– **Expected Results:** Plotting the temperatures and *burnup.dat* values should show that the highest temperatures are associated with highest heat output levels ; likewise, the lowest temperatures are associated with lowest heat output levels.

TEST 2: YEAR OF EMPLACEMENT

– Execute the TPA Version 51betaD code using the basecase *tpa.inp* file with VOLCANO activated for one realization and subarea 1 with maximum simulation times of 10kyr, 100kyr, and 1000kyr. Then, modify the year of emplacement in the *tpa.inp* and *burnup.dat* files to 2133 (i.e., one hundred years later) and execute the TPA Version

51betaD code again. For these simulations, the values for all parameters and data used in calculations will be the same, including the time of the volcanic event; only the emplacement time in the *tpa.inp* and *burnup.dat* files will be different.

– **Expected Results:** Using spreadsheet calculations and comparing results from the two TPA code executions, the inventories in *ebspacsf.nuc* for GW and the GS doses values for specific radionuclides in the *rgsnr.tpa* file should be exponentially decayed by 100 years. Note: selected radionuclides will be evaluated. The acceptable tolerance is less than 1%.

TEST 1 RESULTS: BURNUP

Inspection of data in the file *burnup.dat* is provided below in Table 1.

	TPA5.1betaD			TPA4.1	
Time (yr)	BWR	PWR	Time (yr)	BWR	PWR
1	8666.656	16007.69	1	8407	10510
2	4993.886	8725.222	2	4592	5722
3	3452.021	5661.765	3	3022	3743
5	2260.426	3331.51	5	1829	2238
10	1593.674	2124.147	10	1204	1448
15	1388.692	1796.402	15	1032	1233
20	1252.413	1597.052	20	926.7	1104
25	1132.735	1432.657			
30	1043.49	1310.98	30	773.7	917.8
50	755.1648	934.9177	50	566.9	668
100	408.1607	495.7845	100	317.3	367.3
200	225.2542	268.6157	200	181.7	205.1
300	173.7836	205.8824	300	142	158.9
500	125.5792	147.7668	500	103.2	115.1
1000	71.91241	83.00618	1000	58.32	66.1
2000	37.62872	41.91981	2000	29.54	34.69
5000	23.85442	26.03939	5000	18.52	22.27
10000	17.05174	18.70736	10000	13.46	16.22
20000	9.809821	10.87415	20000	7.978	9.665
50000	3.492567	3.93857	50000	2.928	3.555
100000	1.381935	1.586916	100000	1.123	1.343
200000	0.873423	1.025695	200000	0.6863	0.8022
500000	0.719687	0.84842	500000	0.5834	0.6692
1000000	0.515269	0.605596	1000000	0.4319	0.4851

Table 1. Comparison of *burnup.dat* Files for TPA Versions 5.1betaD and 4.1 Codes.

Plots of data and results from TPA code executions are provided Figures 1 through 4.

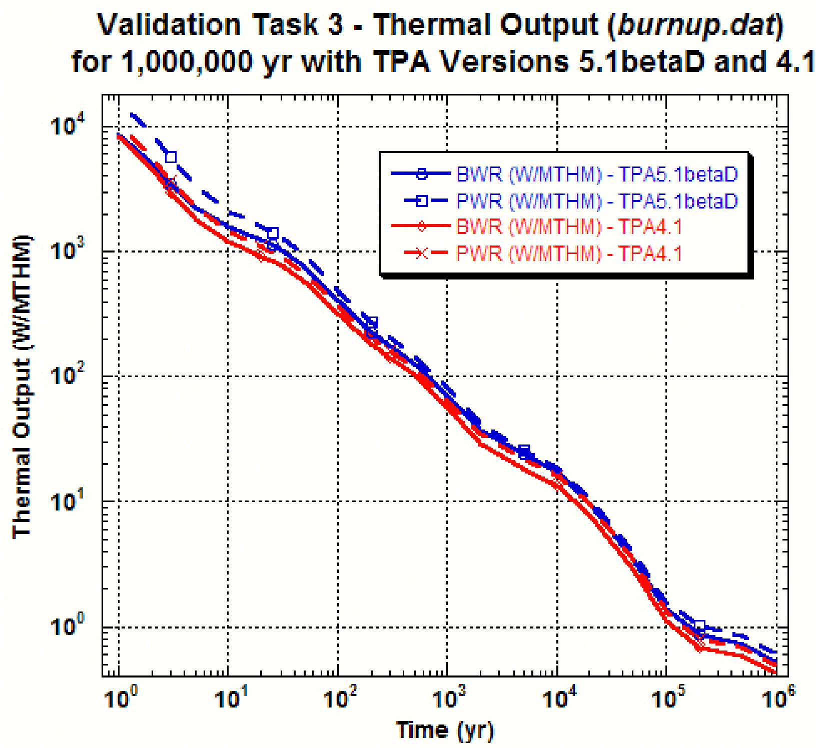


Figure 1. **Plot of BWR and PWR Data in *burnup.dat* files for the TPA Versions 5.1betaD and 4.1 Codes.**

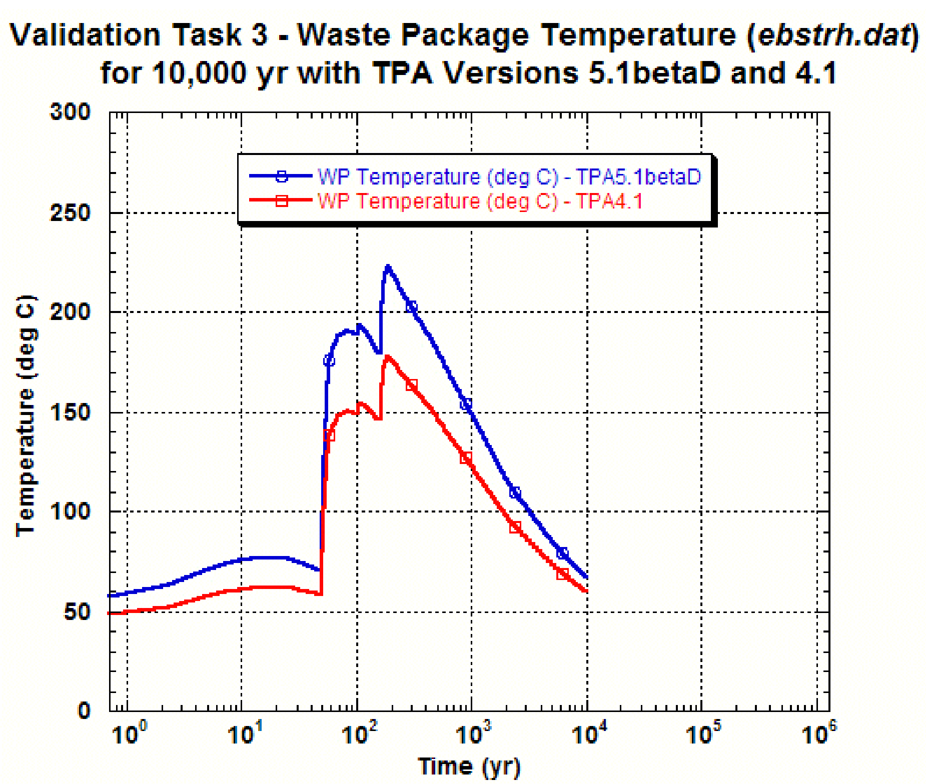


Figure 2. **Plot of Waste Package Temperature at 10,000 yr in *ebstrh.dat* files for TPA Versions 5.1betaD and 4.1 codes.**

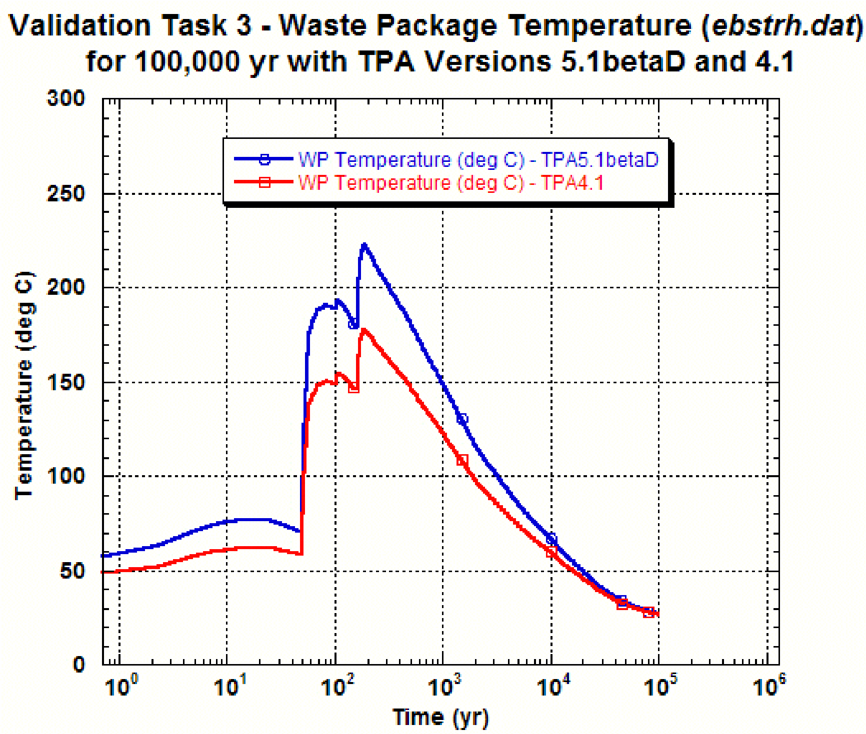


Figure 3. Plot of Waste Package Temperature at 100,000 yr in *ebstrh.dat* files for TPA Versions 5.1betaD and 4.1 codes.

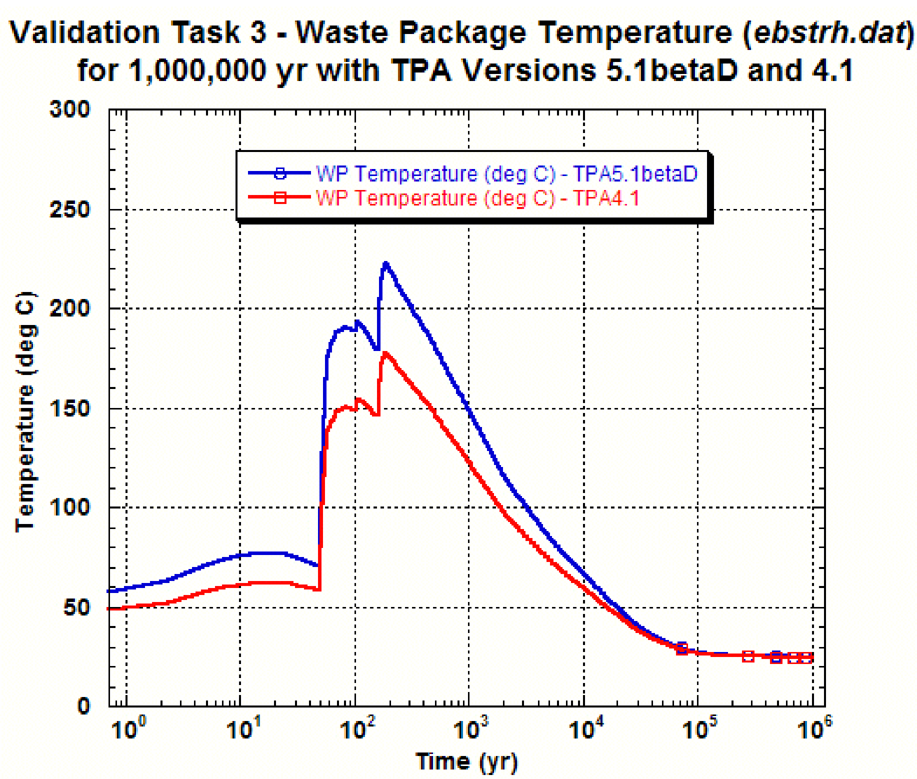


Figure 4. Plot of Waste Package Temperature at 1,000,000 yr in *ebstrh.dat* files for TPA Versions 5.1betaD and 4.1 codes.

The "Expected Results" listed above in the test plan are: "Plotting the temperatures and *burnup.dat* values should show that the highest temperatures are associated with highest heat output levels; likewise, the lowest temperatures are associated with lowest heat output levels." This behavior is evident in the above plots of Figures 1 through 4. Therefore, the test results satisfy the expected results and the test is passed.

TEST 1 Overall Test Status: PASS

TEST 2 RESULTS: YEAR OF EMPLACEMENT

Table 2 below was created, copied, and pasted from an EXCEL spreadsheet. Inventories were decayed using a first-order equation.

Radionuclide (unitless)	t1/2 (yr)	Inventory #1 Year of Emplacement at 2033 (Ci)	Inventory #1 (X) Decayed 100 year (Ci)	Inventory #2 (Y) Year of Emplacement at 2133 (Ci)	% Difference Between X and Y (unitless)
CM246	4.731E+03	**1.617E+00**	**1.593E+00**	**1.594E+00**	**-0.033%**
U238	4.468E+09	2.619E+00	N/A (chain)	2.619E+00	N/A
CM245	8.499E+03	**4.734E+00**	**4.696E+00**	**4.696E+00**	**-0.010%**
AM241	4.322E+02	2.967E+04	N/A (chain)	2.922E+04	N/A
NP237	2.140E+06	3.290E+00	N/A (chain)	4.287E+00	N/A
U233	1.585E+05	6.651E-04	N/A (chain)	2.323E-03	N/A
TH229	7.339E+03	0.000E+00	N/A (chain)	1.371E-05	N/A
AM243	7.380E+03	**2.533E+02**	**2.509E+02**	**2.509E+02**	**0.013%**
PU239	2.406E+04	2.675E+03	N/A (chain)	2.668E+03	N/A
PU240	6.537E+03	4.663E+03	N/A (chain)	4.673E+03	N/A
U234	2.445E+05	1.120E+01	N/A (chain)	1.619E+01	N/A
TH230	7.700E+04	3.740E-03	N/A (chain)	1.635E-02	N/A
RA226	1.600E+03	0.000E+00	N/A (chain)	4.122E-04	N/A
PB210	2.230E+01	0.000E+00	N/A (chain)	2.482E-04	N/A
CS135	2.300E+06	**6.809E+00**	**6.809E+00**	**6.809E+00**	**-0.003%**
I129	1.570E+07	**3.061E-01**	**3.061E-01**	**3.061E-01**	**0.000%**
TC99	2.130E+05	**1.278E+02**	**1.278E+02**	**1.278E+02**	**-0.033%**
NI59	8.000E+04	**3.566E+01**	**3.563E+01**	**3.563E+01**	**-0.002%**
SE79	1.100E+06	**8.521E-01**	**8.520E-01**	**8.521E-01**	**-0.006%**
NB94	2.030E+04	**1.152E+01**	**1.148E+01**	**1.148E+01**	**0.006%**
CL36	3.010E+05	**1.357E-01**	**1.357E-01**	**1.357E-01**	**-0.023%**

Table 2. Percent Differences in the *ebspacsf.nuc* Inventories for Selected Radionuclides With Emplacement at 2,033 and 2,133 from the TPA Version 5.1betaD Code.

The above % differences in Table 2 are all within the acceptable tolerance of 1% for this validation test.

Note that file comparisons conducted using the "fc" in the COMMAND PROMPT window showed no differences between the contents of *ebspacsf.nuc* at 10kyr, 100kyr, and 1,000 kyr for the same year of emplacement.

Also, the "N/A (chain)" and "N/A" above refer to radionuclides that are part of a decay chain in INVENT and are not be subject to first-order decay; consequently, a "% difference" is not calculated for these radionuclides.

For the GS, the same radionuclides as for the GW were selected. These radionuclides are Cm-

246, Cm-245, Am-243, Cs-135, I-129, Tc-99, Ni-59, Se-79, Nb-94, and Cl-36. Results are provided in Tables 3 through 6.

Also, because the GS doses in the *rgsnr.tpa* file are the same for 10kyr, 100kyr, and 1,000 kyr and a number of values are zero, only the non-zero results are shown.

	Cm246	Am243	Cm245	Cs135	I129	Tc99	Nb94	Se79	Ni59	Cl36
Half-Life (yr)	4.73E+03	8.50E+03	7.38E+03	2.30E+06	1.57E+07	2.13E+05	8.00E+04	1.10E+06	2.03E+04	3.01E+05

Time (yr)	Cm246 (rem/yr)	Am243 (rem/yr)	Cm245 (rem/yr)	Cs135 (rem/yr)	I129 (rem/yr)	Tc99 (rem/yr)	Nb94 (rem/yr)	Se79 (rem/yr)	Ni59 (rem/yr)	Cl36 (rem/yr)
9.71E+02	1.40E-05	2.31E-03	4.37E-05	3.21E-09	7.53E-09	1.35E-07	2.75E-08	6.42E-10	1.28E-09	2.21E-10
9.96E+02	1.27E-05	2.09E-03	3.96E-05	2.92E-09	6.83E-09	1.22E-07	2.50E-08	5.82E-10	1.16E-09	2.00E-10
1.02E+03	1.45E-05	2.40E-03	4.54E-05	3.36E-09	7.86E-09	1.40E-07	2.87E-08	6.70E-10	1.34E-09	2.30E-10
1.05E+03	1.54E-05	2.55E-03	4.82E-05	3.57E-09	8.36E-09	1.49E-07	3.05E-08	7.13E-10	1.42E-09	2.45E-10
1.08E+03	1.55E-05	2.57E-03	4.87E-05	3.61E-09	8.47E-09	1.51E-07	3.09E-08	7.22E-10	1.44E-09	2.48E-10
1.10E+03	1.55E-05	2.57E-03	4.87E-05	3.62E-09	8.49E-09	1.51E-07	3.09E-08	7.23E-10	1.44E-09	2.49E-10
1.13E+03	1.54E-05	2.56E-03	4.86E-05	3.62E-09	8.49E-09	1.52E-07	3.09E-08	7.23E-10	1.44E-09	2.49E-10
1.16E+03	1.54E-05	2.56E-03	4.85E-05	3.62E-09	8.49E-09	1.52E-07	3.08E-08	7.23E-10	1.44E-09	2.49E-10
1.19E+03	1.53E-05	2.55E-03	4.84E-05	3.62E-09	8.49E-09	1.52E-07	3.08E-08	7.23E-10	1.44E-09	2.49E-10
1.22E+03	1.52E-05	2.54E-03	4.83E-05	3.62E-09	8.49E-09	1.51E-07	3.08E-08	7.23E-10	1.44E-09	2.49E-10
1.25E+03	1.52E-05	2.54E-03	4.81E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.28E+03	1.51E-05	2.53E-03	4.80E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.31E+03	1.50E-05	2.52E-03	4.79E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.35E+03	1.49E-05	2.51E-03	4.78E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.38E+03	1.49E-05	2.50E-03	4.76E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.42E+03	1.48E-05	2.50E-03	4.75E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.45E+03	1.47E-05	2.49E-03	4.73E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.49E+03	1.46E-05	2.48E-03	4.72E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.52E+03	1.46E-05	2.47E-03	4.71E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.56E+03	1.45E-05	2.46E-03	4.69E-05	3.62E-09	8.49E-09	1.51E-07	3.04E-08	7.23E-10	1.44E-09	2.48E-10
1.60E+03	1.44E-05	2.45E-03	4.68E-05	3.62E-09	8.49E-09	1.51E-07	3.04E-08	7.23E-10	1.44E-09	2.48E-10
1.64E+03	1.43E-05	2.44E-03	4.66E-05	3.62E-09	8.49E-09	1.51E-07	3.03E-08	7.23E-10	1.44E-09	2.48E-10
1.68E+03	1.42E-05	2.44E-03	4.65E-05	3.62E-09	8.49E-09	1.51E-07	3.03E-08	7.23E-10	1.44E-09	2.48E-10
1.72E+03	1.41E-05	2.43E-03	4.63E-05	3.62E-09	8.49E-09	1.51E-07	3.02E-08	7.23E-10	1.44E-09	2.48E-10
1.77E+03	1.41E-05	2.42E-03	4.61E-05	3.62E-09	8.49E-09	1.51E-07	3.02E-08	7.23E-10	1.44E-09	2.48E-10
1.81E+03	1.40E-05	2.41E-03	4.60E-05	3.62E-09	8.49E-09	1.51E-07	3.02E-08	7.23E-10	1.44E-09	2.48E-10
1.85E+03	1.39E-05	2.40E-03	4.58E-05	3.62E-09	8.49E-09	1.51E-07	3.01E-08	7.23E-10	1.43E-09	2.48E-10
1.90E+03	1.38E-05	2.39E-03	4.56E-05	3.62E-09	8.49E-09	1.51E-07	3.01E-08	7.23E-10	1.43E-09	2.48E-10
1.95E+03	1.37E-05	2.38E-03	4.55E-05	3.62E-09	8.49E-09	1.51E-07	3.00E-08	7.23E-10	1.43E-09	2.48E-10
1.99E+03	1.36E-05	2.36E-03	4.53E-05	3.62E-09	8.49E-09	1.51E-07	3.00E-08	7.23E-10	1.43E-09	2.48E-10
2.04E+03	1.35E-05	2.35E-03	4.51E-05	3.62E-09	8.49E-09	1.51E-07	2.99E-08	7.23E-10	1.43E-09	2.48E-10
2.09E+03	1.34E-05	2.34E-03	4.49E-05	3.62E-09	8.49E-09	1.51E-07	2.99E-08	7.23E-10	1.43E-09	2.48E-10
2.15E+03	1.33E-05	2.33E-03	4.47E-05	3.62E-09	8.49E-09	1.51E-07	2.98E-08	7.23E-10	1.43E-09	2.48E-10
2.20E+03	1.32E-05	2.32E-03	4.45E-05	3.62E-09	8.49E-09	1.51E-07	2.98E-08	7.23E-10	1.43E-09	2.48E-10
2.25E+03	1.31E-05	2.31E-03	4.44E-05	3.62E-09	8.49E-09	1.51E-07	2.97E-08	7.23E-10	1.43E-09	2.48E-10
2.31E+03	1.30E-05	2.30E-03	4.42E-05	3.62E-09	8.49E-09	1.51E-07	2.96E-08	7.23E-10	1.43E-09	2.48E-10
2.36E+03	1.29E-05	2.28E-03	4.40E-05	3.62E-09	8.49E-09	1.51E-07	2.96E-08	7.23E-10	1.43E-09	2.48E-10
2.42E+03	1.28E-05	2.27E-03	4.37E-05	3.62E-09	8.49E-09	1.51E-07	2.95E-08	7.23E-10	1.43E-09	2.48E-10
2.48E+03	1.27E-05	2.26E-03	4.35E-05	3.62E-09	8.49E-09	1.51E-07	2.95E-08	7.23E-10	1.43E-09	2.48E-10
2.54E+03	1.26E-05	2.25E-03	4.33E-05	3.62E-09	8.49E-09	1.51E-07	2.94E-08	7.23E-10	1.43E-09	2.48E-10
2.60E+03	1.24E-05	2.23E-03	4.31E-05	3.62E-09	8.49E-09	1.51E-07	2.94E-08	7.23E-10	1.43E-09	2.48E-10

Table 3. Half-Life and Ground Surface Dose in the *rgsnr.tpa* File for Selected Radionuclides With Emplacement at 2,033 from the TPA Version 5.1betaD Code.

Time (yr)	Cm246 (rem/yr)	Am243 (rem/yr)	Cm245 (rem/yr)	Cs135 (rem/yr)	I129 (rem/yr)	Tc99 (rem/yr)	Nb94 (rem/yr)	Se79 (rem/yr)	Ni59 (rem/yr)	Cl36 (rem/yr)
9.71E+02	1.38E-05	2.29E-03	4.33E-05	3.21E-09	7.53E-09	1.35E-07	2.75E-08	6.42E-10	1.28E-09	2.21E-10
9.96E+02	1.25E-05	2.07E-03	3.92E-05	2.92E-09	6.83E-09	1.22E-07	2.50E-08	5.82E-10	1.16E-09	2.00E-10
1.02E+03	1.43E-05	2.38E-03	4.50E-05	3.36E-09	7.86E-09	1.40E-07	2.87E-08	6.70E-10	1.34E-09	2.30E-10
1.05E+03	1.52E-05	2.53E-03	4.77E-05	3.57E-09	8.36E-09	1.49E-07	3.05E-08	7.13E-10	1.42E-09	2.45E-10
1.08E+03	1.53E-05	2.55E-03	4.82E-05	3.61E-09	8.47E-09	1.51E-07	3.09E-08	7.22E-10	1.44E-09	2.48E-10
1.10E+03	1.53E-05	2.55E-03	4.82E-05	3.62E-09	8.49E-09	1.51E-07	3.09E-08	7.23E-10	1.44E-09	2.49E-10
1.13E+03	1.52E-05	2.54E-03	4.81E-05	3.62E-09	8.49E-09	1.52E-07	3.09E-08	7.23E-10	1.44E-09	2.49E-10
1.16E+03	1.52E-05	2.54E-03	4.80E-05	3.62E-09	8.49E-09	1.52E-07	3.08E-08	7.23E-10	1.44E-09	2.49E-10
1.19E+03	1.51E-05	2.53E-03	4.79E-05	3.62E-09	8.49E-09	1.52E-07	3.08E-08	7.23E-10	1.44E-09	2.49E-10
1.22E+03	1.50E-05	2.52E-03	4.78E-05	3.62E-09	8.49E-09	1.51E-07	3.08E-08	7.23E-10	1.44E-09	2.49E-10
1.25E+03	1.50E-05	2.52E-03	4.77E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.28E+03	1.49E-05	2.51E-03	4.76E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.31E+03	1.48E-05	2.50E-03	4.75E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.35E+03	1.47E-05	2.49E-03	4.74E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.38E+03	1.47E-05	2.48E-03	4.72E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.42E+03	1.46E-05	2.48E-03	4.71E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.45E+03	1.45E-05	2.47E-03	4.69E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.49E+03	1.44E-05	2.46E-03	4.68E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.52E+03	1.44E-05	2.45E-03	4.67E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.56E+03	1.43E-05	2.44E-03	4.65E-05	3.62E-09	8.49E-09	1.51E-07	3.04E-08	7.23E-10	1.44E-09	2.48E-10
1.60E+03	1.42E-05	2.43E-03	4.64E-05	3.62E-09	8.49E-09	1.51E-07	3.04E-08	7.23E-10	1.44E-09	2.48E-10
1.64E+03	1.41E-05	2.42E-03	4.62E-05	3.62E-09	8.49E-09	1.51E-07	3.03E-08	7.23E-10	1.44E-09	2.48E-10
1.68E+03	1.40E-05	2.42E-03	4.61E-05	3.62E-09	8.49E-09	1.51E-07	3.03E-08	7.23E-10	1.44E-09	2.48E-10
1.72E+03	1.39E-05	2.41E-03	4.59E-05	3.62E-09	8.49E-09	1.51E-07	3.02E-08	7.23E-10	1.44E-09	2.48E-10
1.77E+03	1.39E-05	2.40E-03	4.57E-05	3.62E-09	8.49E-09	1.51E-07	3.02E-08	7.23E-10	1.44E-09	2.48E-10
1.81E+03	1.38E-05	2.39E-03	4.56E-05	3.62E-09	8.49E-09	1.51E-07	3.02E-08	7.23E-10	1.44E-09	2.48E-10
1.85E+03	1.37E-05	2.38E-03	4.54E-05	3.62E-09	8.49E-09	1.51E-07	3.01E-08	7.23E-10	1.43E-09	2.48E-10
1.90E+03	1.36E-05	2.37E-03	4.52E-05	3.62E-09	8.49E-09	1.51E-07	3.01E-08	7.23E-10	1.43E-09	2.48E-10
1.95E+03	1.35E-05	2.36E-03	4.51E-05	3.62E-09	8.49E-09	1.51E-07	3.00E-08	7.23E-10	1.43E-09	2.48E-10
1.99E+03	1.34E-05	2.34E-03	4.49E-05	3.62E-09	8.49E-09	1.51E-07	3.00E-08	7.23E-10	1.43E-09	2.48E-10
2.04E+03	1.33E-05	2.33E-03	4.47E-05	3.62E-09	8.49E-09	1.51E-07	2.99E-08	7.23E-10	1.43E-09	2.48E-10
2.09E+03	1.32E-05	2.32E-03	4.45E-05	3.62E-09	8.49E-09	1.51E-07	2.99E-08	7.23E-10	1.43E-09	2.48E-10
2.15E+03	1.31E-05	2.31E-03	4.43E-05	3.62E-09	8.49E-09	1.51E-07	2.98E-08	7.23E-10	1.43E-09	2.48E-10
2.20E+03	1.30E-05	2.30E-03	4.41E-05	3.62E-09	8.49E-09	1.51E-07	2.98E-08	7.23E-10	1.43E-09	2.48E-10
2.25E+03	1.29E-05	2.29E-03	4.40E-05	3.62E-09	8.49E-09	1.51E-07	2.97E-08	7.23E-10	1.43E-09	2.48E-10
2.31E+03	1.28E-05	2.28E-03	4.38E-05	3.62E-09	8.49E-09	1.51E-07	2.96E-08	7.23E-10	1.43E-09	2.48E-10
2.36E+03	1.27E-05	2.26E-03	4.36E-05	3.62E-09	8.49E-09	1.51E-07	2.96E-08	7.23E-10	1.43E-09	2.48E-10
2.42E+03	1.26E-05	2.25E-03	4.33E-05	3.62E-09	8.49E-09	1.51E-07	2.95E-08	7.23E-10	1.43E-09	2.48E-10
2.48E+03	1.25E-05	2.24E-03	4.31E-05	3.62E-09	8.49E-09	1.51E-07	2.95E-08	7.23E-10	1.43E-09	2.48E-10
2.54E+03	1.24E-05	2.23E-03	4.29E-05	3.62E-09	8.49E-09	1.51E-07	2.94E-08	7.23E-10	1.43E-09	2.48E-10
2.60E+03	1.22E-05	2.21E-03	4.27E-05	3.62E-09	8.49E-09	1.51E-07	2.94E-08	7.23E-10	1.43E-09	2.48E-10

Table 4. Ground Surface Dose in the *rgsnr.tpa* File Decayed 100 yr for Selected Radionuclides With Emplacement at 2,033 from the TPA Version 5.1betaD Code.

Time (yr)	Cm246 (rem/yr)	Am243 (rem/yr)	Cm245 (rem/yr)	Cs135 (rem/yr)	I129 (rem/yr)	Tc99 (rem/yr)	Nb94 (rem/yr)	Se79 (rem/yr)	Ni59 (rem/yr)	Cl36 (rem/yr)
9.71E+02	1.38E-05	2.29E-03	4.33E-05	3.21E-09	7.53E-09	1.35E-07	2.74E-08	6.42E-10	1.28E-09	2.21E-10
9.96E+02	1.25E-05	2.07E-03	3.92E-05	2.92E-09	6.83E-09	1.22E-07	2.49E-08	5.82E-10	1.16E-09	2.00E-10
1.02E+03	1.43E-05	2.38E-03	4.51E-05	3.36E-09	7.86E-09	1.40E-07	2.86E-08	6.70E-10	1.34E-09	2.30E-10
1.05E+03	1.52E-05	2.52E-03	4.78E-05	3.57E-09	8.36E-09	1.49E-07	3.04E-08	7.13E-10	1.42E-09	2.45E-10
1.08E+03	1.53E-05	2.55E-03	4.83E-05	3.61E-09	8.47E-09	1.51E-07	3.07E-08	7.22E-10	1.44E-09	2.48E-10
1.10E+03	1.53E-05	2.55E-03	4.83E-05	3.62E-09	8.49E-09	1.51E-07	3.08E-08	7.23E-10	1.44E-09	2.48E-10
1.13E+03	1.52E-05	2.54E-03	4.82E-05	3.62E-09	8.49E-09	1.51E-07	3.08E-08	7.23E-10	1.44E-09	2.49E-10
1.16E+03	1.51E-05	2.53E-03	4.81E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.19E+03	1.51E-05	2.53E-03	4.80E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.22E+03	1.50E-05	2.52E-03	4.79E-05	3.62E-09	8.49E-09	1.51E-07	3.07E-08	7.23E-10	1.44E-09	2.49E-10
1.25E+03	1.49E-05	2.51E-03	4.77E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.28E+03	1.49E-05	2.50E-03	4.76E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.31E+03	1.48E-05	2.50E-03	4.75E-05	3.62E-09	8.49E-09	1.51E-07	3.06E-08	7.23E-10	1.44E-09	2.48E-10
1.35E+03	1.47E-05	2.49E-03	4.74E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.38E+03	1.47E-05	2.48E-03	4.72E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.42E+03	1.46E-05	2.47E-03	4.71E-05	3.62E-09	8.49E-09	1.51E-07	3.05E-08	7.23E-10	1.44E-09	2.48E-10
1.45E+03	1.45E-05	2.47E-03	4.70E-05	3.62E-09	8.49E-09	1.51E-07	3.04E-08	7.23E-10	1.44E-09	2.48E-10
1.49E+03	1.44E-05	2.46E-03	4.68E-05	3.62E-09	8.49E-09	1.51E-07	3.04E-08	7.23E-10	1.44E-09	2.48E-10
1.52E+03	1.44E-05	2.45E-03	4.67E-05	3.62E-09	8.49E-09	1.51E-07	3.03E-08	7.23E-10	1.44E-09	2.48E-10
1.56E+03	1.43E-05	2.44E-03	4.65E-05	3.62E-09	8.49E-09	1.51E-07	3.03E-08	7.23E-10	1.44E-09	2.48E-10
1.60E+03	1.42E-05	2.43E-03	4.64E-05	3.62E-09	8.49E-09	1.51E-07	3.03E-08	7.23E-10	1.44E-09	2.48E-10
1.64E+03	1.41E-05	2.42E-03	4.62E-05	3.62E-09	8.49E-09	1.51E-07	3.02E-08	7.23E-10	1.44E-09	2.48E-10
1.68E+03	1.40E-05	2.41E-03	4.61E-05	3.62E-09	8.49E-09	1.51E-07	3.02E-08	7.23E-10	1.44E-09	2.48E-10
1.72E+03	1.39E-05	2.40E-03	4.59E-05	3.62E-09	8.49E-09	1.51E-07	3.01E-08	7.23E-10	1.44E-09	2.48E-10
1.77E+03	1.39E-05	2.39E-03	4.58E-05	3.62E-09	8.49E-09	1.51E-07	3.01E-08	7.23E-10	1.43E-09	2.48E-10
1.81E+03	1.38E-05	2.38E-03	4.56E-05	3.62E-09	8.49E-09	1.51E-07	3.01E-08	7.23E-10	1.43E-09	2.48E-10
1.85E+03	1.37E-05	2.37E-03	4.54E-05	3.62E-09	8.49E-09	1.51E-07	3.00E-08	7.23E-10	1.43E-09	2.48E-10
1.90E+03	1.36E-05	2.36E-03	4.53E-05	3.62E-09	8.49E-09	1.51E-07	3.00E-08	7.23E-10	1.43E-09	2.48E-10
1.95E+03	1.35E-05	2.35E-03	4.51E-05	3.62E-09	8.49E-09	1.51E-07	2.99E-08	7.23E-10	1.43E-09	2.48E-10
1.99E+03	1.34E-05	2.34E-03	4.49E-05	3.62E-09	8.49E-09	1.51E-07	2.99E-08	7.23E-10	1.43E-09	2.48E-10
2.04E+03	1.33E-05	2.33E-03	4.47E-05	3.62E-09	8.49E-09	1.51E-07	2.98E-08	7.23E-10	1.43E-09	2.48E-10
2.09E+03	1.32E-05	2.32E-03	4.46E-05	3.62E-09	8.49E-09	1.51E-07	2.98E-08	7.23E-10	1.43E-09	2.48E-10
2.15E+03	1.31E-05	2.31E-03	4.44E-05	3.62E-09	8.49E-09	1.51E-07	2.97E-08	7.23E-10	1.43E-09	2.48E-10
2.20E+03	1.30E-05	2.30E-03	4.42E-05	3.62E-09	8.49E-09	1.51E-07	2.97E-08	7.23E-10	1.43E-09	2.48E-10
2.25E+03	1.29E-05	2.29E-03	4.40E-05	3.62E-09	8.49E-09	1.51E-07	2.96E-08	7.23E-10	1.43E-09	2.48E-10
2.31E+03	1.28E-05	2.27E-03	4.38E-05	3.62E-09	8.49E-09	1.51E-07	2.95E-08	7.23E-10	1.43E-09	2.48E-10
2.36E+03	1.27E-05	2.26E-03	4.36E-05	3.62E-09	8.49E-09	1.51E-07	2.95E-08	7.23E-10	1.43E-09	2.48E-10
2.42E+03	1.26E-05	2.25E-03	4.34E-05	3.62E-09	8.49E-09	1.51E-07	2.94E-08	7.23E-10	1.43E-09	2.48E-10
2.48E+03	1.25E-05	2.24E-03	4.32E-05	3.62E-09	8.49E-09	1.51E-07	2.94E-08	7.23E-10	1.43E-09	2.48E-10
2.54E+03	1.24E-05	2.23E-03	4.30E-05	3.62E-09	8.49E-09	1.51E-07	2.93E-08	7.23E-10	1.43E-09	2.48E-10
2.60E+03	1.23E-05	2.21E-03	4.28E-05	3.62E-09	8.49E-09	1.51E-07	2.93E-08	7.23E-10	1.42E-09	2.48E-10

Table 5. Ground Surface Dose in the *rgsnr.tpa* File for Selected Radionuclides With Emplacement at 2,133 from the TPA Version 5.1betaD Code.

Time (yr)	Cm246 (rem/yr)	Am243 (rem/yr)	Cm245 (rem/yr)	Cs135 (rem/yr)	I129 (rem/yr)	Tc99 (rem/yr)	Nb94 (rem/yr)	Se79 (rem/yr)	Ni59 (rem/yr)	Cl36 (rem/yr)
9.71E+02	-0.026%	0.054%	-0.020%	-0.003%	0.000%	-0.033%	0.277%	-0.006%	-0.342%	-0.023%
9.96E+02	0.122%	0.146%	0.076%	-0.003%	0.000%	-0.033%	0.314%	-0.006%	-0.342%	-0.023%
1.02E+03	-0.076%	0.021%	-0.277%	-0.003%	0.000%	-0.033%	0.262%	-0.006%	-0.342%	-0.023%
1.05E+03	-0.158%	0.367%	-0.106%	-0.003%	0.000%	-0.033%	0.241%	-0.006%	-0.342%	-0.023%
1.08E+03	-0.167%	-0.034%	-0.115%	-0.003%	0.000%	-0.033%	0.561%	-0.006%	-0.342%	-0.023%
1.10E+03	-0.167%	-0.034%	-0.115%	-0.003%	0.000%	-0.033%	0.237%	-0.006%	-0.342%	0.379%
1.13E+03	-0.158%	-0.031%	-0.113%	-0.003%	0.000%	0.626%	0.237%	-0.006%	-0.342%	-0.023%
1.16E+03	0.501%	0.363%	-0.111%	-0.003%	0.000%	0.626%	0.238%	-0.006%	-0.342%	-0.023%
1.19E+03	-0.149%	-0.028%	-0.109%	-0.003%	0.000%	0.626%	0.238%	-0.006%	-0.342%	-0.023%
1.22E+03	-0.141%	-0.025%	-0.108%	-0.003%	0.000%	-0.033%	0.238%	-0.006%	-0.342%	-0.023%
1.25E+03	0.527%	0.372%	-0.104%	-0.003%	0.000%	-0.033%	0.239%	-0.006%	-0.342%	0.379%
1.28E+03	-0.132%	0.377%	-0.102%	-0.003%	0.000%	-0.033%	0.239%	-0.006%	-0.342%	0.379%
1.31E+03	-0.123%	-0.019%	-0.101%	-0.003%	0.000%	-0.033%	0.239%	-0.006%	-0.342%	0.379%
1.35E+03	-0.114%	-0.016%	-0.099%	-0.003%	0.000%	-0.033%	0.240%	-0.006%	-0.342%	-0.023%
1.38E+03	-0.114%	-0.012%	-0.095%	-0.003%	0.000%	-0.033%	0.240%	-0.006%	-0.342%	-0.023%
1.42E+03	-0.105%	0.391%	-0.094%	-0.003%	0.000%	-0.033%	0.240%	-0.006%	-0.342%	-0.023%
1.45E+03	-0.095%	-0.009%	-0.303%	-0.003%	0.000%	-0.033%	0.241%	-0.006%	-0.342%	-0.023%
1.49E+03	-0.086%	-0.006%	-0.088%	-0.003%	0.000%	-0.033%	0.241%	-0.006%	-0.342%	-0.023%
1.52E+03	-0.086%	-0.003%	-0.086%	-0.003%	0.000%	-0.033%	0.570%	-0.006%	-0.342%	-0.023%
1.56E+03	-0.076%	0.001%	-0.083%	-0.003%	0.000%	-0.033%	0.243%	-0.006%	-0.342%	-0.023%
1.60E+03	-0.067%	0.004%	-0.081%	-0.003%	0.000%	-0.033%	0.243%	-0.006%	-0.342%	-0.023%
1.64E+03	-0.057%	0.007%	-0.077%	-0.003%	0.000%	-0.033%	0.244%	-0.006%	-0.342%	-0.023%
1.68E+03	-0.047%	0.421%	-0.075%	-0.003%	0.000%	-0.033%	0.244%	-0.006%	-0.342%	-0.023%
1.72E+03	-0.037%	0.426%	-0.072%	-0.003%	0.000%	-0.033%	0.245%	-0.006%	-0.342%	-0.023%
1.77E+03	-0.037%	0.431%	-0.287%	-0.003%	0.000%	-0.033%	0.245%	-0.006%	0.355%	-0.023%
1.81E+03	-0.026%	0.436%	-0.066%	-0.003%	0.000%	-0.033%	0.245%	-0.006%	0.355%	-0.023%
1.85E+03	-0.016%	0.441%	-0.062%	-0.003%	0.000%	-0.033%	0.246%	-0.006%	-0.342%	-0.023%
1.90E+03	-0.005%	0.447%	-0.280%	-0.003%	0.000%	-0.033%	0.246%	-0.006%	-0.342%	-0.023%
1.95E+03	0.005%	0.452%	-0.056%	-0.003%	0.000%	-0.033%	0.247%	-0.006%	-0.342%	-0.023%
1.99E+03	0.016%	0.035%	-0.052%	-0.003%	0.000%	-0.033%	0.247%	-0.006%	-0.342%	-0.023%
2.04E+03	0.027%	0.039%	-0.048%	-0.003%	0.000%	-0.033%	0.248%	-0.006%	-0.342%	-0.023%
2.09E+03	0.039%	0.043%	-0.269%	-0.003%	0.000%	-0.033%	0.248%	-0.006%	-0.342%	-0.023%
2.15E+03	0.050%	0.047%	-0.266%	-0.003%	0.000%	-0.033%	0.249%	-0.006%	-0.342%	-0.023%
2.20E+03	0.062%	0.050%	-0.263%	-0.003%	0.000%	-0.033%	0.249%	-0.006%	-0.342%	-0.023%
2.25E+03	0.073%	0.054%	-0.034%	-0.003%	0.000%	-0.033%	0.250%	-0.006%	-0.342%	-0.023%
2.31E+03	0.085%	0.496%	-0.030%	-0.003%	0.000%	-0.033%	0.251%	-0.006%	-0.342%	-0.023%
2.36E+03	0.097%	0.065%	-0.026%	-0.003%	0.000%	-0.033%	0.251%	-0.006%	-0.342%	-0.023%
2.42E+03	0.110%	0.069%	-0.251%	-0.003%	0.000%	-0.033%	0.253%	-0.006%	-0.342%	-0.023%
2.48E+03	0.122%	0.073%	-0.247%	-0.003%	0.000%	-0.033%	0.253%	-0.006%	-0.342%	-0.023%
2.54E+03	0.135%	0.077%	-0.244%	-0.003%	0.000%	-0.033%	0.254%	-0.006%	-0.342%	-0.023%
2.60E+03	-0.658%	0.085%	-0.241%	-0.003%	0.000%	-0.033%	0.254%	-0.006%	0.360%	-0.023%

Table 6. Percent Differences With Emplacement at 2,033 and 2,133 in Ground Surface Dose from the *rgsnr.tpa* File for Selected Radionuclides using the TPA Version 5.1betaD Code.

The above % differences in Table 6 are all within the acceptable tolerance of 1% for this validation test.

The "Expected Results" listed above in the test plan are: "Using spreadsheet calculations and comparing results from the two TPA code executions, the inventories in *ebspacsf.nuc* for GW and the GS dose~~s~~ values for specific radionuclides in the *rgsnr.tpa* file should be exponentially decayed by 100 years. Note: selected radionuclides will be evaluated. The acceptable tolerance is less than 1%." All % differences are within the acceptable tolerance of 1%. Therefore, the test results satisfy the expected results and the test is passed.

Test 2 Overall Test Status: PASS

SOFTWARE VALIDATION TEST REPORT (SVR)

SVTR#:	Project#: 20.06002.01.354
Software Name: **TPA**	Version: 5.1betaU
Test ID: **P-4**	Test Series Name: **Climate and Subarea-Averaged Net Infiltration**

Test Method

x code inspection	x spreadsheet
x output inspection	x graphical
x hand calculation	x comparison with external code results

Test Objective: Verify the functionalities implemented in UZFLOW in accordance with the Software Validation Plan for TPA Code Version 5.1.

Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): XP

Input Data (files, data base, mode settings): See below.

Assumptions, constraints, and/or scope of test: (none)

Test Procedure: See Attachments A and B.

Test Results

Location: Attached CD labeled "TPA Version 5.1 Validation Task P-4"

Test Criterion and Analysis of Results: see Attachment B

Test Evaluation (Pass/Fail): PASS

Notes:

Tester: Razvan Nes	Date: 4/27/2007

Attachment A

TPA Version 5.1 Validation, Task P-4 Test Plan

Task Title: "Climate and Subarea-Averaged Net Infiltration " - The climate and infiltration abstraction was modified to permit specifying a constant net infiltration rate after 10,000 years. Accordingly, *uzflow.f* and related input data and subroutines have been modified to permit this specification. Other changes include modification to the ITYM standalone code, which resulted in generation of new *maidtbl.dat* and *smaidtbl.dat* data files.

Task Lead: R. Nes

Other team member(s): S. Stothoff,

Test Suite: See below

Files to be modified: Listed below.

Output files: Listed below.

<u>TESTS:</u>

Test 1

Test verifies bullets 1 and 5 of Section 6.1.5 of the Software Validation Plan for TPA Code Version 5.1.

The test verifies that:

- Parameter values in *tpa.inp* for average net infiltration after 10,000 years are consistent with the specified range of 0.27-126[mm/yr], based on external analyses; and
- Mean annual infiltration (MAI) after 10,000 years is correctly computed when a correlation to MAI at the start is specified.

The testing process is described below:

- Tester will review the 500-realization output *samplpar.res* for the distribution of sampled mean annual infiltration (MAI) after 10,000 years, checking parameter distributions and ranges; and
- Tester will check the correlation between MAI at start and MAI after 10,000 years; by using a software of choice, tester will plot MAI after 10,000 years as a function of MAI at start from *samplpar.res*, and/or will calculate the correlation factor (usually known as r^2); the calculated r^2 will then be compared with the correlation coefficient given as input in the tpa.inp file.

The results of the test will be reported as PASS/FAIL, if the error is within or exceeding 5%, respectively. The two parameters in question, MAI after 10,000yr and MAI at start, are separately correlated to several other parameters, so an error within 5% was considered satisfactory.

Test 2

Test verifies bullets 2, 3, and 4 of the Software Validation Plan for TPA Code Version 5.1.

The test verifies that:

- The correct value for subarea averaged net infiltration is used for constant climate after 10,000 years when flag* in *tpa.inp* is set to 1, and the correct value based on scaling factor in *climato2.dat* is calculated when the flag is set to 0;

- The TPA output either reports or permits calculation of subarea averaged net infiltration at each time step; and

- The spatial variability of infiltration among subareas is preserved when constant infiltration after 10,000 years is specified (i.e., specified or sampled value is for entire repository, but different average infiltration rates should be calculated for each subarea).

*Note that there is no flag in *tpa.inp* that turns on a constant climate after 10,000 years. Instead, a parameter describing the onset time for a constant climate is specified; this parameter is given a value of 10,000 years if a constant climate is desired and a value larger than the simulation time if the scaling factor in *climato2.dat* is to be calculated.

The testing process is described below:

- Tester will execute the TPA code Version 5.1 two times, with one realization for all 10 subareas using mean values of the input parameters (*tpameans.out*) as input file. The output file *uzflow.rlt* will be generated by setting the appropriate *appendfiles* flag.

    - 1st execution with the long-term-average onset time and the maximum simulation time set to 10,000 yr;
    - 2nd execution with the long-term-average onset time set to 10,000 yr and the maximum simulation time set to 1,000,000 yr.

- Tester will inspect the corresponding *infilper.res* files to verify:

    - Net infiltration is constant after 10,000 yr when the onset time is 10,000 yr;
    - Net infiltration changes with time in proportion to climate data presented in the climato2.dat file when the onset time is 10,000 yr.

- Tester will then inspect the *uzflow.rlt* file to verify that, when the onset time is 10,000 yr, average infiltration after 10,000 yr is different for each subarea, but the area-weighted average for the entire repository matches the value in *infilper.res*

Maximum simulation time of 1,000,000yr was arbitrarily chosen by the tester. This does not significantly change the output, and does not affect the test results.

The results of the test will be reported as PASS/FAIL, accordingly.

Attachment B

TPA 5.1 Software Validation Task P-4 Test Results

Following are test results for the validation test cases described in Attachment A for TPA Version 5.1 code Software Validation Task P-4. Additional details related to test procedures are also provided.

<u>Test 1.</u> The test verifies that:

- **Parameter values in *tpa.inp* for average net infiltration after 10,000 years are consistent with the specified range of 0.27-126[mm/yr];**
- **Mean annual infiltration (MAI) after 10,000 years is correctly computed when a correlation to MAI at the start is specified.**

Version of TPA code

Test case : tpa51betaU

Path for run directory:

Test case : 500-realization run, by O.Pensado

Environment variable:

Test case : -

Path for archive of results

Test case : -

Special input files or modifications to input files required : -

Special diagnostic code modifications required : -

Program modes to be used (append flags, scenario/model switches, etc.): -

Utility scripts needed to perform the test: -

Utility codes needed in the analysis of the test data: Wolfram Mathematica®

Assumptions: -

Constraints -

Output files to compare or examine:

Test Procedure: see Attachment A

Test results:

-The analysis of *samplpar.res*) output file (in the *500realiz* attached folder) shows that sampled values for mean annual infiltrations *uzflow_LongTermAverageFootprintAverageMAI[mm/yr]* and *uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]* are compatible with the quantiles indicated in the *tpa.inp* file; this is summarized in Table 1. Test1 bullet #1 result: PASSED.

Table 1: Mean annual infiltrations (quantile)- input parameter and sampled value

	Input Parameters		Sampled Values	
Quantile	0.001	0.999	0.001	0.999
Mean Annual Infiltration-at Start [mm/yr]	0.27	126	0.27	119
Mean Annual Infiltration-10K yr [mm/yr]	4.2	288.1	4.2	265.1

-sampled values of *uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]* (MAI) and *uzflow_LongTermAverageFootprintAverageMAI[mm/yr]* (10K MAI) from *samplpar.res* are plotted, on a log-log scale, in Fig.1; the correlation factor (usually known as r^2) of the two parameters was calculated, and its value was found to be approximately ***0.942***, which is in good agreement -within 5%-with ***0.98*** value of,

correlateinputs
uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]

indicated in *tpa.inp*.

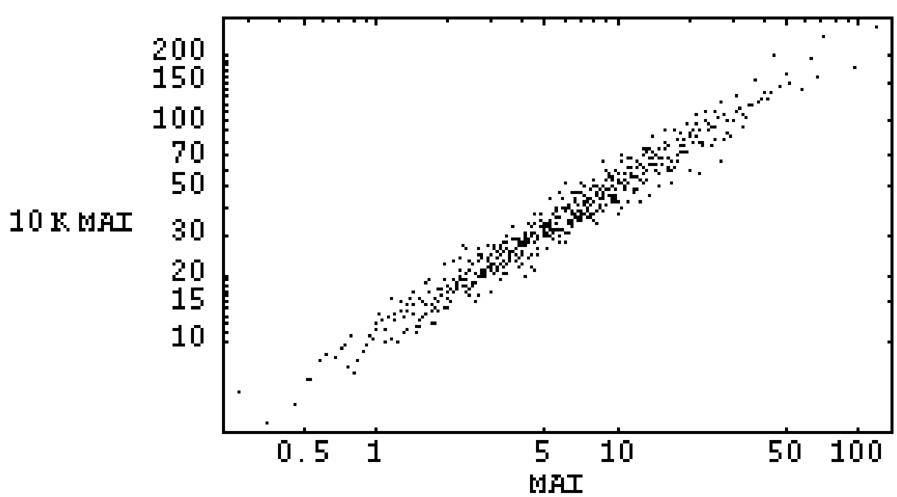


Fig. 1: Correlation between Mean Annual Infiltrations

-Test 1 bullet #2 result: PASS.

<u>Test 2.</u> The test verifies that:

- **The correct value for subarea averaged net infiltration is used for constant climate after 10,000 years when flag* *uzflow_LongTermAverageOnsetTime[yr]* in *tpa.inp* is set to 1, and the correct value based on scaling factor in *climato2.dat* is calculated when the flag is set to 0;**

- **The TPA output either reports or permits calculation of subarea averaged net infiltration at each time step;**

- **The spatial variability of infiltration among subareas is preserved when constant infiltration after 10,000 years is specified (i.e., specified or sampled value is for entire repository, but different average infiltration rates should be calculated for each subarea).**

***see Attachment A.**

Version of TPA code

Test case : tpa51betaU

Path for run directory:

Test case : TPA machine: D:\Public\RNes

Environment variable:

Test case : -

Path for archive of results

Test case : attached CD

Special input files or modifications to input files required : generate the *tpameans.out* file by a one-realization run

Special diagnostic code modifications required : -

Program modes to be used (append file flags, scenario/model switches, etc.):

-append file flags in the *tpa.inp* file
- *OutputMode = 2* (user-defined output)
- *SelectAppendFiles = 0,* or *1* (append all output files, or *uzflow.ech* and *uzflow.rlt* only)

-one-relization run flag in the *tpa.inp* file
- *UserDefinedLowerRealizationAppended =1*
- *UserDefinedUpperRealizationAppended =1*

-simulation time flags
- *MaximumTime[yr]= 10,000 or 1,000,001*
- *DurationOfCompliancePeriod[yr]= 10,000*;

-all subareas

Utility scripts needed to perform the test: -

Utility codes needed in the analysis of the test data: Wolfram Mathematica®

Assumptions: - see Attachment A

Constraints - see Attachment A

Output files to compare or examine:

-tpa.inp
-tpameans.out
-climato2.dat
-uzflow.rlt
-infilper.res

Test Procedure: see Attachment A

Test results:

- Tester inspected the corresponding *infilper.res* files to verify that net infiltration is constant after 10,000 yr when the *uzflow_LongTermAverageOnsetTime[yr] flag* is 10,000 and simulation time is 1,000,001 yr; the *infilper.res* files of interest are located in the attached *10Mrun* folder;

-Test2, bullet #3 result: PASS.

-Net infiltration (INFIL[mm/yr]) changes with time and mean annual precipitation (MIP[mm/yr]) changes with time, derived* based on climate data presented in the *climato2.dat* file when the simulation time is 1,000,001 yr, are presented in Fig. 2 a) and b), respectively;

--Test2, bullet #1 result: PASS.

*Derivations were made based on *uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum* equal to 2.05, as per *tpa.inp*.

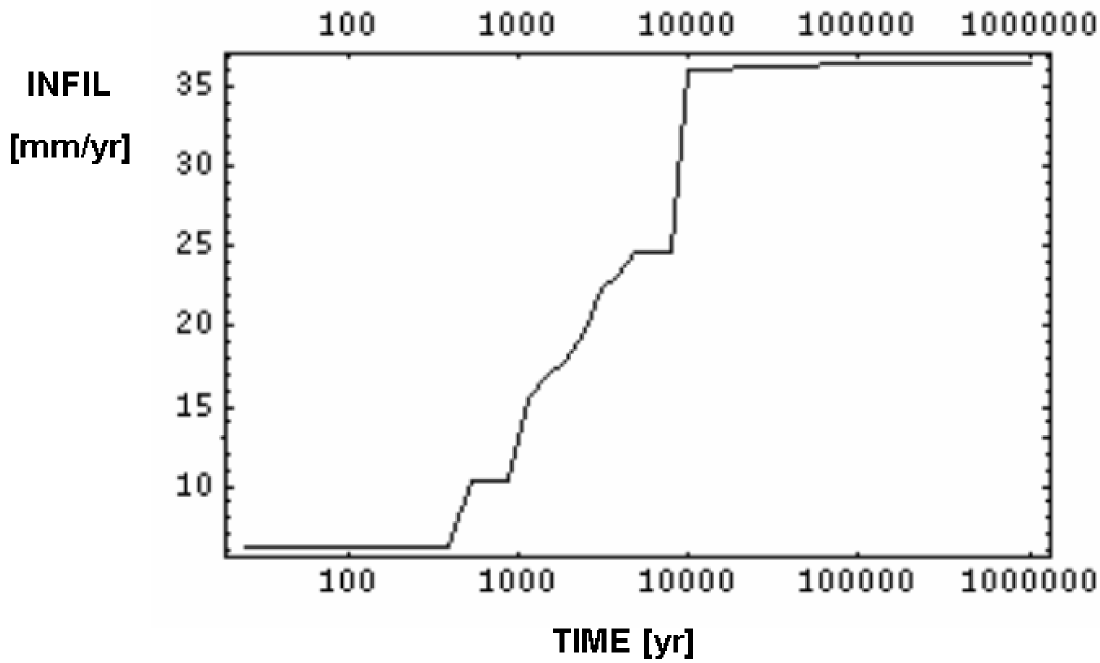


Fig. 2 a)

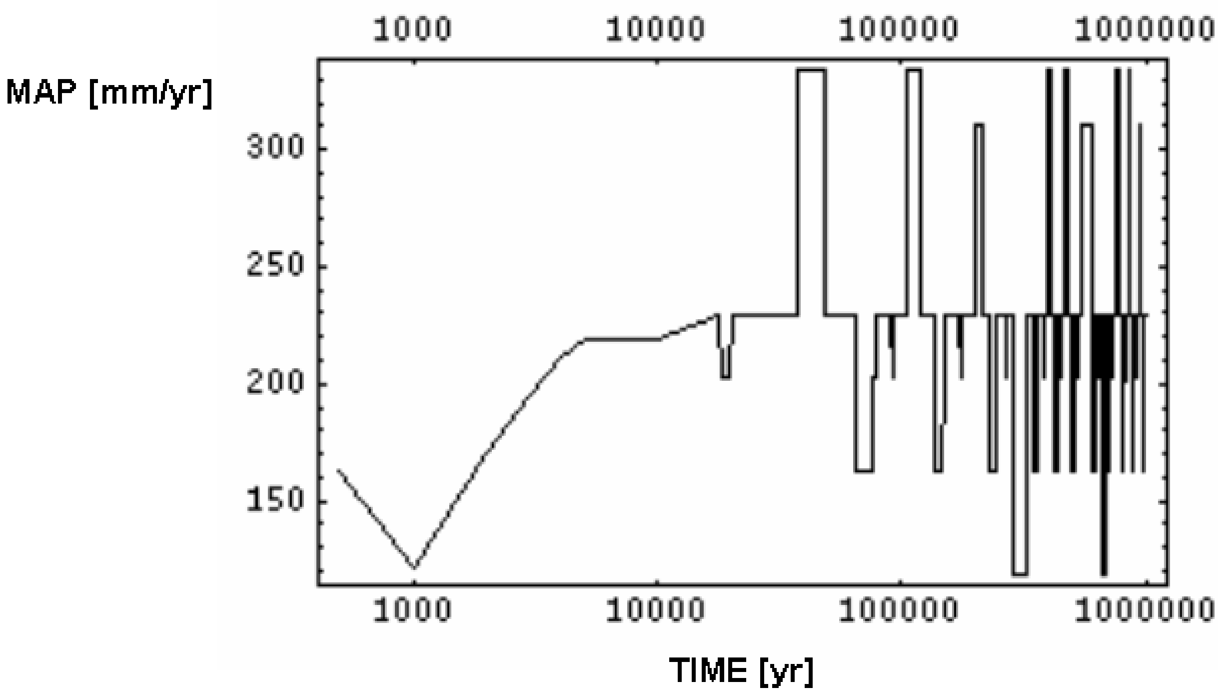


Fig. 2 b)

Fig. 2: Net infiltration (a) and mean annual precipitation (b) functions of time.

NOTE:
Both graphs show flat portions (constant values) after approximately 10,000 yr. Mean annual precipitation, however, shows after 10,000 yr additional alternate climate changes due to the nature of the data in *climato2.dat*, changes not reflected by the net infiltration (constant after 10,000 yr).

-Tester inspected the *uzflow.rlt* file, calculating the area-weighted mean infiltration at time=10,000yr from flow data provided in *uzflow.rlt* (Eq. 1) and by area-weighted average (Eq. 2) from *infilper.res*:

$$\bar{I} = \frac{\sum_{i=1}^{10} \Phi_i}{\sum_{i=1}^{10} A_i} \qquad \text{(Eq. 1)}$$

$$\bar{I} = 10^{-3} \times \frac{\sum_{i=1}^{10} I_i \times A_i}{\sum_{i=1}^{10} A_i} \qquad \text{(Eq. 2)}$$

Where: i = subarea index, from 1 to 10 [-]

Φ_i = flow through subarea *i*[m^3/yr]

A_i = area of subarea *i*[m^2], as per *tpa.out*

I_i = infiltration through subarea *i*[mm/yr]

-Data used to calculate average infiltration with Eq.1 and Eq.2 are summarized in Table 2. The table shows also areas, infiltrations by subarea, and flow by subarea.:

Table 2: Mean annual infiltration calculations.

i	A_i [m^2]	Φ_i [m^3/yr] simulation time=10,000yr	Φ_i [m^3/yr] simulation time=1,000,001yr	I_i [mm/yr] simulation time=10,000yr	I_i [mm/yr] simulation time=1,000,001yr
1	224091.0	5.5404E+03	8.1025E+03	2.4724E+01	3.6157E+01
2	448476.0	1.4871E+04	2.1245E+04	3.3160E+01	4.7371E+01
3	1241313.5	2.6437E+04	3.9246E+04	2.1297E+01	3.1617E+01
4	775953.1	1.7345E+04	2.5914E+04	2.2354E+01	3.3397E+01
5	605892.0	1.3969E+04	2.0741E+04	2.3055E+01	3.4232E+01
6	152357.0	2.6973E+03	4.0905E+03	1.7704E+01	2.6848E+01

7	318122.0	1.1846E+04	1.6725E+04	3.7237E+01	5.2573E+01
8	439350.0	9.1675E+03	1.3669E+04	2.0866E+01	3.1112E+01
9	305880.0	5.8272E+03	8.8206E+03	1.9051E+01	2.8837E+01
10	747165.5	1.5270E+04	2.2824E+04	2.0437E+01	3.0547E+01

- Based on data in Table 2, average infiltrations calculated by **both** Eq.1 and Eq.2 were:

    - $\overline{I}$ = *2.3385E-02 m/yr*, for simulation time = 10,000yr
    - $\overline{I}$ = *3.4492E-02 m/yr*, for simulation time = 1,000,001yr

- Overall result for Test 2 bullet #2 result: PASS.

Software Validation Report (SVR)

<table>
<tr><td>SVTR#:</td><td colspan="2">Project #: 20.060002.01.354</td></tr>
<tr><td colspan="2">Software Name: TPA</td><td>Versions: 5.1betaU, 5.1betaV</td></tr>
<tr><td>Test ID: P-5</td><td colspan="2">Test Series Name: Near Field Thermo-hydrologic and chemical environment</td></tr>
<tr><td colspan="3">Test Method
☐ <u>code inspection</u> ☒ <u>spreadsheet</u>
☒ <u>output inspection</u> ☒ <u>graphical</u>
☐ <u>hand calculation</u> ☐ <u>comparison with external code</u></td></tr>
<tr><td colspan="3">Test Objective: Process-level validation of NFENV module. See Attachment A for full description of test objectives.</td></tr>
<tr><td colspan="3"><u>Test Environment Setup</u>

<u>Hardware (platform, peripherals):</u> Pentium IV, 3.4 Ghz, 512 MB RAM 2.5 GB Virtual RAM

<u>Software (OS, compiler, libraries, auxiliary codes or scripts):</u> Microsoft Windows XP Professional, Version 2002, SP2

<u>Input Data (files, database, mode settings):</u> tpa.inp changes required for a specific test are listed in the test procedure. The external data file drythick.dat is required for the test.</td></tr>
<tr><td colspan="3"><u>Assumptions, constraints, and/or scope of test:</u> See Attachment A
Assumptions or constraints: none
Scope of the test: To verify the process level thermohydrological and chemical calculations performed by the NFENV module of TPA 5.1 code. Tests include verification of temperature and reflux computations for different modeling assumptions and numerical techniques as well as confirmatory calculations for near field chemical environment.</td></tr>
<tr><td colspan="3"><u>Test Procedure</u>:
Tested in accordance with the procedure in Attachment A and results presented in Attachment-B</td></tr>
<tr><td colspan="3">Test Results
Location: See attached CD labeled “TPA Version 5.1 Validation Task P-5"

Test Criteria and Analysis of Results: See Attachment B

<u>Test Evaluation (Pass/Fail):</u> Pass</td></tr>
<tr><td colspan="3"><u>Notes:</u> None.</td></tr>
<tr><td>Testers: K. Das, M. Juckett, R. Fedors, and J. Myers</td><td colspan="2">Date: March 27, 2007</td></tr>
</table>

Attachment A

TPA Version 5.1 Validation, Planned Test Cases

Six different aspects of the near field thermohydrological and chemical processes need to be tested. The requirements of each test and the proposed test plan are listed below.

General Assumptions

For the purposes of this validation test, it is assumed:

1. The input parameters and their distributions supplied by *tpa.inp* are consistent with the abstractions of the modeled processes.
2. Previous validation testing of this module and testing of subsequent SCRs affecting this module have been properly performed, and may be cited as evidence of module performance.
3. Majority of the simulations will be carried out for 10k years as the majority of the tests involve events that will occur up to or before 5k years and unlikely to have any effect beyond 10k years. However, a limited number of TPA runs will be made for 1 million years for calculation verification of near-field variables beyond 10k years.
4. Tests will be done using input parameters from *tpameans.out* file with seismic and igneous disruptive scenarios turned off.
5. In most of the cases deterministic simulations will be used (1 realization) for subarea 3, which is the subarea that best represents average behavior of the repository.

Test-1

For REFLUX3 computations, the dryout zone thickness data should be selected based on the rate of drift degradation. When the rate of drift degradation is very low, the drift is considered as intact for the REFLUX3 computations and will use drythick.dat for an intact drift. The appropriate dryout thickness data (from drythick.dat) should be selected as a function of the specified drift degradation rate.

Objectives

For computation of reflux water, the dryout thickness is supplied externally with separate data sets for intact and degraded drift. The switch from intact to a degraded dryout thickness occurs when the top of the drip shield begins to be covered by the rubble as the sides of the drip shield fill first. The objective of the test is to verify if the TPA code chooses the appropriate dryout thickness values based on drift degradation rate.

Proposed procedure for Test-1

To check that the degraded dryout thickness data set is used once the drip shield begins to be covered by rubble vertically, all we need to compare are the Outer diameter of the backfill (BF_Out_Dia) in *thermal.dbg* and dryout zone thickness in used in the calculations. The *thermal.dbg* file is a standard output file. The dryout thickness used in the calculation for each time-step will be obtained by modifying the *nfenv.f* file.

To vary the rate of degradation, either the "TimePulseEnd" parameter (set as 4000 years in *drythick.dat*) needs to be varied. It should be set to a value lower than the degradation time for rock type-1 and 2 which is 369.32 years. An alternative way is to change the degradation time for the rock. This test will set the *DegradationTimeRockType3[]*=200 years to achieve fast degradation and 10000 years to achieve slow degradation rates.

Expected results should show appropriate selection of dryout thickness that matches with the values supplied by the file *drythick.dat*.

<u>Test-2</u>

Temperatures for the waste package, drift wall, and drip shield are consistent and include the effects of drift degradation and increasing rubble thickness with time.

<u>Objectives</u>

Study the sensitivity of the temperature profiles for drift degradation and rubble thickness.

<u>Proposed procedure for Test</u>-2

The height of rubble accumulation above the drip shield is determined by the bulking factor of rock type 1 and 2. By default, the bulking factor follows a beta distribution with limiting values of 1 and 2. The bulking factor value will be changed to three constant value of 1.15, 1.2 and 1.25 to obtain three different rubble thickness above the drip shield. Subsequently the waste package and the drip shield temperatures will be compared for Thermal-Mode-1 and Thermal-Mode-2 to determine the sensitivity of the temperature distribution with rubble thickness.

The starting point of the test would be the mean case using input values from *tpameans.out*. The perturbations to the repository closure time and end of active ventilation period will be applied in the next step. The relevant information needed to check for consistency are included in the *thermal.dbg* standard output file. Temperatures for the waste package (tempwp), outer surface of drip shield (tempdsoA and tempdsoB), and drift wall (temprw) as a function of time are in the *thermal.dbg* file. Timing of rubble filling the side of the drift, and then covering the top of the drip shield can be inferred from equivalent diameter in the *thermal.dbg* file. The entries of Drift_Dia and BF_Out_Dia represent equivalent diameters of the "A" leg (vertical); and Drift_DiaB and BF_Out_DiaB are the "B" leg (lateral).

It is expected that a lower bulking factors will result in greater thickness of rubble that in turn will result in higher waste package temperature.

Test-3

Temperature calculations appropriately account for and distinguish between time of ventilation and time of closure.

Objectives

Study the effect of ventilation time and time of repository closure on temperatures of drip shield, waste package and drift wall.

Proposed procedure for Test-3

Currently, the time of active ventilation and time of closure are set to 50 and 100 years respectively in *tpa.inp*. These parameters will be varied to examine their effect on the temperature profile for the intact drift case. The time of active ventilation will be changed to 30, 50 and 70 years with fixed time of closure of 100 years. The time of closure will be changed to 60,100 and 150 years with a fixed time of active ventilation of 50 years.

The starting point of the test will be the mean case using input values from *tpameans.out*. The perturbations to the repository closure time and end of active ventilation period will be applied in the next step. Results are available in the *thermal.dbg* or *nfenv.rlt* files, which are available as standard output file. The waste package temperature (tempwp), dripshield temperatures (tempdsoA and tempdsoB) and the repository wall temperature (temprw) will be studied.

It is expected that a longer active ventilation period will cause increased heat removal from the drift and result in lower temperatures and vice-versa. Change in active cooling period will be reflected as low temperature values in the temperature profiles for waste package, drift wall and drip shield. Usually drift closure results in an abrupt increase in temperature immediately following the closure time. This point of sudden change is expected to vary with different closure time points and will be reflected in the temperature curves for waste package, drift wall and drip shield.

Test-4

Estimates of seepage versus time are consistent with reflux abstraction and the specified seepage threshold temperature.

Objective

Test 4 evaluate the sensitivity of the code to seepage the threshold temperature that determines the onset of seepage. This test will also be carried out for mean parameters from *tpameans.out.* Then perturbations will be applied through the input parameter *SeepageThresholdTemperature*.

Proposed procedure for Test-4

Currently the SeepageThresholdTemperature follows a triangular distribution with 100.0, 105.0, 125.0 as limiting parameters. It will be varied to three different constant values of 90, 110, and 130 C (194, 230 and 266 deg F) to study the sensitivity of the seepage rate to change in onset temperature. As constant values of the threshold temperatures will be used instead of random sample, computing multiple realizations will not be necessary.

Results for these runs will be obtained from *nfenv.rlt* and *thermal.dbg*. The output variables used for the analysis include repository wall temperature (temprw), drip shield temperatures (tempdsoA and tempdsoB) and the quantity of seepage that could potentially contact the waste package (qm3hit).

An additional sensitivity study will be carried out to understand the effect of drift degradation on seepage rate. TPA will be used to generate results for both degraded and intact drift scenario to verify whether the seepage threshold temperature is being compared with the correct reference temperature. The drift wall temperature is the reference temperature for an intact drift. Whereas for a degraded drift (nominal case in TPA), the drip shield temperature is the reference temperature. Once the two sides of the drip shield are full with rubble (in the simplified geometry assumed in TPA) and accumulation starts over the drip shield, the drift is considered degraded and the corresponding reference temperature is the drip shield temperature. So, the effective side diameter on the side or the accumulated rubble height over the drip shield will be the testing parameter for drift degradation. The drift will be considered intact for side diameters less than or equal to the original drift wall diameter and will be considered degraded otherwise. The rubble diameter in the side, quantity of seepage, drip shield, and drift wall temperatures will be recorded in a file and the output will be used to study the effect of drift degradation on seepage rate.

It is expected that the quantity qm3hit will change with change in seepage threshold temperature. It is also expected that the reference temperature for comparison with seepage threshold temperature will be the drift wall temperature for an intact drift and drip shield temperature for a degraded drift.

Test-5

Numerical resolution issues or time stepping algorithms that may affect calculated waste package, drip shield, or drift wall temperatures do not result in errors in temperature values used in calculations.

Objective

Test 5 assesses the effect of integration parameters in temperature calculations. The Gauss Legendre integration technique is used to compute the drift wall temperature from the mountain scale heat transfer equation. The number of weighting factors of the integration specified by the constant *NumberOfWeightsForGaussLegendreIntegration* in *tpa.inp* will have some effect in the stepwise temporal variation in drift wall temperature. This value will subsequently affect the calculation of waste package and drip shield temperatures. However, the final impact of this temperature will be in the radionuclide release rates from the engineered barrier and it needs to be ensured that the release rates are not dependent on any numerical parameters.

Proposed procedure for Test-5

The mean input parameters from *tpameans.out* will be used. Currently a fixed value of Gauss-Lagendre integration weighting factor of 20 is being for computational economy. The weighting factor for the Gauss-Lagendre integration will be varied to three constants, 20, 50, and 100. This is the only parameter associated with numerics in the mountain scale model and will affect the integration. The corresponding waste package temperature will be plotted to see if the results are sensitive to integration weighting factor.

It is expected that the drift wall and waste package temperature will converge to a fixed value as weight factor increases.

Test-6

Temperature, relative humidity, and seepage onset information are correctly used to determine near-field chemical environments. When the relative humidity is low (below a threshold value), the system is considered dry and aqueous corrosion does not take place. If seepage does not contact the waste package, Environment I is assumed to form. Environment II is assumed to occur when the relative humidity is above a threshold value and seepage contacts the waste package. Environment III occurs when the relative humidity is high (close to 90%) and seepage contacts the waste package.

Changes in pH, chloride and nitrate concentrations with time are correctly computed.

Objective

The objective of this test is to verify the sampling of input values and distributions performed by the TPA module NFENV. One of the objectives of this test is to ensure that the input data provided to the *nfenv.f* code is correctly read. The second objective is to verify that the temperature, relative humidity, and seepage onset information are correctly used to determine near-field chemical environments. Finally, changes in pH, chloride, and nitrate will be checked for correct implementation. The following criteria define each chemical environment.

Criteria for Each Chemical Environment	
Environment	**Criteria**
Dry	RH < CriticalRelativeHumidityAqueousCorrosion[]
I	RH ≥ CriticalRelativeHumidityAqueousCorrosion[]
II	Qhit > 0 and t ≥ time of drip shield failure
III	RH ≥ RewettingHumidity[]

Proposed procedure for Test-6

A procedure is proposed to achieve the stated objective, however, during the conduction of validation testing the validation teams may conduct additional testing, to be documented in the SVR as necessary, to understand and verify software performance related to the NFENV module. The TPA code will be executed for single reference case realization of 1,000,000 yrs for one subarea. The output mode will be selected as 1 to enable *nfenv.rlt* output files. Ten realizations will be executed, which will cover several humidity and temperature scenarios. Comparison of the chemistry and environmental switches will demonstrate that the values are properly sampled. Using the output data from *nfenv.rlt*, chloride concentration vs. time for the duration of the time period will be plotted. Values from the output file will be compared to inflection values given for environments I, II, and III. Inflection points in the graph should mimic appropriate changes in values for relative humidity, temperature and time of drip shield failure. File *dsfail.rlt* will be checked to determine drip shield failure time by subarea. The transition in chemistry will also be verified to determine if environment function switches properly. Also, the output files will be used to determine whether pH, chloride, and nitrate values are sampled correctly.

Attachment B

TPA 5.1 Software Validation Task P-5 Test Results

Following are test results for the validation test cases described in Attachment A for TPA Version 5.1 code Software Validation Task P- 5. Additional details related to test procedures are also provided.

Test 1. Proper Selection of Dry thickness values from drythick.dat

<u>Path for run directory:</u>

Test case 1a	:	Cuda: D\TPA\TEST-1\No-Degradation
Test case 1b	:	Cuda: D\TPA\TEST-1\Degradation-before-pulse
Test case 1c	:	Cuda: D\TPA\TEST-1\Degradation-after-pulse

<u>Environment variable:</u>

Test case 1a	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 1b	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 1c	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV

<u>Special input files or modifications to input files required :</u> None

<u>Special diagnostic code modifications required :</u>

The following segment was added to the end of the subroutine thickness_reader to get the interpolated thickness values out. This is done in order to write the dryout thickness values (*drycheck.dat*) that is being used in the computation in an output file. This will provide a better understanding of what exact values of dryout zone thickness are being used.

```
c-------outputfile added to check if correct data is read----
c-------
          idrycheck = igetunitnumber('nfenv   ')
          open(idrycheck,file='drycheck.dat')
          write(idrycheck,*)'flagDegrade =',flagDegrade
          write(idrycheck,*)'timeDegrade =',timeDegrade
          write(idrycheck,*)'timePulseEnd =',timePulseEnd

        do i=1,nreflux,10
           write(idrycheck,*) xinterp_tim(i), xinterp_thick(i)
        enddo
```

The modified code with the source and compiled executable is stored at
Cuda: D:\TPA\code-to-check-drythick\

Program modes to be used (append flags, scenario/model switches, etc.):

All three tests were performed for subarea 3 and for 1 realization and 10k years. TPA mean values are generally used for the calculations. Output files for all the modules were written out and one additional file “drycheck.dat” that is created with the code above is also written out. For all the cases the seismic scenario flag was turned off.

Specific input changes made for each specific case is described below;

Case 1.1

TPA runs without any degradation and the thickness reader reads in data that is specified for use in an intact drift.

Case 1.2

TPA runs with degradation and the time of degradation is before the end of the thermal pulse. So, the thickness reader is supposed to read in data that is specified for use in a degraded drift.

Case 1.3

TPA runs with degradation and the time of degradation is long after the end of thermal pulse. So, the thickness reader is supposed to read in data that is specified for use in a degraded drift.

Case No	Input Variable Name	Default Value	Modified Value
1.1	DriftDegradationScenarioFlag	1	0
	DegradationTimeRockTypeOneSubarea_3	749.99	749.99
	DegradationTimeRockTypeTwoSubarea_3	749.99	749.99
1.2	DriftDegradationScenarioFlag	1	1
	DegradationTimeRockTypeOneSubarea_3	749.99	200.000
	DegradationTimeRockTypeTwoSubarea_3	749.99	200.000
1.3	DriftDegradationScenarioFlag	1	1
	DegradationTimeRockTypeOneSubarea_3	749.99	1000000.
	DegradationTimeRockTypeTwoSubarea_3	749.99	1000000.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: TECPLOT-360

Objective: Verify the thickness reader reads the correct dryout thickness values from *drythick.dat*. There are three checks that needs to be done.

(i) For an intact drift, it should use dryout thickness values specified for an intact drift from *drythick.dat*.

(ii) For a degraded drift, where total degradation takes place before thermal pulse ends, it should use the data specified for the degraded drift from *drythick.dat*. Under this scenario, the drift is considered a "closed drift".

(iii) For a degraded drift, where total drift degradation does not take place before thermal pulse ends, it should use the data specified for the intact drift from *drythick.dat*. Under this scenario, the drift is considered a "open drift".

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *drycheck.dat* and *drythick.dat*

Test Procedure:

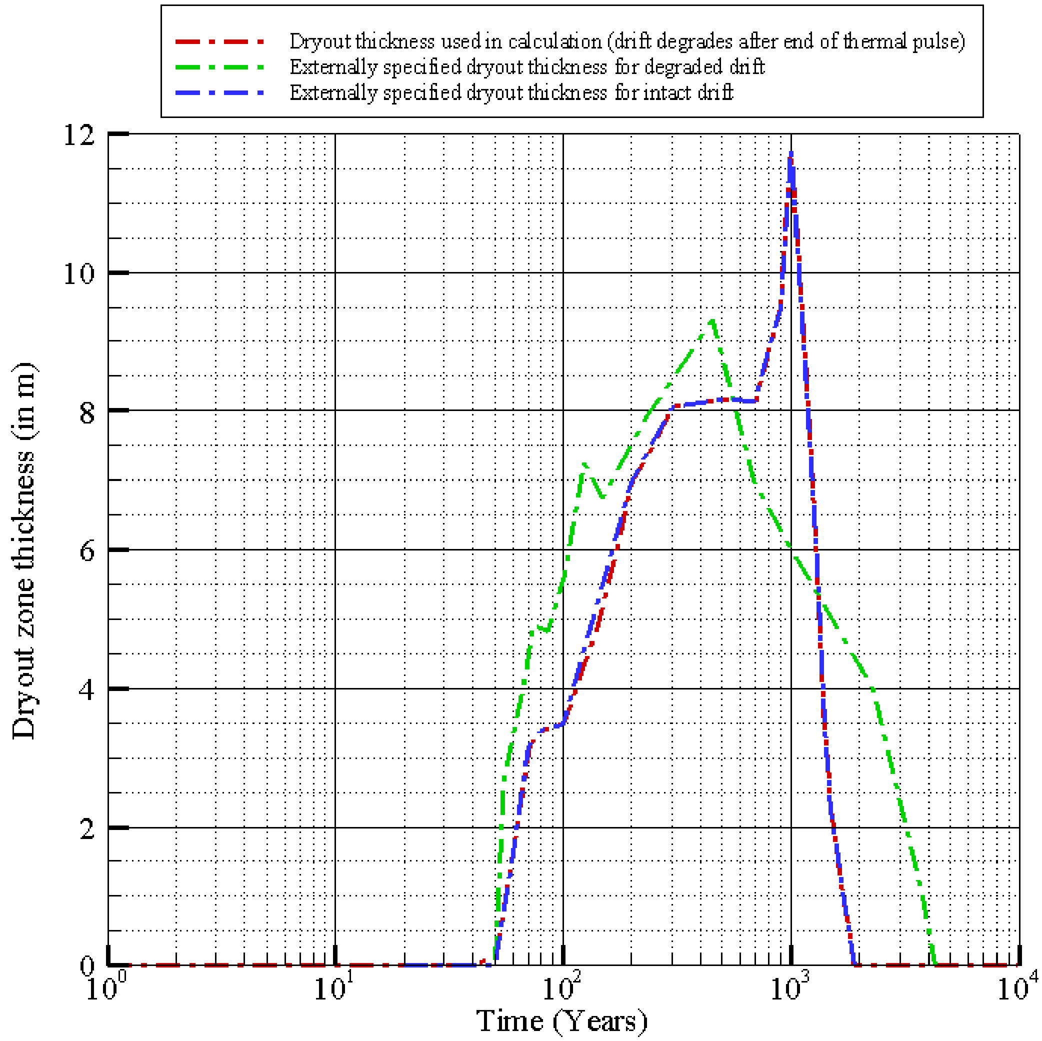
1) Execute the TPA code thrice, using the modified tpa.inp file and the new executable build with modified *nfenv.f*, and evaluate the results.
2) Compare the dryout thickness values used in calculations (*drycheck.dat*) and *drythick.dat*

Pass/Fail criteria:

1) For test 1.1, the values recorded in *drycheck.dat* should match with data corresponding to intact drift in *drythick.dat*
2) For test 1.2, the values recorded in *drycheck.dat* should match with data corresponding to degraded drift in *drythick.dat*
3) For test 1.3, the values recorded in *drycheck.dat* should match with data corresponding to intact drift in *drythick.dat*

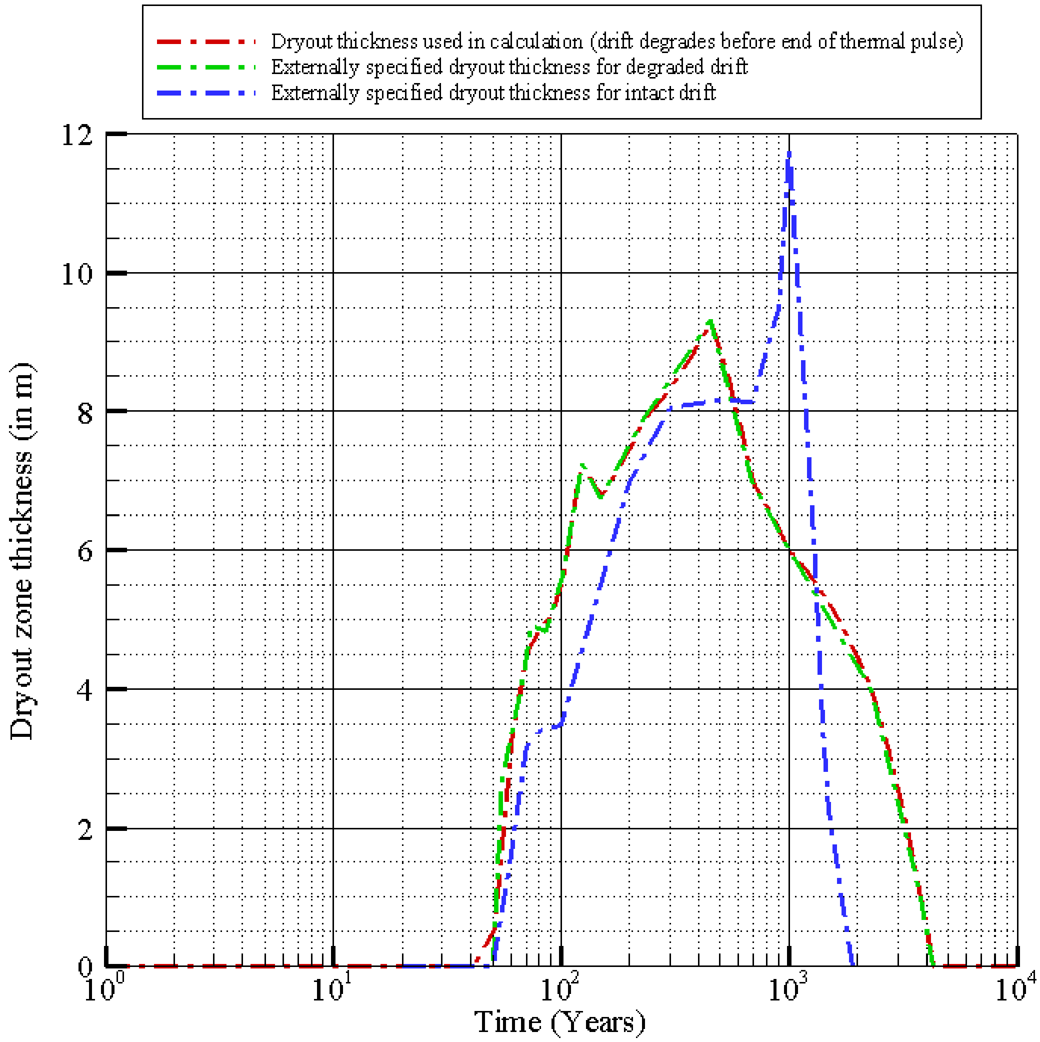
Test results:

Test 1.1: Intact Drift



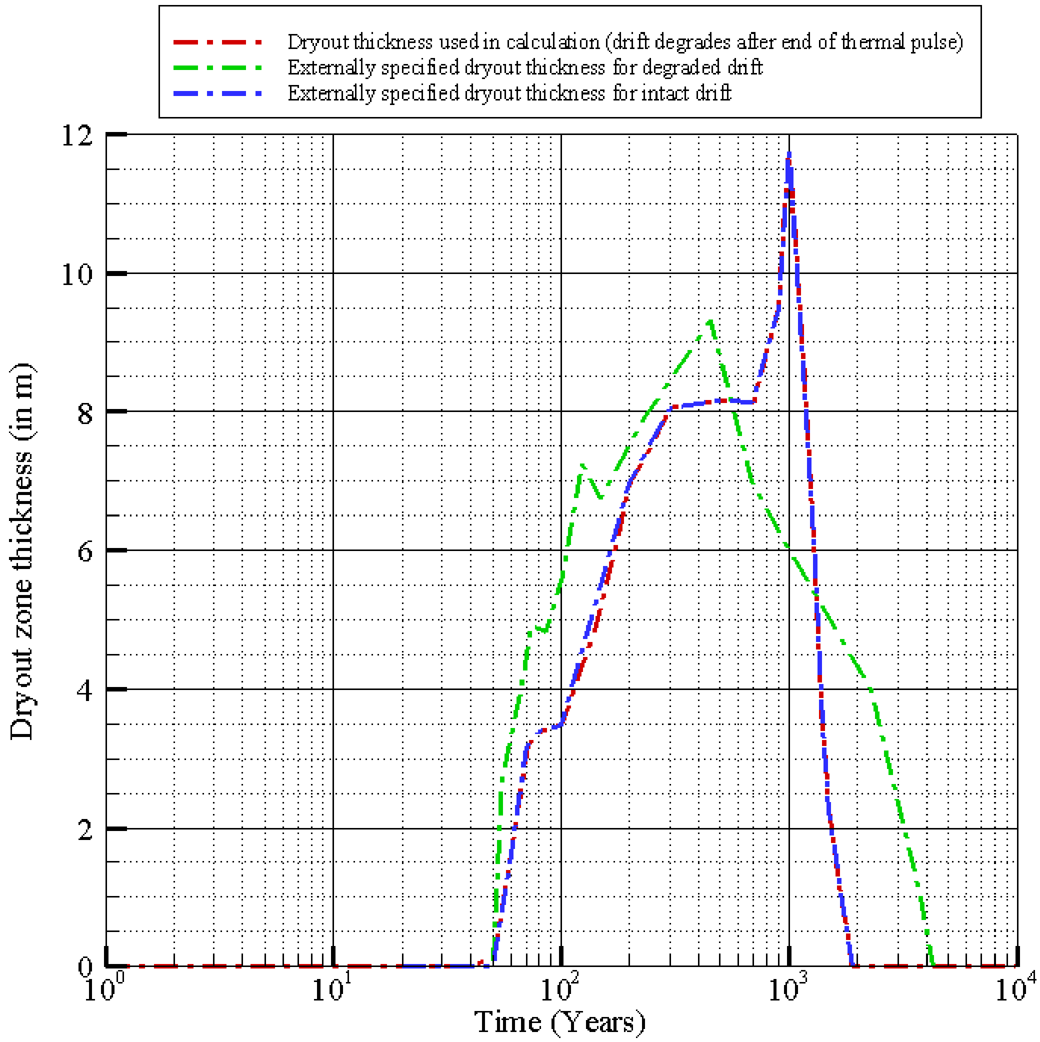
Observation: The dryout thickness values used in the computation matches exactly with the dryout values for the intact drift in *drythick.dat*

Test 1.2: Total degradation before the end of thermal pulse



Observation: The dryout thickness values used in the computation matches exactly with the dryout values for the degraded drift in *drythick.dat*

Test 1.3 **Total degradation after the end of thermal pulse**



Observation: The dryout thickness values used in the computation matches exactly with the dryout values for the intact drift in *drythick.dat*

<u>Test 1 Results (PASS/FAIL):</u> **PASS**

Test 2. Effect of Rubble Accumulation of Temperature Calculation

Path for run directory:

Test case 2.1.1	:	Cuda: D\TPA\TEST-2\Bulkfact1.15
Test case 2.1.2	:	Cuda: D\TPA\TEST-2\Bulkfact1.20
Test case 2.1.3	:	Cuda: D\TPA\TEST-2\Bulkfact1.25
Test case 2.2.1	:	Cuda: D\TPA\TEST-2\Th-mode-2-Bulkfact1.15
Test case 2.2.2	:	Cuda: D\TPA\TEST-2\Th-mode-2-Bulkfact1.20
Test case 2.2.3	:	Cuda: D\TPA\TEST-2\Th-mode-2-Bulkfact1.25

Environment variable:

Test case 2.1.1	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 2.1.2	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 2.1.3	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 2.2.1	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 2.2.2	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 2.2.3	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

All tests were performed for subarea 3 and for 1 realization and 10k years. TPA mean values from *tpameans.out* are generally used for the calculations. Specific input changes made for each specific case is described below; Test cases 2.1.1, 2.1.2 and 2.1.3 are for Thermal Mode-1 and 2.2.1, 2.2.2 and 2.2.3 are for Thermal Mode-2.

Case No	Input Variable Name	Default Value	Modified Value
2.1.1	FractionAllowedToDegrade[]	0.25	0.25
	BulkingFactorRockTypeOneSubarea_3[]	1.19	1.15
	BulkingFactorRockTypeTwoSubarea_3[]	1.19	1.15
2.1.2	FractionAllowedToDegrade[]	0.25	0.25
	BulkingFactorRockTypeOneSubarea_3[]	1.19	1.20
	BulkingFactorRockTypeTwoSubarea_3[]	1.19	1.20
2.1.3	FractionAllowedToDegrade[]	0.25	0.25
	BulkingFactorRockTypeOneSubarea_3[]	1.19	1.25
	BulkingFactorRockTypeTwoSubarea_3[]	1.19	1.25

Case No	Input Variable Name	Default Value	Modified Value
2.2.1	FractionAllowedToDegrade[]	0.25	0.80
	BulkingFactorRockTypeOneSubarea_3[]	1.19	1.15
	BulkingFactorRockTypeTwoSubarea_3[]	1.19	1.15
2.2.2	FractionAllowedToDegrade[]	0.25	0.80
	BulkingFactorRockTypeOneSubarea_3[]	1.19	1.20
	BulkingFactorRockTypeTwoSubarea_3[]	1.19	1.20
2.2.3	FractionAllowedToDegrade[]	0.25	0.80
	BulkingFactorRockTypeOneSubarea_3[]	1.19	1.25
	BulkingFactorRockTypeTwoSubarea_3[]	1.19	1.25

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: TECPLOT-360

Objective: To study the sensitivity of the code in calculating temperature with varying rubble thickness.

Variation of bulking factor is expected to change the volume and thickness of rubble accumulation over the drip shield and influence the temperature calculation. Bulking factor determines the volume that will be generated after rock spalling and hence the thickness of it on the engineered system.

In the TPA-5.1, there are two different modes that are used to calculate temperature fields that are known as Thermal-mode-1 and Thermal-mode-2. The objective of the present test is also to see if the code is sensitive to changes in rubble thickness for both these modes.

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *nfenv.rlt* and *driftfail.rlt*

Test Procedure:

1) Execute the TPA code six times, using the modified *tpa.inp* file and saving the results for examination.
2) Examine the drift ceiling heights in the output files *driftfail.rlt*
3) Examine temperatures obtained from file *nfenv.rlt*

Pass/Fail criteria:

For all the cases, the temperature profile should show some sensitivity to changes in rubble thickness or the bulking factor. It is expected that lower values of rubble thickness results in lower waste package temperature and with a higher value of rubble thickness results in higher values of waste package temperature. So, the following criteria is used in the analysis for both thermal mode-1 and 2.

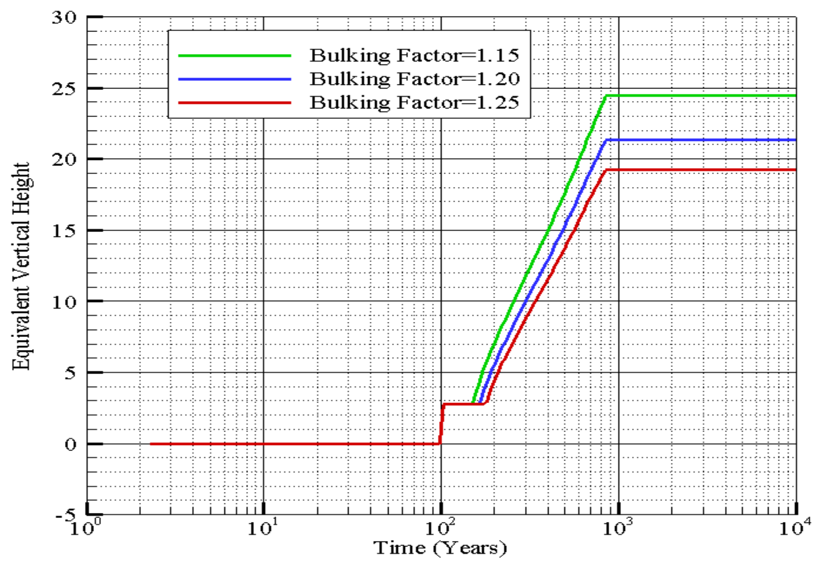
(1) Change in bulking factor should change the effective drift height, with lower bulking factor giving higher drift height.

(2) Change in bulking factor should change the temperature profile of the waste package and drip shield. The lower bulking factor creates a larger thickness of rubble on drip shield and should result in higher temperature.

(3) Change in bulking factor should not affect the drift wall temperature as it is calculated separately using a mountain scale model and is not affected by the accumulated rubble on the drip shield.

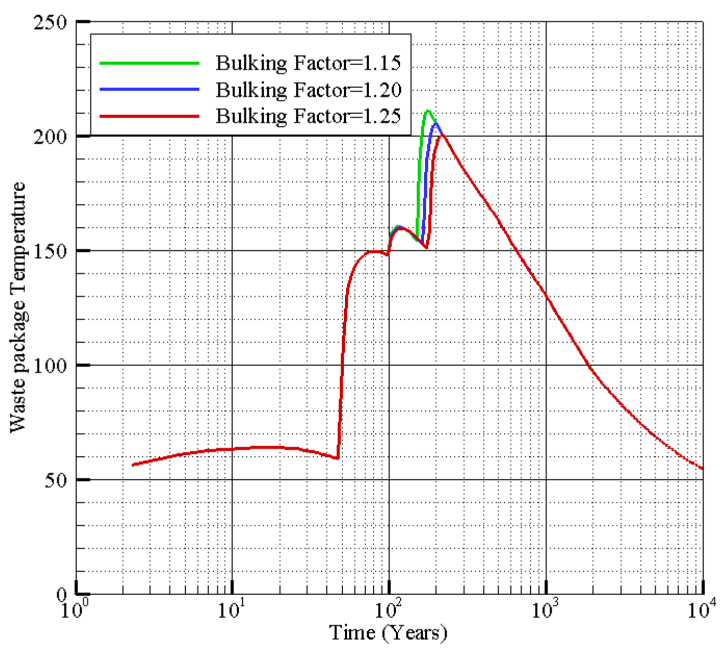
Test results:

Variation of drift height with bulking factor Thermal-Mode-1



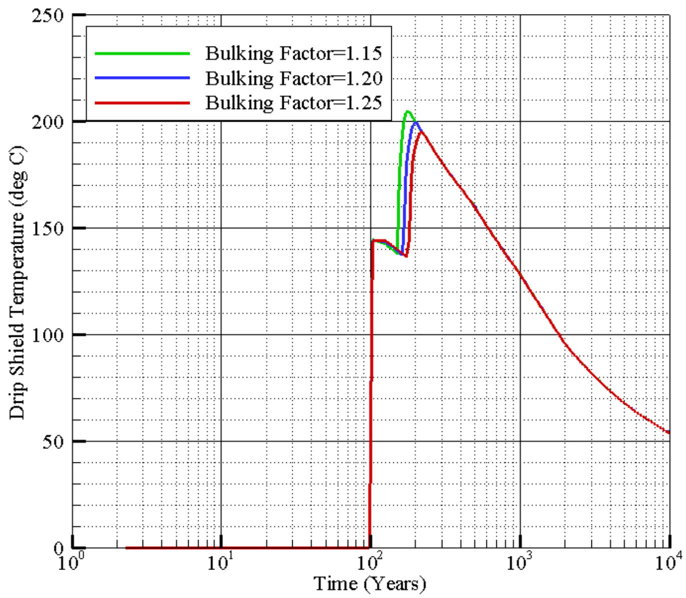
Observation
Change in bulking factor affects the equivalent drift height with lower bulking factor resulting in higher drift height.

Variation of waste package temperature with bulking factor in Thermal-Mode-1



Observation
Change in bulking factor affects the temperature distribution on the waste package. Higher the bulking factor, lower the waste package temperature.

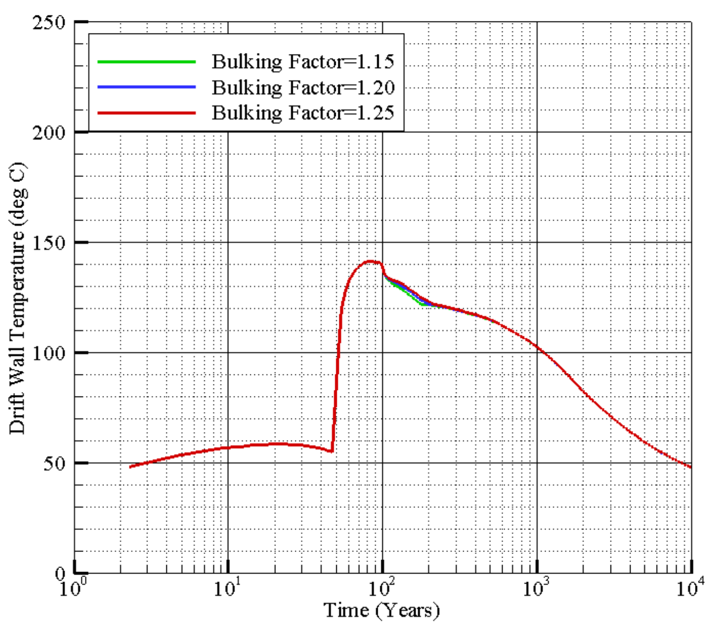
Variation of drip shield temperature with bulking factor in Thermal-Mode-1



Observation

Change in bulking factor affects the temperature distribution on the drip shield. Higher the bulking factor, lower the drip shield temperatures.

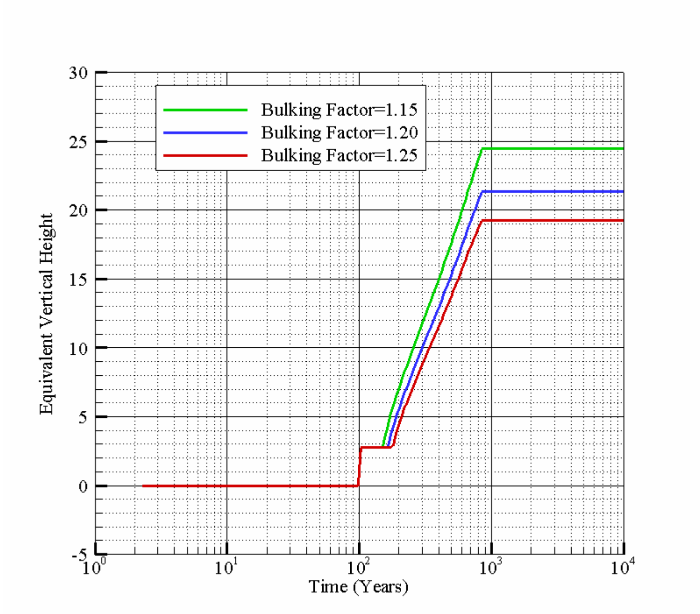
Variation of drift wall temperature with bulking factor in Thermal-Mode-1



Observation

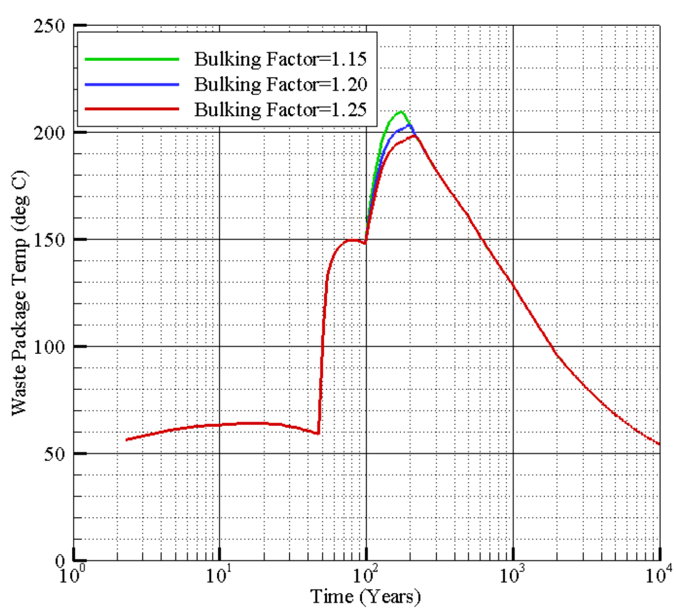
Change in bulking Factor does not significantly affect the drift wall temperatures.

Variation of drift height with bulking factor Thermal-Mode-2



Observation
Change in bulking factor affects the equivalent drift height with lower bulking factor having greater height.

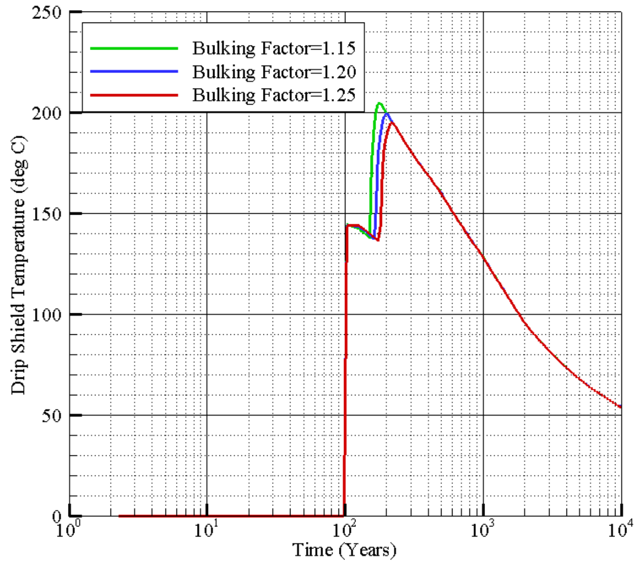
Variation of waste package temperature with bulking factor in Thermal-Mode-2



Observation

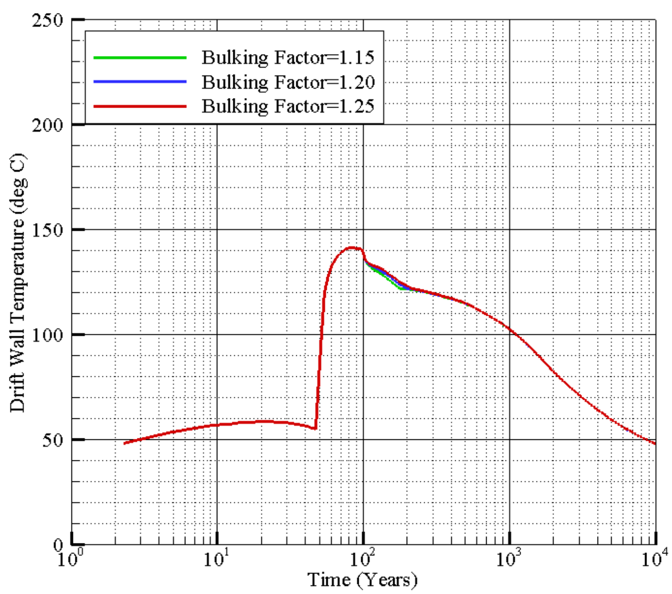
Change in bulking factor affects the temperature distribution on the waste package. Higher the bulking factor, lower the waste package temperature.

Variation of drip shield temperature with bulking factor in Thermal-Mode-2



Observation
Change in bulking factor affects the temperature distribution on the drip shield. Higher the bulking factor, lower the drip shield temperature.

Variation of drift wall temperature with bulking factor in Thermal-Mode-2



Observation
Change in bulking factor does not significantly change the drift wall temperature

<u>Test 2 Results (PASS/FAIL):</u> **PASS**

Test 3. Effect of Closure and Active Ventilation Period

Path for run directory:

Test case 3.1.1 :	Cuda: D\TPA\TEST-3\vent=30 years
Test case 3.1.2 :	Cuda: D\TPA\TEST-3\vent=50 years
Test case 3.1.3 :	Cuda: D\TPA\TEST-3\vent=70 years
Test case 3.2.1 :	Cuda: D\TPA\TEST-3\Closure=60 years
Test case 3.2.2 :	Cuda: D\TPA\TEST-3\Closure=100 years
Test case 3.2.3 :	Cuda: D\TPA\TEST-3\Closure=150 years

Environment variable:

Test case 3.1.1 :	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 3.1.2 :	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 3.1.3 :	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 3.2.1 :	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 3.2.2 :	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 3.2.3 :	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

All tests were performed for subarea 3 and for 1 realization and 10k years. TPA mean values from *tpameans.out* are generally used for the calculations. Specific input changes made for each specific case is described below; All the tests were done for intact drifts.

Cases 3.1

This set of test cases examine the effect of active ventilation period while the time of repository closure is kept constant at 100 years. All the tests were done for intact drift.

Case No	Input Variable Name	Default Value	Modified Value
3.1.1	TimeOfRepositoryClosure[yr]	100	100
	TimeActiveVentilationEnds[yr]	50	30
3.1.2	TimeOfRepositoryClosure[yr]	100	100
	TimeActiveVentilationEnds[yr]	50	60
3.1.3	TimeActiveVentilationEnds[yr]	100	100
	TimeOfRepositoryClosure[yr]	50	90

Cases 3.2

This set of test cases examine the effect of the repository closure time will be studied with the active ventilation time at a constant value of 50 years. All the tests were done for intact drift.

Case No	Input Variable Name	Default Value	Modified Value
3.2.1	TimeOfRepositoryClosure[yr]	100	60
	TimeActiveVentilationEnds[yr]	50	50
3.2.2	TimeOfRepositoryClosure[yr]	100	100
	TimeActiveVentilationEnds[yr]	50	50
3.2.3	TimeActiveVentilationEnds[yr]	100	150
	TimeOfRepositoryClosure[yr]	50	50

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: TECPLOT-360

Objective: To study the sensitivity of the code in calculating temperature with varying closure time and active ventilation period.

Currently the active ventilation period is set at 50 years. During this period, heat is removed from the repository by forced convection. Reducing this period will result in less heat removal and higher in-drift temperature. Similarly, a longer period of active ventilation means higher total heat removal and lower temperatures at the drift wall and in-drift components.

Repository closure time is currently set at 100 years. An earlier closure time, with everything else fixed, will result in an abrupt increase in waste package temperature immediately after closure. This increase in temperature is due to inclusion of drip-shield in the temperature calculation in the post-closure period. The drip shield is excluded from temperature calculation in the pre-closure period. The drift wall temperature, however, should not show any change as the change in repository closure time does not alter the amount of heat removed from the waste package.

<u>Assumptions:</u> None, other than those made within the TPA code.

<u>Constraints:</u> None

<u>Output files to compare or examine:</u> *thermal.dbg*

<u>Test Procedure:</u>

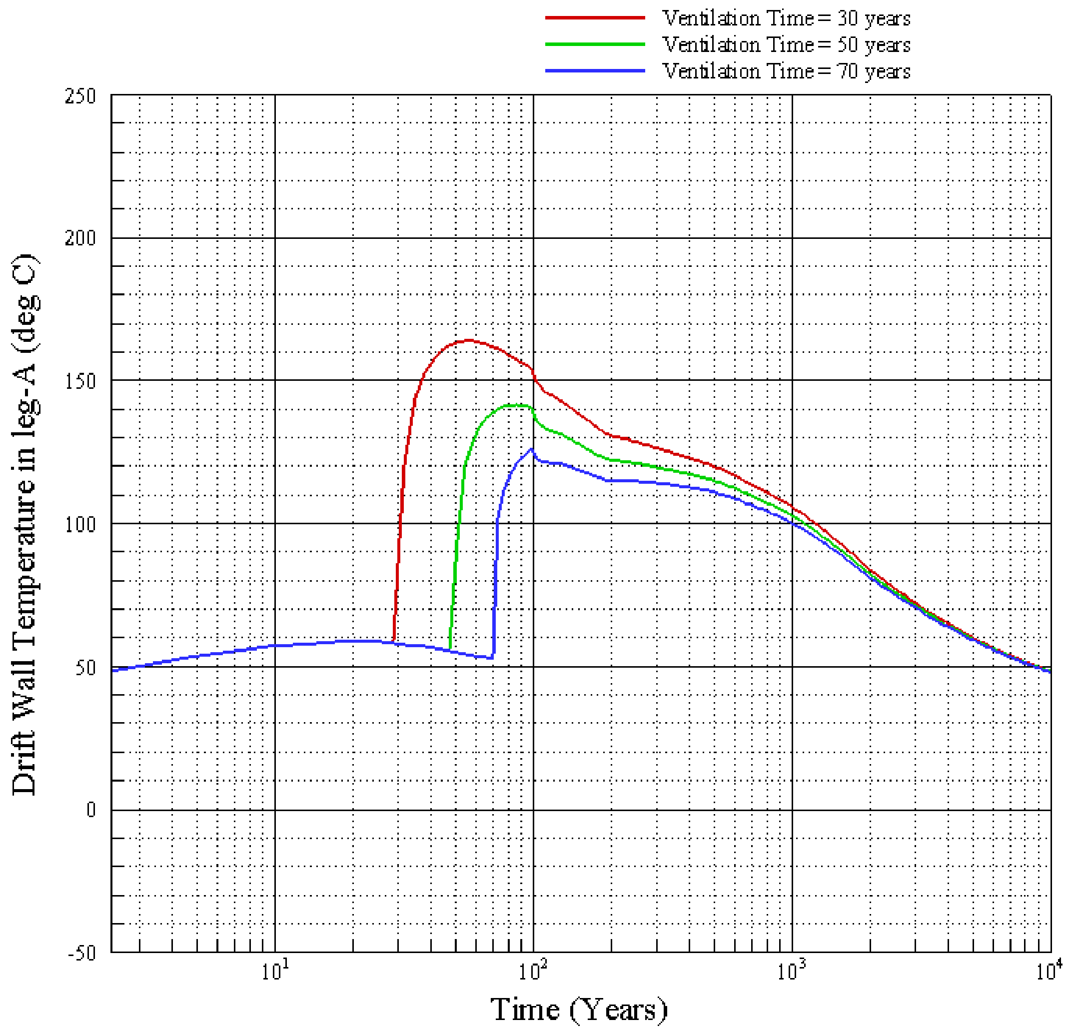
1) Execute the TPA code six times, using the modified *tpa.inp* file and saving the results for examination.
2) Examine the temperatures in the output file *thermal.dbg*

<u>Pass/Fail criteria:</u>

(1) Lower value of active ventilation must result in higher temperature of drift components and drift wall as less heat is being removed by forced convection.
(2)Repository closure results in a jump in waste package temperature immediately after the closure. Early closure will cause this abrupt increase early and a late closure will have it later. This increase in WP temperature should occur almost at the same time a repository closure is specified by the user.
(3) Change in closure time should not affect the drift wall temperature distribution.

Test results:

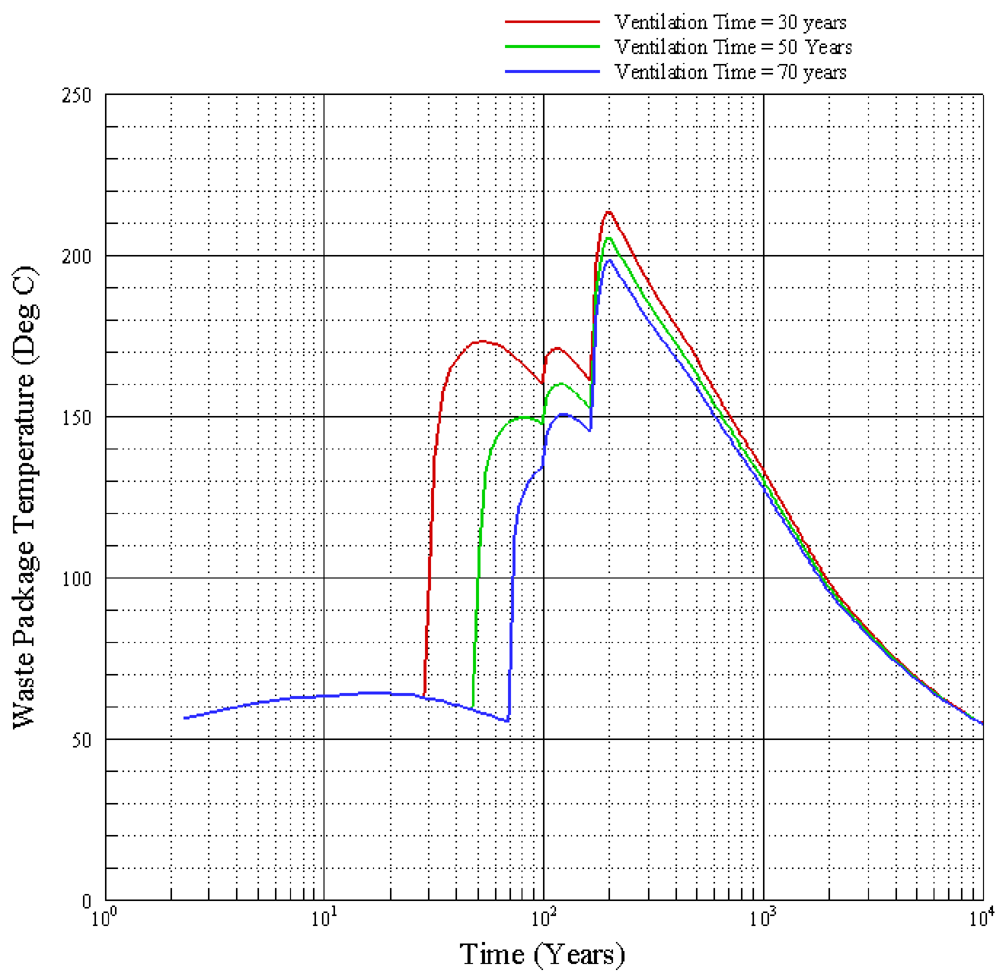
Effect of active ventilation time on drift wall temperature



Observation

The drift wall temperature shows a jump immediately after the active ventilation period. Shorter active ventilation periods result in higher drift wall temperatures.

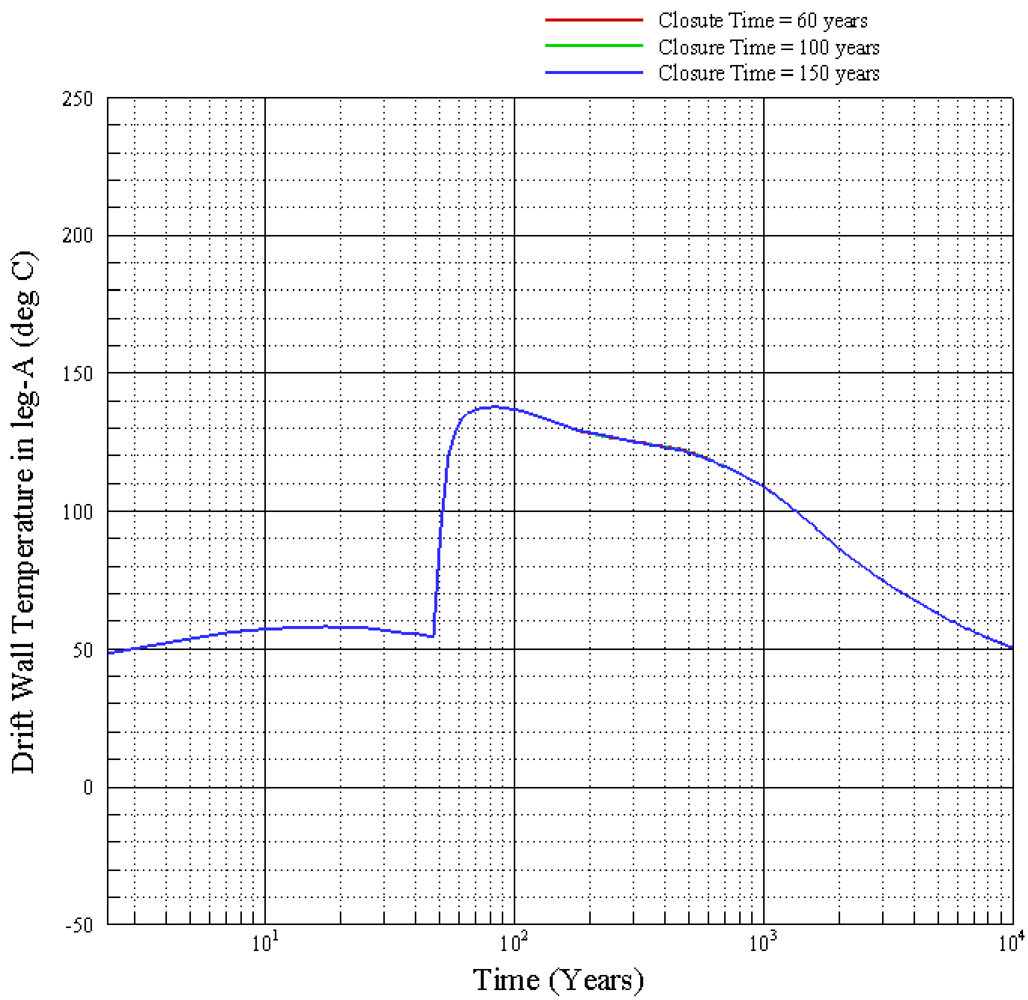
Effect of active ventilation time on waste package temperature



Observation

The waste package temperature shows a jump in immediately after the active ventilation period. Shorter active ventilation period results in higher waste package temperatures.

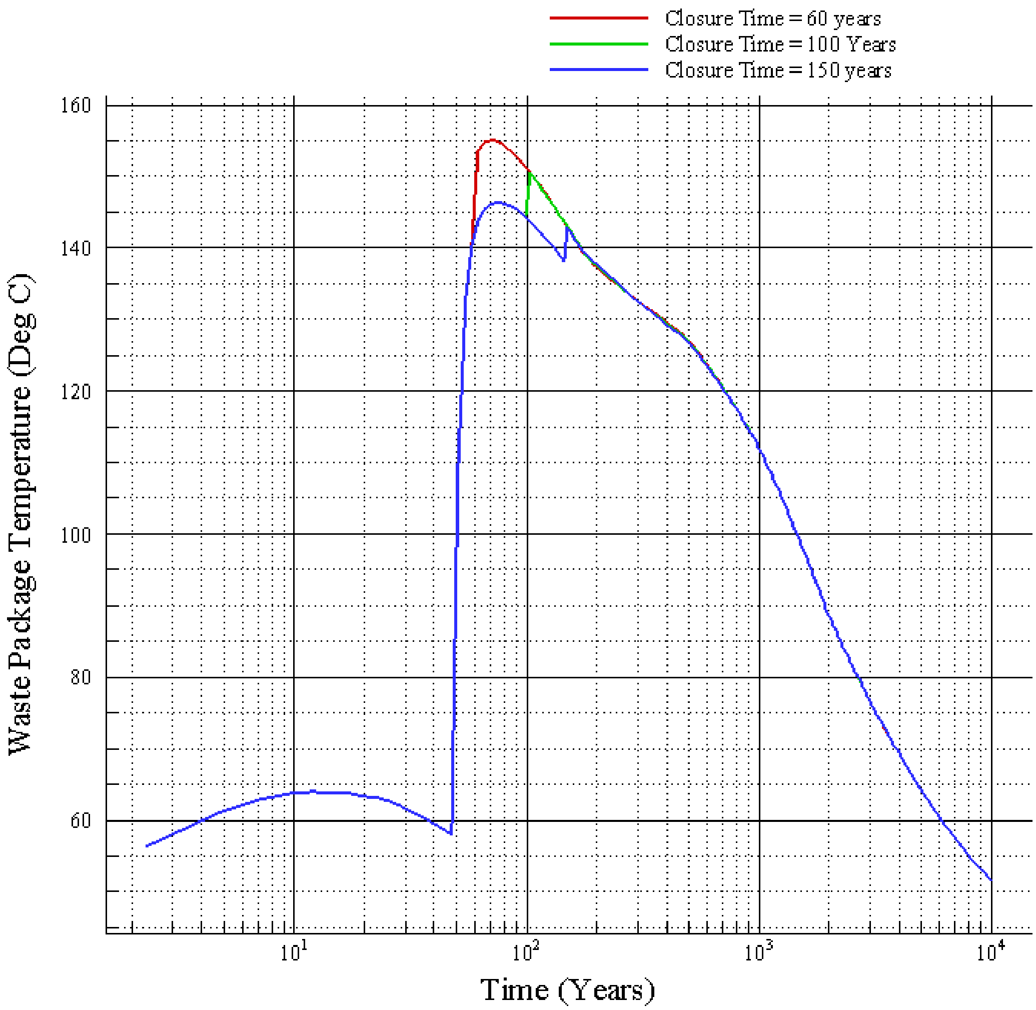
Effect of repository closure time on drift wall temperature



Observation

Change in closure time does not affect the drift wall temperature distribution. All the lines are coincident.

Effect of repository closure time on waste package temperature



Observation

Repository closure results in a jump in waste package temperature immediately after the closure. Early closure will cause this spike to happen early and a late closure will have this spike late.

Test 3 Results (PASS/FAIL): **PASS**

Test 4. Effect of Seepage Threshold temperature

Path for run directory:

Test case 4.1	:	Cuda: D\TPA\TEST-4\SeepThT=80
Test case 4.2	:	Cuda: D\TPA\TEST-4\SeepThT=90
Test case 4.3	:	Cuda: D\TPA\TEST-4\SeepThT=110
Test case 4.4	:	Cuda: D\TPA\TEST-4\SeepThT=120
Test case 4.5	:	Cuda: D\TPA\TEST-4\SeepThT=130
Test case 4.6	:	Cuda: D\TPA\TEST-4\SeepThT=None
Test case 4.7	:	Cuda: D\TPA\TEST-4\Intact
Test case 4.8	:	Cuda: D\TPA\TEST-4\Degraded

Environment variable:

Test case 4.1	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 4.2	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 4.3	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 4.4	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 4.5	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 4.6	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 4.7	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 4.8	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV

Special input files or modifications to input files required : None

Special diagnostic code modifications required :

The following segment was modified to get the comparison temperature written out in an output file. Comparison temperature is the temperature that is considered for comparison with the seepage threshold temperature. For a degraded drift with rubble above the drip-shield, the comparison temperature should be the drip shield temperature. For any other case, the comparison temperature is the drift wall temperature. The outputfile *seepcheck.dat* will contain time, drip shield temperature, drift wall temperature and comparison temperature.

```
c-------outputfile added to check if correct data is read----
c-------

  iseepcheck = igetunitnumber('nfenv   ')
      open(iseepcheck,file='seepcheck.dat')

     if (FlagSeepage .eq. 1) then
```

```
               do it = 1, ntim

          cc rwr 6/16/06; SCR651; determine waste package general corrosion
cc                    failure time, in addition to the time of
cc                    weld failure
cc (when the drift has degraded, use drip shield temperature instead
cc  of "temprep")
cc          if (temprep(it) .GT. ThrSeepage) then
cc              qm3peryrperwpinsamisswp(it) =
cc     &           qm3peryrperwpinsamisswp(it) +
cc     &           qm3peryrperwpinsahitwp(it)
cc              qm3peryrperwpinsahitwp(it)=0.0
cc            endif
cc rwr 7/31/06; SCR658; Ensure the following logic is used to
cc                    determine the onset of seepage:
cc                    when the drift [eqBFDiaB()] has not
cc                    failed, then seepage will not occur
cc                    if the drift wall temperature [temprep()]
cc                    is greater than the seepage threshold
cc                    temperature; otherwise, once the drift
cc                    has failed, seepage will not occur if the
cc                    temperature of the drip shield [tempdsoB()]
cc                    is greater than the seepage temperature
cc                    threshold
cc           if (eqBFDiaB(it) .ge. driftdia) then


          if (eqBFDiaB(it) .lt. driftdia) then
            if (temprep(it) .GT. ThrSeepage) then
              tseepchk=temprep(it)
              qm3peryrperwpinsamisswp(it) =
     &           qm3peryrperwpinsamisswp(it) +
     &           qm3peryrperwpinsahitwp(it)
              qm3peryrperwpinsahitwp(it)=0.0
            endif
          else
            if (tempdsoB(it) .GT. ThrSeepage) then
              tseepchk=tempdsoB(it)
              qm3peryrperwpinsamisswp(it) =
     &           qm3peryrperwpinsamisswp(it) +
     &           qm3peryrperwpinsahitwp(it)
              qm3peryrperwpinsahitwp(it)=0.0
            endif
          endif
           write(iseepcheck,*) tim(it),temprep(it),
     &                     tempdsoB(it),tseepchk,
     &                     qm3peryrperwpinsahitwp(it)
        enddo
        close(iseepcheck)
      endif
```

The modified code with the source and compiled executable is stored at
Cuda: D:\TPA\code-to-check-seepage\

<u>Program modes to be used (append flags, scenario/model switches, etc.):</u>

All three tests were performed for subarea 3 and for 1 realization and 10k years. TPA mean values from *tpameans.out* are generally used for the calculations. Output files for all the modules were written out. Additionally *seepcheck.dat* that is created with the code above is also written out.

Tests 4.1-4.6 study the effect of change in seepage threshold temperature on the quantity of water contacting the waste package . For tests 4.1-4.6, the drift degradation switch is turned off, i.e. no drift degradation takes place. Tests 4.7 and 4.8 explore the use of seepage threshold temperature in the code with and without drift degradation. Test 4.7 simulates a drift with degradation time large enough so that the drift will be effectively considered open and the reference temperature for comparison should be the drift wall temperature. Test case 4.8 simulates it with degradation time small enough so that the drip shield will have rubble accumulated on top of it soon after closure and the drift will be considered closed. The reference temperature for comparison for this case will be drip shield temperature. For all the tests (4.1-4.7) the seismic scenario flag is turned off.

Specific input changes made for each specific case is described below.

Case No	Input Variable Name	Default Value	Modified Value
41	DriftDegradationScenarioFlag	1	0
	FlagSeepageThreshold	1	1
	SeepageThresholdT[c]	110	80
4.2	DriftDegradationScenarioFlag	1	0
	FlagSeepageThreshold	1	1
	SeepageThresholdT[c]	110	90
4.3	DriftDegradationScenarioFlag	1	0
	FlagSeepageThreshold	1	1
	SeepageThresholdT[c]	110	110
4.4	DriftDegradationScenarioFlag	1	0
	FlagSeepageThreshold	1	1
	SeepageThresholdT[c]	110	120
4.5	DriftDegradationScenarioFlag	1	0
	FlagSeepageThreshold	1	1
	SeepageThresholdT[c]	110	130
4.6	DriftDegradationScenarioFlag	1	0
	FlagSeepageThreshold	1	0
	SeepageThresholdT[c]	110	110
4.7	DriftDegradationScenarioFlag	1	1
	SeepageThresholdT[c]	110	110
	DegradationTimeRockTypeOneSubarea_3	749.99	10000
	DegradationTimeRockTypeTwoSubarea_3	749.99	10000
4.8	DriftDegradationScenarioFlag	1	1
	SeepageThresholdT[c]	110	110
	DegradationTimeRockTypeOneSubarea_3	749.99	150
	DegradationTimeRockTypeTwoSubarea_3	749.99	150

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *nfenv.rlt* and *seepcheck.dat*

Test Procedure:

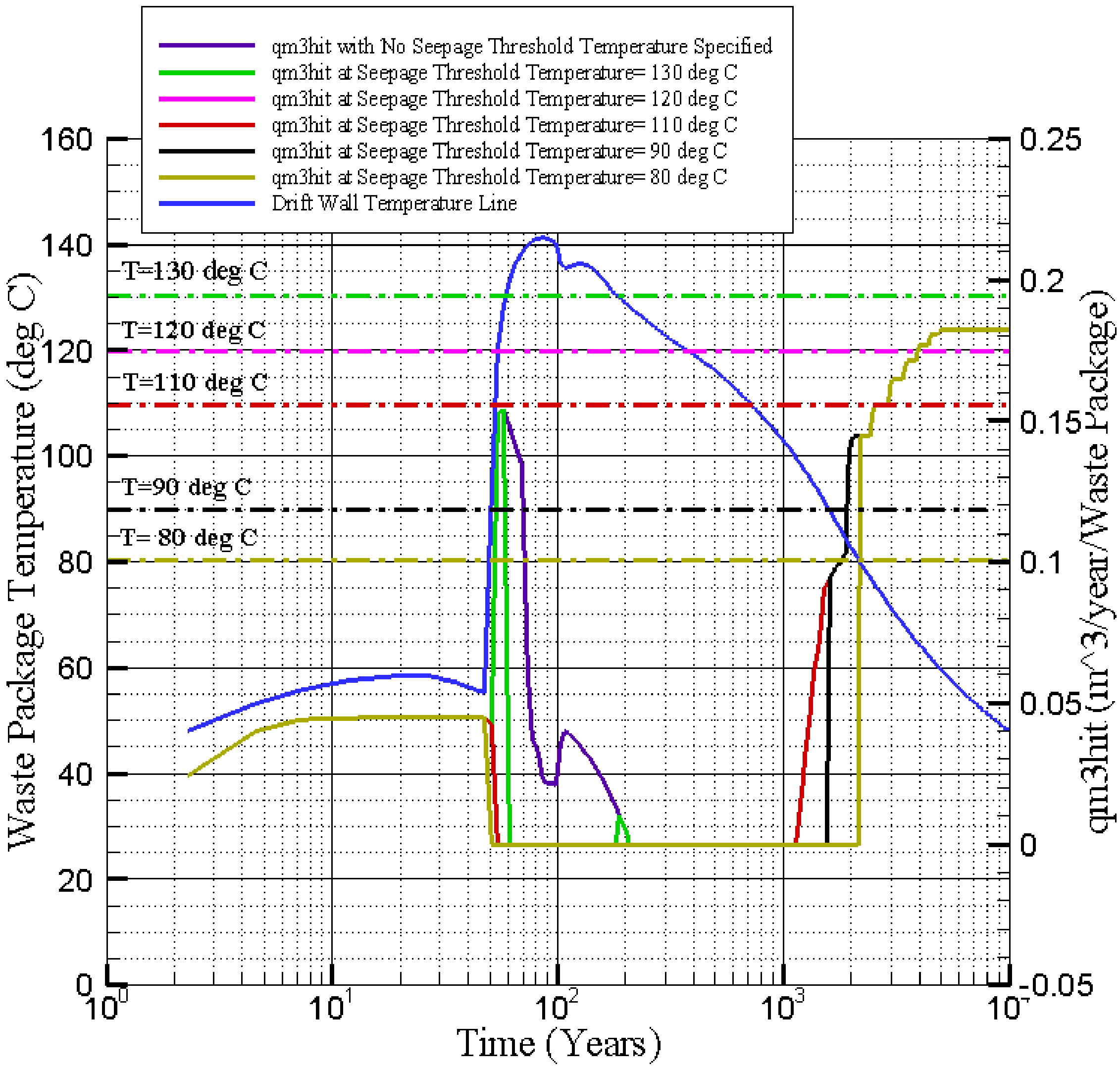
1) Execute the TPA code eight times, using the modified tpa.inp file and the new executable build with modified *nfenv.f*, and saving the results for examination.
2) Examine the drift wall temperature and the quantity of water that is available as seepage and has the potential to hit the waste packages (qm3hit) from the *nfenv.rlt* file and observe the temperature at which seepage starts.
3) Examine the wall, drip shield and comparison temperatures in *seepcheck.dat* and observe whether the comparison temperature is equal to the drip shield temperature for a drift with accumulated rubble above drip shield and equal to drift wall temperature for an intact drift.

Pass/Fail criteria:

1)Water could potentially contact the waste package when the drift wall temperature is at or below the seepage threshold temperature. So at or below seepage threshold temperature, the quantity of water that is available as seepage and has the potential to hit the waste packages (qm3hit) may be positive, but above the seepage threshold temperature, it must be zero.
2)For an intact drift, the comparison temperature should be equal to the drift wall temperature
3) For a degraded drift, comparison temperature should be equal to drip shield temperature after rubble starts accumulating above the drip shield.

Test results:

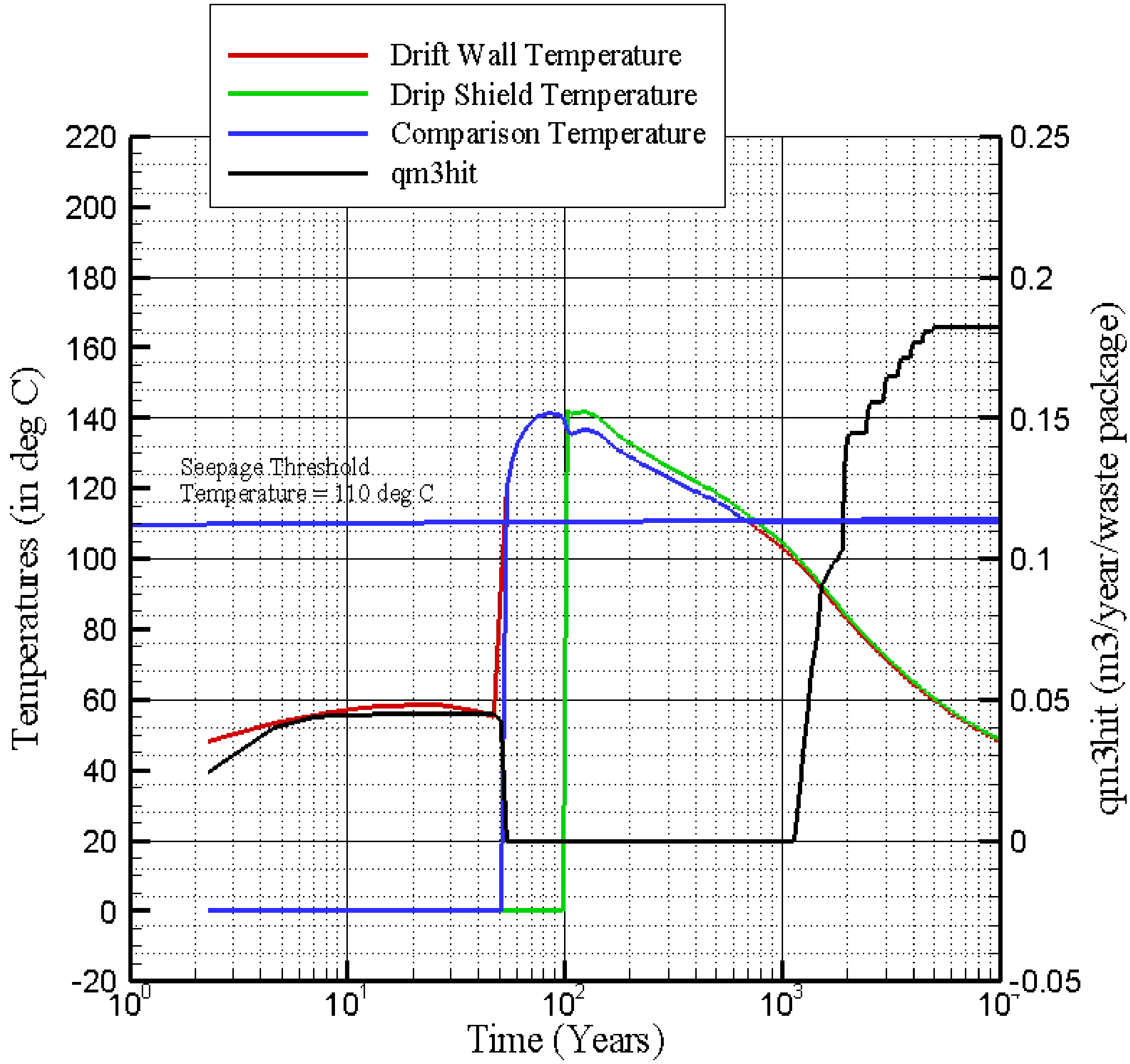
Effect of Seepage Threshold Temperature on the Quantity of Seepage Water in an Intact Drift



Observation

The solid lines show the seepage that contacts the waste package. The dotted lines show different temperatures. The solid green line shows the seepage with seepage threshold temperature=130° C [266° F]. The seepage starts when the drift wall temperature reaches 130° C. (At the intersection of the horizontal continuous green line indicating the constant T=130° C and the waste package temperature line). Seepage pattern at other threshold temperatures also show the same trend. So there is seepage only below the seepage threshold temperature and no seepage above it. Results are also presented for threshold temperatures of 80, 90, 110, 120° C [176, 194, 230 and 248 ° F].

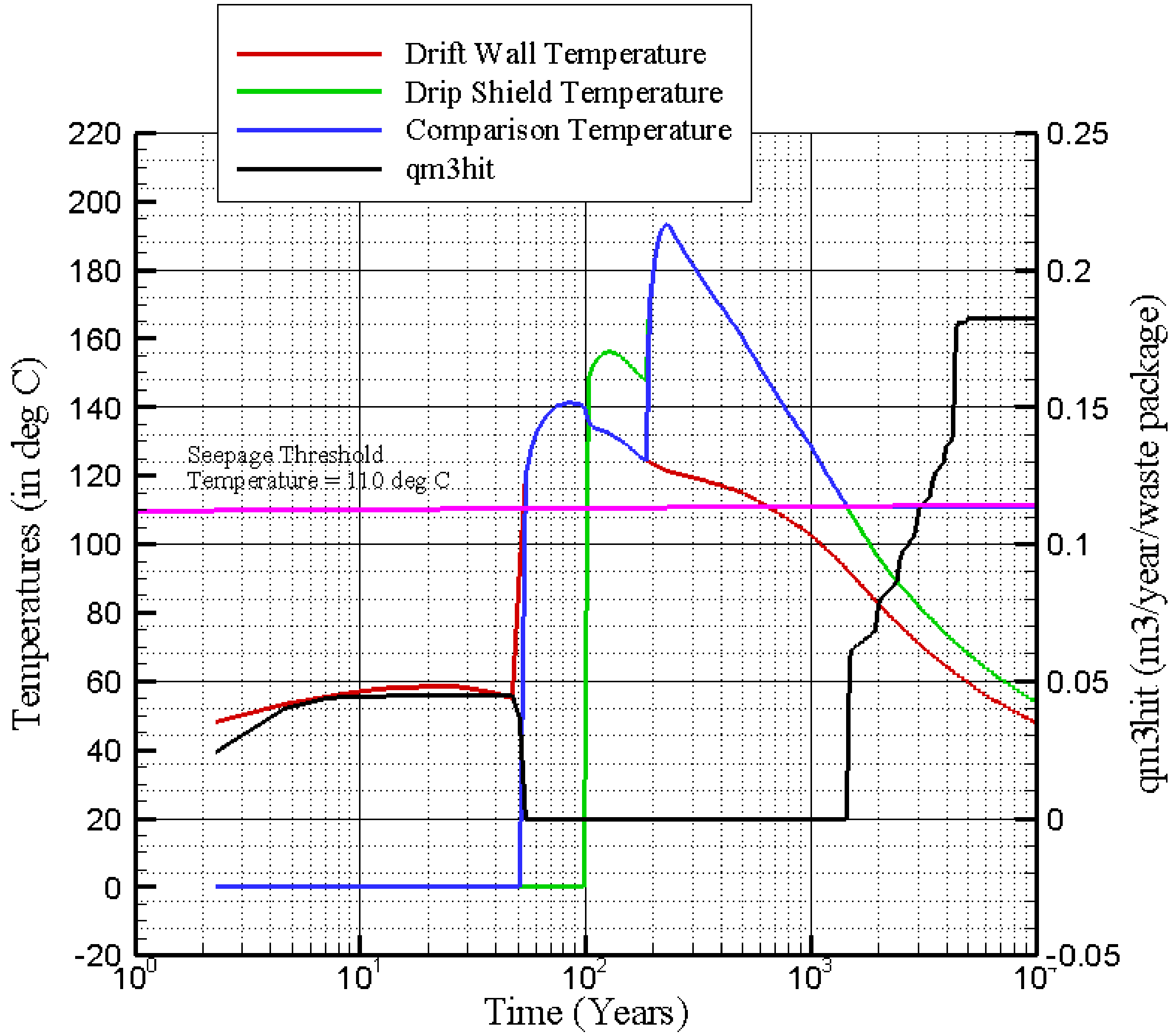
The comparison temperature for an intact drift



Observation

The comparison temperature is equal to the drift wall temperature for an intact drift.

The comparison temperature for a degraded drift



Observation

The comparison temperature is equal to the drift wall temperature before rubble starts to accumulate on the drift wall and after that it switches to the drip shield temperature for a degraded drift.

Test 4 Results (PASS/FAIL): **PASS**

Test 5. Effect of Numerical Resolution on Temperature Calculation [Weighting factors used in Gauss Lagendre Integration]

Path for run directory:

Test case 5.1	:	Cuda: D\TPA\TEST-5\LI-w-fac=10
Test case 5.2	:	Cuda: D\TPA\TEST-5\LI-w-fac=20
Test case 5.3	:	Cuda: D\TPA\TEST-5\LI-w-fac=30
Test case 5.4	:	Cuda: D\TPA\TEST-5\LI-w-fac=40
Test case 5.5	:	Cuda: D\TPA\TEST-5\LI-w-fac=50
Test case 5.6	:	Cuda: D\TPA\TEST-5\LI-w-fac=60
Test case 5.7	:	Cuda: D\TPA\TEST-5\LI-w-fac=100
Test case 5.8	:	Cuda: D\TPA\TEST-5\LI-w-fac=200

Environment variable:

Test case 5.1	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 5.2	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 5.3	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 5.4	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 5.5	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 5.6	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 5.7	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV
Test case 5.8	:	TPA_TEST=d:\TPA\tpa51betaV TPA_DATA=d:\TPA\tpa51betaV

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

All tests were performed for subarea 3 and for 1 realization and 10k years. Tpa mean values are generally used for the calculations. For different runs the number of weighting factors required for Gauss-Lagendre integration is varied between 10 and 200. Specific input changes made for each specific case is described below;

Case No	Input Variable	Default Value	Used Value
1	NumberOfWeightsForGauss LegendreIntegration	20	10
2	NumberOfWeightsForGauss LegendreIntegration	20	20
3	NumberOfWeightsForGauss LegendreIntegration	20	30
4	NumberOfWeightsForGauss LegendreIntegration	20	40
5	NumberOfWeightsForGauss LegendreIntegration	20	50
6	NumberOfWeightsForGauss LegendreIntegration	20	60
7	NumberOfWeightsForGauss LegendreIntegration	20	100
8	NumberOfWeightsForGauss LegendreIntegration	20	200

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *nfenv.rlt*

Test Procedure:

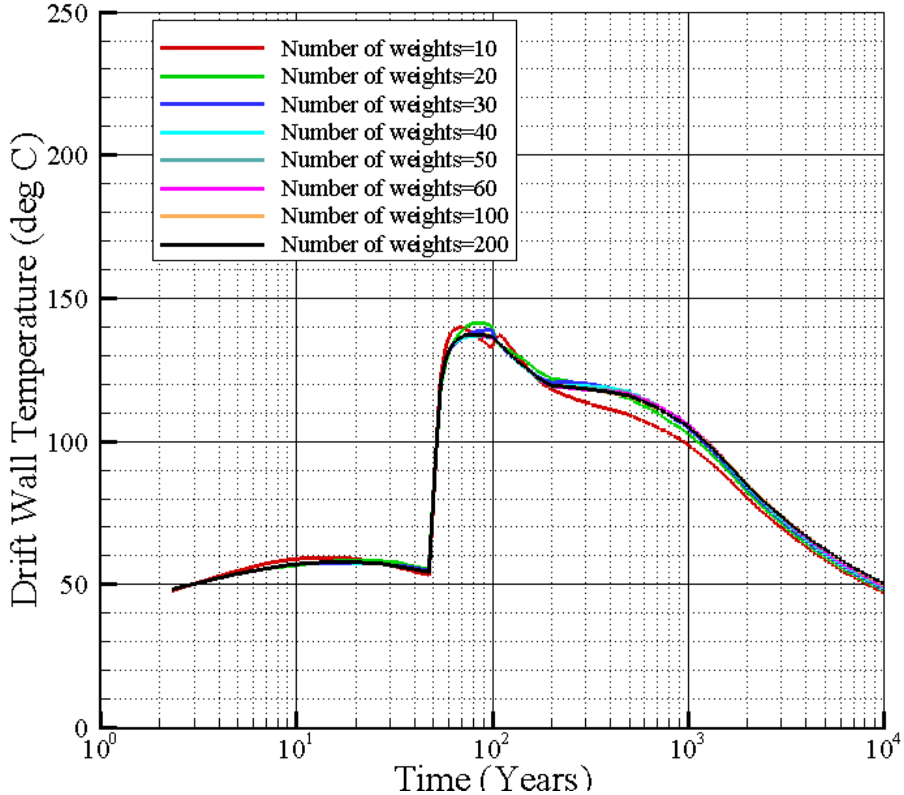
1) Execute the TPA code eight times, using the modified tpa.inp file and the standard tpa executable .
2) Plot the drift wall, waste package and drip shield temperature to see what effect the number of weighting factors for integration has

Pass/Fail criteria:

The number of weighting factors does not significantly alter the pattern of temperature distribution

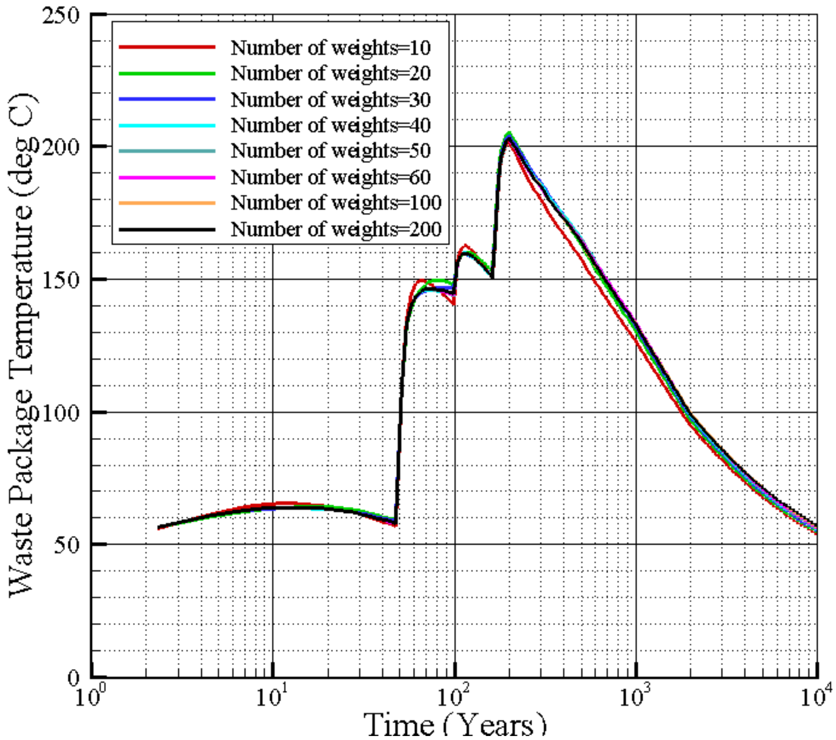
Test results:

Effect of the number of weighting factors on drift wall temperature



Observation
The temperature at the driftwall is affected when the number of weights is 10. At higher number of weights, the results do not change significantly.

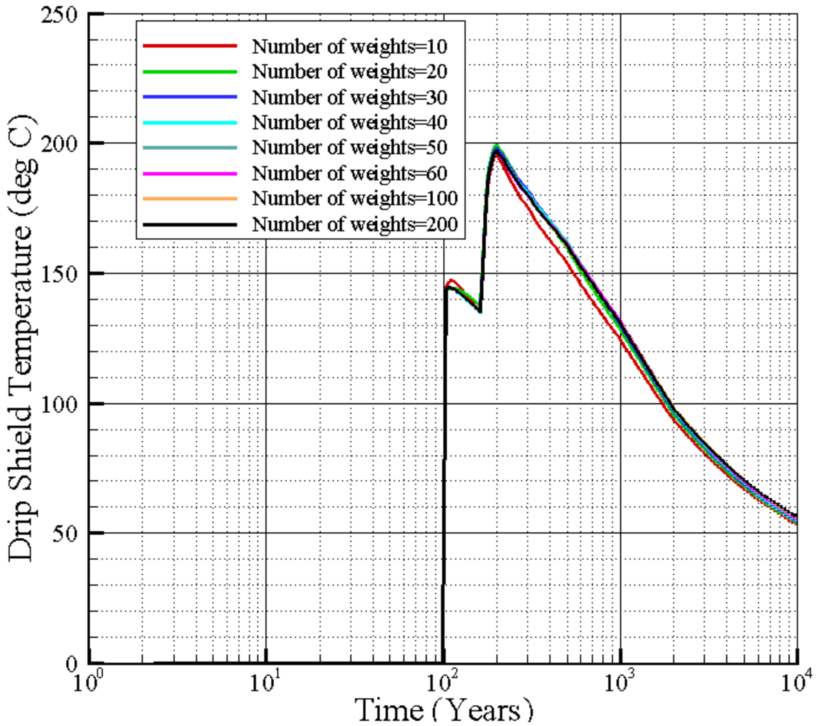
Effect of the number of weighting factors on waste package temperature



Observation

Waste package temperature is almost independent of the number of weights except at the lowest number of weights.

Effect of the number of weighting factors on drip shield temperature

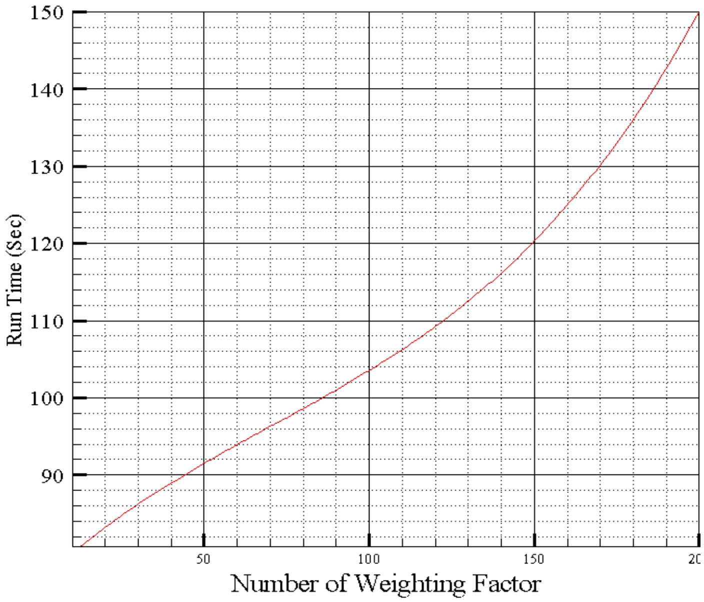


Observation
Drip shield temperature is almost independent of the number of weights except at the lowest number of weights

Test 5 Results (PASS/FAIL): **PASS**

Comment on test-5

Run Time with different number of weighting factors



Observation

Run time increases significantly with number of weights. It seems that a value of 30 will be a suitable one.

Test 6. Correct Use of Temperature, Relative Humidity, and Seepage Onset Information to Determine Near Field Chemical Environments

Path for run directory:
Gerbil: d:\TPA_Runs

Environment variable:
TPA_TEST=d:\TPA\tpa51betaU

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

All three tests were performed for subarea 3, which is representative of the entire repository. 10 realizations were run with compliance period of one million years. Output files for all the modules were written out.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify that the sampling of input values and distributions in the NFENV module are correct, such that environmental switches are triggered properly.

(i) Test 6.1: Determine that the onset of Environment I, the time at which the repository RH reaches the input parameter CriticalRelativeHumidityAqueousCorrosion = 0.2 is also the time at first chloride (Cl^-) concentration increases.

(ii) Test 6.2: Determine that the onset of Environment II, the time of Flow Hit (Q_{hit}) > 0 corresponds to the time of second Cl^- concentration increase.

(iii) Test 6.3: Determine that the onset of Environment III, the time that the relative humidity reaches a value within the input parameter RewettingHumidity range of 0.95 to 0.98 (uniform distribution) is also the time that the Cl^- concentration decreases.

Assumptions: The switches that trigger a change Cl- concentration also correctly trigger a change in the other chemistry parameters (fluoride, carbonate, nitrate, sulfate, and pH) that are implemented in the same manner in the TPA version 5.1 code.

Constraints: None

Output files to compare or examine: *nfenv.rlt; tpa.out*

Test Procedure:

1) Execute the TPA code, using the modified *tpa.inp* file.

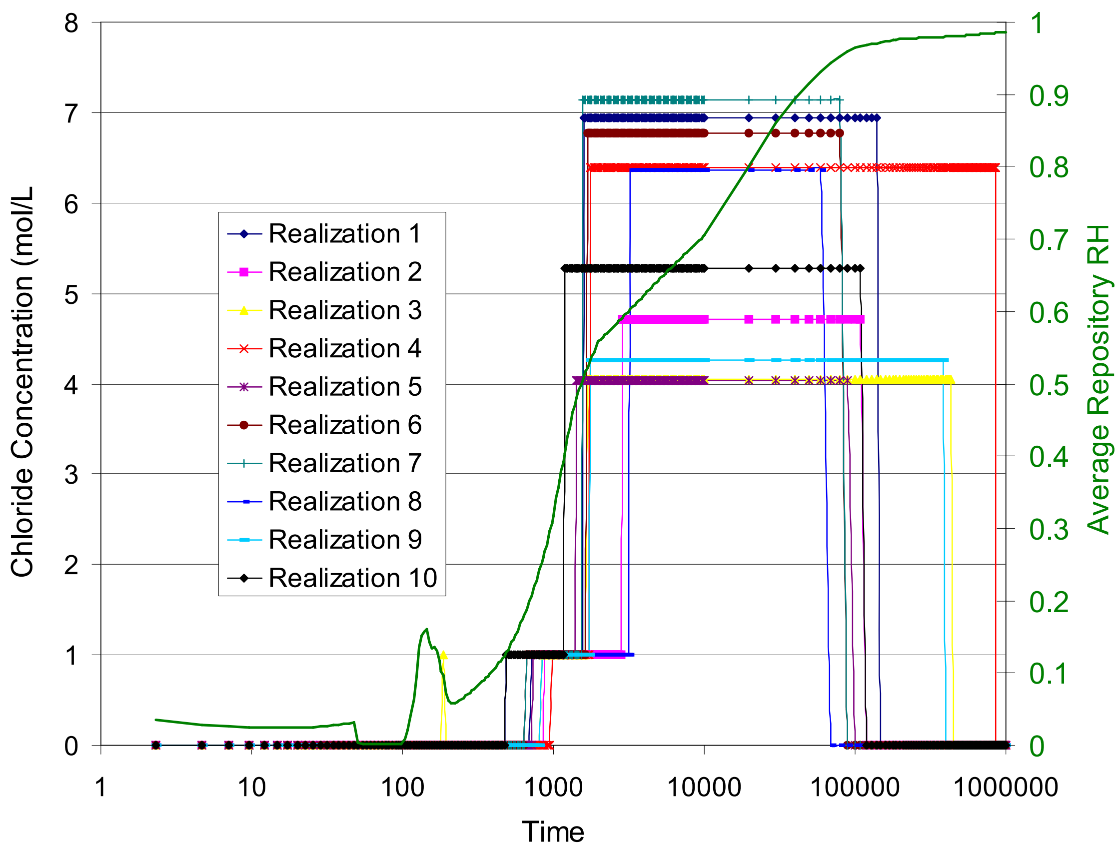
2) Examine the data to compare output values for each Environment.

Pass/Fail criteria:

1) For test 6.1, for each realization, the time values for Environment I at which RH reaches 0.2 is also the time at first Cl^- concentration increase
2) For test 6.2, for each realization, the time values for Environment II, the time of Flow Hit >0 corresponds to the time of second Cl^- concentration increase
3) For test 6.3, for each realization, the time values for Environment III, the time of 0.95 $\geq$relative humidity $\leq$ 0.98 corresponds to the time of Cl^- concentration decrease

Test results:

Chloride Concentration As a Function of Time For All Tests



Observation: The Chloride concentration generally follows the expected pattern. Initially the concentration is zero during the dry period. The concentration increases to one molar during environment I. The concentrations increase to between four and eight molar during environment II. Finally concentrations drop down to near zero molar during environment III.

Test 6.1

Realization	Time at 1st Cl^- step (years)	Time at RH ≥ 0.2 (years)
1	7.12E+02	7.12E+02
2	8.77E+02	8.77E+02
3	8.33E+02	8.33E+02
4	9.71E+02	9.71E+02
5	7.31E+02	7.31E+02
6	6.58E+02	6.58E+02
7	6.58E+02	6.58E+02
8	4.88E+02	4.88E+02
9	8.33E+02	8.33E+02
10	4.88E+02	4.88E+02

Observation: The time at which relative humidity reaches a value of 0.2 or greater corresponds to the time of the first increase in chloride concentration, indicating that Environment I switch is properly triggered in every realization.

Test 6.2

Realization	Time at 2nd Cl^- step (years)	Time at $Q_{hit}>0$ (years)
1	1601.1	1601.1
2	2863.4	2863.4
3	1681.6	1681.6
4	1765.9	1765.9
5	1415.4	1415.4
6	1681.6	1681.6
7	1562.2	1562.2
8	3226.8	3226.8
9	1765.9	1765.9
10	1188.9	1188.9

Observation: The time of $Q_{hit} > 0$ corresponds to the time of the second chloride concentration step. This indicates that the Environment II switch is correctly triggered in every realization.

Test 6.3

Realization	Time at 3^{rd} Cl^- step (years)	Time at $0.95 \leq RH \leq 0.98$ (years)
1	148600	148600
2	118900	118900
3	445600	445600
4	861400	861400
5	99100	99100
6	89200	89200
7	89200	89200
8	69400	69400
9	396100	396100
10	118900	118900

Observation: The time that $0.95 \leq RH \leq 0.98$ corresponds to the time of the chloride concentration decrease (3^{rd} step). This indicates that the Environment III switch is correctly triggered in every realization.

Test 6 Results (PASS/FAIL): **PASS**

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 20.06002.01.354
Software Name: TPA	Version: TPA5.1betaT
Test ID: **P-6**	Test Series Name: **Drift Degradation**

Test Method

- ■ code inspection
- ■ output inspection
- ■ hand calculation
- ■ spreadsheet
- ■ graphical
- □ comparison with external code results

Test Objective: See Attachment A:
Task P-6 Test Plan Objectives, Assumptions, Planned Tests

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): WindowsXP (SP2)

Input Data (files, data base, mode settings):

Assumptions, constraints, and/or scope of test:

See Attachment A: Task P-6 Test Plan Objectives, Assumptions, Planned Tests

Test Procedure:

See Attachment A: Task P-6 Test Plan Objectives, Assumptions, Planned Tests
See Attachment B: TPA 5.1 Software Validation Task P-6 Test Results

Test Results

Location: See attached CD labeled "TPA Version 5.1 Validation Task P-6"

Test Criterion and Analysis of Results:
See Attachment B: TPA 5.1 Software Validation Task P-6 Test Results

Test Evaluation (Pass/Fail): **PASS**

Notes:

Tester: James Mancillas	Date: 4/25/07

Attachment A

Task P-6 Test Plan
Objectives, Assumptions, Planned Tests

The following describes the objectives, assumptions, and planned tests for Task P-6 of the TPA Version 5.1 code Software Validation Plan.

OBJECTIVES

The objective of Software Validation Task P-6 is to validate process level calculations performed by the TPA module DRIFTFAIL. The specific issues to be addressed by SVR #6 are the following:

1. Thermally induced drift degradation can be turned off to permit comparisons of scenarios with and without drift degradation.
2. Drift fill up times should be consistent with the input for drift degradation times for thermally induce degradation scenarios, and drift fill time should occur at earlier times when seismically induced drift degradation occurs.
3. Vertical pressures for the trapezoidal configuration should approach the pressures for the chimney configuration when trapezoidal base angle is increased to 90 degrees.
4. Drift heights, vertical pressures and equivalent diameters are calculated correctly for eight potential degradation scenarios.
    a. Chimney shape, thermally induced drift degradation only
    b. Chimney shape, thermally induced drift degradation and seismically induced drift degradation
    c. Chimney shape, drift degradation with early seismicity (prior to complete drift degradation)
    d. Chimney shape, seismically induced drift degradation only
    e. Trapezoidal shape, thermally induced drift degradation only
    f. Trapezoidal shape, thermally induced drift degradation and seismically induced drift degradation
    g. Trapezoidal shape, drift degradation with early seismicity (prior to complete drift degradation)
    h. Trapezoidal shape, seismically induced drift degradation only.

5 Seismically induced drift degradation does not occur for seismic events which occur prior to repository closure.

ASSUMPTIONS

For the purposes of this validation test, it is assumed:

- The input parameters and their distributions supplied by *tpa.inp* are consistent with the abstractions of the modeled processes.
- Previous validation testing of this module and testing of subsequent SCRs affecting this module have been properly performed, and may be used as confirmation of TPA code performance.

TEST

The following tests sequentially address the objectives of this SVR. During validation testing the validation teams may conduct additional testing, to be documented in the SVR, as necessary to understand and verify software performance related to the DRIFTFAIL module.

1. Execute one reference case realization for 10ky with the append all option set. Then execute a second realization for 10ky with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DriftDegradationScenarioFlag(yes=1,no=0)	0

Then compare the general TPA screen output and *ebsrel.rlt, driftfail.rlt*. The second realization should have skipped the DRIFTFAIL and MECHFAIL modules, and no WP should have mechanically failed.

2. Execute a reference case realization of 10ky for one subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DegradationTimeRockTypeOneSubarea_1[yr]	Constant, 2000

Then execute 10 realizations of 10ky for one subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	1
DegradationTimeRockTypeOneSubarea_1[yr]	Constant, 2000

Then examine the *driftfail.rlt* files to verify that drift failure times are properly evaluated without seismicity and that seismic events accelerate drift degradation.

3. Execute one reference case realization of 10ky for one subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
FractionDriftDegradationOccursbyChimney	1
DegradationTimeRockTypeOneSubarea_1[yr]	Constant, 1000

Then execute three realizations of 10ky for one subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table.

Parameter	Value
FractionDriftDegradationOccursbyChimney	0
DegradationTimeRockTypeOneSubarea_1[yr]	Constant, 1000
TrapezoidBaseAngle	Constant, 50.7, 75, 90

Then compare the drift heights recorded in *driftfail.rlt* files for each of the realizations. The trapezoidal shape drift degradation realizations for base angles 50.7, 75, and 90 degrees should have drift heights which converge to the chimney drift height, as the base angle approaches 90 degrees.

The fourth objective of this SVT requires 8 testing scenarios. These test will be listed as test 4a through test 4h.

4a. Perform a single reference case realization of the TPA code for a single subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DriftDegradationGeometrySelectionValue	Uniform 0.0, 0.2

Then compare the results recorded in *driftfail.rlt* and d*riftfail.dat* with hand calculations of drift height, vertical pressures and equivalent diameters performed using MS Excel.

4b. Perform a single reference case realization of the TPA code for a single subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	1
DriftDegradationGeometrySelectionValue	Uniform 0.0, 0.2

Then compare the results recorded in *driftfail.rlt* and *driftfail.dat* with hand calculations of drift height, vertical pressures and equivalent diameters performed using MS Excel.

4c. Perform a single reference case realization of the TPA code for a single subarea with the append all option set and additionally modify the tpa.inp file in accordance with the following table

Parameter	Value

SeismicDisruptiveScenarioFlag(yes=1,no=0)	1
DriftDegradationGeometrySelectionValue	Uniform 0.0, 0.2

Execute the TPA code for subarea one. Then copy the *driftfail.inp* file and *driftfail.exe* file into a separate directory. Then modify the *driftfail.inp* file to create a seismic event at 450 yr and setting the bulking factors to 1.19 and 1.21 for rock types one and two. Then compare the results recorded in *driftfail.rlt* and *driftfail.dat* with hand calculations of drift height, vertical pressures and equivalent diameters performed using MS Excel. A time of 450 yr is selected such that the event will occur about midway between the beginning of drift degradation (100 yr) and the time the drift is fully degraded (about 1000 yr).

4d. Perform a single reference case realization of the TPA code for a single subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	1
DriftDegradationGeometrySelectionValue	Uniform 0.0, 0.2
DriftDegradationScenarioFlag(yes=1,no=0)	0

Then compare the results recorded in driftfail.rlt and driftfail.dat with hand calculations of drift height, vertical pressures and equivalent diameters performed using MS Excel.

4e. Perform a single reference case realization of the TPA code for a single subarea with the append-all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DriftDegradationGeometrySelectionValue	Uniform 0.8, 1.0

Then compare the results recorded in driftfail.rlt and driftfail.dat with hand calculations of drift height, vertical pressures and equivalent diameters performed using MS Excel.

4f. Perform a single reference case realization of the TPA code for a single subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value

SeismicDisruptiveScenarioFlag(yes=1,no=0)	1
DriftDegradationGeometrySelectionValue	Uniform 0.8, 1.0

Then compare the results recorded in *driftfail.rlt* and *driftfail.dat* with hand calculations of drift height, vertical pressures and equivalent diameters performed using MS Excel.

4g. Perform a single reference case realization of the TPA code for a single subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	1
DriftDegradationGeometrySelectionValue	Uniform 0.8, 1.0

Execute the TPA code for subarea one. Then copy the *driftfail.inp* file and *driftfail.exe* file into a separate directory. Then modify the *driftfail.inp* file to create a seismic event at 450 yr and set the bulking factors to 1.19 and 1.21 for rock types one and two. Then compare the results recorded in *driftfail.rlt* and *driftfail.dat* with hand calculations of drift height, vertical pressures and equivalent diameters performed using MS Excel. A time of 450 yr is selected such that the event will occur about midway between the beginning of drift degradation (100 yr) and the time the drift is fully degraded (about 1000 yr).

4h. Perform a single reference case realization of the TPA code for a single subarea with the append all option set, and additionally modify the tpa.inp file in accordance with the following table:

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	1
DriftDegradationGeometrySelectionValue	Uniform 0.8, 1.0
DriftDegradationScenarioFlag(yes=1,no=0)	0

Then compare the results recorded in *driftfail.rlt* and *driftfail.dat* with hand calculations of drift height, vertical pressures and equivalent diameters performed using MS Excel.

5. Perform 500 reference case realizations of the TPA code for a single subarea with the append all option set. The examine the files *driftfail.ech* and *driftfail.rlt* to identify when an event occurred prior to repository closure, and to ensure drift degradation did not result from an event prior to closure.

Attachment B

TPA 5.1 Software Validation Task P-6 Test Results

Following are test results for the validation test cases described in Attachment A for TPA Version 5.1 code Software Validation Task P-6. Additional details related to test procedures are also provided.

Test 1. Drift degradation can be turned off

Path for run directory:
Reference case: Manta: D\ValidationTPA\reference_case
Test case : Manta: D\ValidationTPA\test1

Environment variable:
Reference case: TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Test case: TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Path for archive of results
Reference case : [CD: titled P6 Testing]: \SVT6\reference_case
Test case: [CD: titled P6 Testing]: \SVT6\test1

Special input files or modifications to input files required : None

Special diagnostic code modifications required: None

Program modes to be used (append flags, scenario/model switches, etc.):
Reference case: append all
Test case: append all, and the following

Table 1: Test1

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DriftDegradationScenarioFlag(yes=1,no=0)	0

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify that drift degradation can be turned off to permit comparisons of scenarios with and without drift degradation

Assumptions None, other than those made within the TPA code.

Constraints None

Output files to compare or examine: Screen output (tpa.exe>*out*) , *driftfail.rlt*

Test Procedure

1. Perform one reference case TPA run for 10ky, with the file output option set to append all.
2. Perform one test case realization for 10ky, with the file output option set to append all, and the tpa.inp file modified as described in Table 1.
3. Examine and compare results of the test case with the reference case

Pass/Fail criteria

1. The testcase realization should have no mechanical failures of the drip shield or waste packages.

2. When no drift degradation, thermal or seismic, occurs the values for equivalent diameters of the drift and drift backfill are properly calculated.

Test results:

-criterion 1

The reference case and test case realization both successfully executed under the test conditions.

In the reference case, an examination of the screen output, \Validation_test\SVR6\reference_case*out*, shows mechanical failure of the drip shields (in all subareas). An examination of the output file \Validation_test\reference_case*driftfail.rlt* shows that under these conditions, drift degradation occur and rubble accumulates on top of the drip shield results in vertical pressures which are sufficient to fail drip shields.

The following excerpt is from the screen output Validation_test\SVR6\reference_case*out*

```
*************************************************************************************
------------------------------------------------------------------------
    subarea   1 of  10           realization    1 of  500
------------------------------------------------------------------------
exec: calling uzflow
        Mean Annual Infiltration at Start(AAI0):    6.9049E+00
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
dataFile= dsfailt.dat
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      435.7  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1167.8  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     27 at TPA time =   1159.5 yr
 *** failed WPs:  27   out of  526   ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                Highest release rates from Sub Area 1
             Tc99    8.0694E-04 [Ci/yr/SA] at  1.000E+04 yr
             Ni59    5.1995E-05 [Ci/yr/SA] at  1.000E+04 yr
             Ja241   2.7481E-05 [Ci/yr/SA] at  1.189E+03 yr
             Cs135   1.8479E-05 [Ci/yr/SA] at  1.000E+04 yr
```

```
            Am241   7.5963E-06 [Ci/yr/SA] at  1.562E+03 yr
            Np237   5.8459E-06 [Ci/yr/SA] at  1.000E+04 yr
exec: calling uzft
                    Highest release rates from UZ
            Tc99    7.8320E-04 [Ci/yr/SA] at  1.000E+04 yr
            Ni59    3.4316E-05 [Ci/yr/SA] at  1.000E+04 yr
            Ja241   1.4257E-05 [Ci/yr/SA] at  1.524E+03 yr
            Cs135   1.2196E-05 [Ci/yr/SA] at  1.000E+04 yr
            Am241   4.2627E-06 [Ci/yr/SA] at  2.044E+03 yr
            Np237   3.8582E-06 [Ci/yr/SA] at  7.551E+03 yr
exec: calling szft
                    Highest release rates from SZ
            Tc99    2.8016E-04 [Ci/yr/SA] at  1.000E+04 yr
            I129    5.1374E-07 [Ci/yr/SA] at  1.000E+04 yr
            Se79    4.8468E-07 [Ci/yr/SA] at  1.000E+04 yr
            Ja243   4.3171E-07 [Ci/yr/SA] at  1.000E+04 yr
            Ja241   2.8987E-07 [Ci/yr/SA] at  1.000E+04 yr
            Jc245   2.7115E-07 [Ci/yr/SA] at  1.000E+04 yr
*************************************************************************************
```

An examination of the screen output from the test case realization (\SVR6\test1*out*), with no thermal or seismic drift degradation, shows the DRIFTDRIVER and MECHDRIVER modules were not called for any subareas. The screen output also shows no mechanical failure of the drip shields or waste packages and no radio nuclide releases occurred . Because DRIFTDRIVE and MECHDRIVE were not called; no drift degradation calculations were performed, no mechanical failures of the drip shields or waste packages are evaluated, no result files for the drift failure calculations (*driftfail.rlt, driftfail.ech mechfail_wp.rlt*, and *mechfail_ds.rlt*) were generated.

The following excerpt is from the screen output\SVR6\test1*out*

```
*************************************************************************************
------------------------------------------------------------------------
    subarea   1 of  10           realization    1 of  500
------------------------------------------------------------------------
exec: calling uzflow
        Mean Annual Infiltration at Start(AAI0):    6.9049E+00
exec: calling nfenvFl
exec: calling dsfail
dataFile= dsfailt.dat
     *** No Drip Shield Mechanical Failure ***
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
 *** failed WPs:  0   out of  526  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
*************************************************************************************
```

- criterion 2

An examination of the executive module shows that the equivalent drift diameters A and B, the equivalent backfill diameters A and B are initialized. The drift diameters are initialized to the drift diameter. The backfill equivalent diameters are initialized to zero prior to repository closure. After closure the backfill equivalent diameters are initialized to the equivalent outer diameter of the drip shield plus the thickness of any engineered backfill. The following text is an excerpt from *exec.f*

```
******************************************************************************
cc Equivalent diameters for the drift and backfill
c     GADAMS PA-SCR-480 7-19-04: Initialize equivalent drift diameter
c     and seismic backfill diameter arrays in the executive because the
c     mechanical failure module is not always invoked.
      do index_backfill = 1, ntim
        equivdriftdiaAsubarea(index_backfill, isa) = driftdia
        equivdriftdiaBsubarea(index_backfill, isa) = driftdia

c       GADAMS PA-SCR-553 2-6-2005: Replaced backfill time with time of
c       repository closure
c        if(tim(index_backfill) .lt. backfill_time) then
        if(tim(index_backfill) .lt. closure_time) then
c       GADAMS PA-SCR-553 2-6-2005: End of change

c         Backfill is not yet present
          equivbfdiaAsubarea(index_backfill, isa) = 0.0d0
          equivbfdiaBsubarea(index_backfill, isa) = 0.0d0
        else
          if(backfill_thickness .GT. 0.0D0) then
c           Engineered backfill is present at this time
            equivbfdiaAsubarea(index_backfill, isa) =
     &        dsidia + 2.0d0 * dsthick + 2.0d0 * backfill_thickness
            equivbfdiaBsubarea(index_backfill, isa) =
     &        dsidia + 2.0d0 * dsthick + 2.0d0 * backfill_thickness
          else
c           After closure, initialize to drip shield outer diameter
c           when engineered backfill is not present
            equivbfdiaAsubarea(index_backfill, isa) =
     &        dsidia + 2.0d0 * dsthick
            equivbfdiaBsubarea(index_backfill, isa) =
     &        dsidia + 2.0d0 * dsthick
          endif
        endif
      enddo
******************************************************************************
```

This excerpt shows that the equivalent diameters are properly initialized if no drift degradation calculations are performed. If drift degradation does not occur these initial values are not altered during the remaining calculations of the realization.

The vertical pressures are initialized to zero at the beginning of each realization, which is the expected values if no drift degradation occurs. If drift degradation does not occur these initial values are not altered during the remaining calculations of the realization. The following text is an excerpt from *exec.f*

```
******************************************************************************
       call zero( maxseismic*maxnsubarea, vert_pressure1_seismic(1,1))
        call zero( maxseismic*maxnsubarea, vert_pressure2_seismic(1,1))
        call zero( maxntime*maxnsubarea, vert_pressure1_subarea(1,1))
        call zero( maxntime*maxnsubarea, vert_pressure2_subarea(1,1))
******************************************************************************
```

These results show that objective of test 1 of Task P-6 has been successfully tested.

Test 1 Results (PASS/FAIL): **PASS**

Test 2. Drift failure time consistent with drift degradation times

Path for run directory:

Test case 2a : Manta: D\Validation_test\test2a
Test case 2b : Manta: D\Validation_test\test2b

Environment variable:

Test case 2a : TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Test case 2b : TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Path for archive of results

Test case 2a : [CD: titled P6 Testing]: \SVT6\test2a
Test case 2b : [CD: titled P6 Testing]: \SVT6\test2b

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

Test2a and Test2b were performed by executing the TPA code for subarea 1, for ten realizations of 10kys. In addition the *tpa.inp* files were modified to include the following changes.

Test case 2a : append all, and the following

Table 2: Test2a

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DegradationTimeRockTypeOneSubarea_1[yr]	Constant, 2000

Test case 2b: append all, and the following

Table 3: Test2b

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	1
DegradationTimeRockTypeOneSubarea_1[yr]	Constant, 2000

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: MS Excel

Objective: Verify the drift failure times are consistent with the drift degradation times for non-seismic scenarios and drift failure times should occur at earlier times when seismicity occurs.

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *driftfail.rlt*

Test Procedure:

1) Execute the TPA code twice, using the modified tpa.inp file, and saving the results for examination.
2) Examine the drift ceiling heights in the output files *driftfail.rlt*.

Pass/Fail criteria:

1) The drift failure time should be consistent with the drift degradation time (**DegradationTimeRockTypeOneSubarea_1[yr]**).
2) The degradation of the drift should be accelerated when seismicity occurs prior to drift failure.

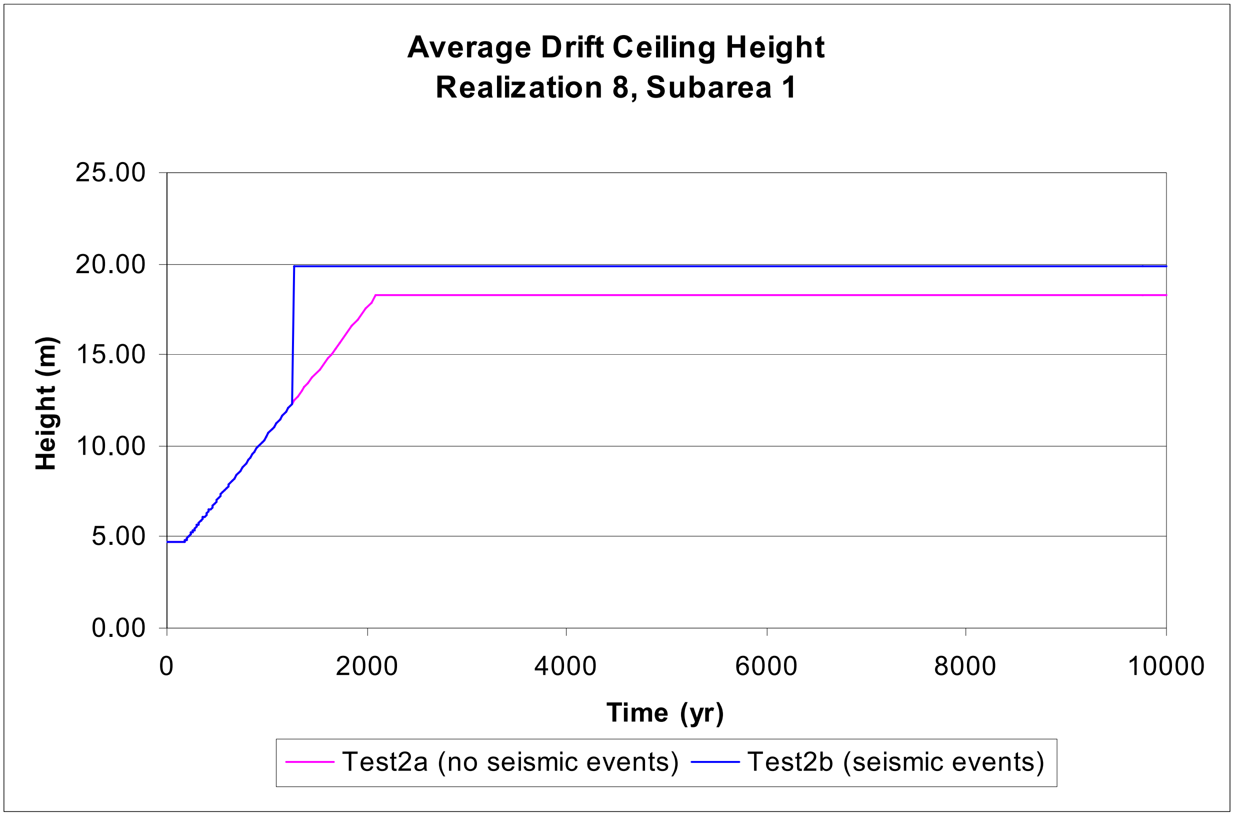
Test results:
Both tests, test2a and test2b, were successfully executed under the test conditions.

- criterion 1
The time at which the drift is completely filled with rubble for a drift which does not experience seismic degradation should be directly related to the degradation time of the drift. Recorded in the output file \SVR6\test2a*driftfail.rlt*, the drift fill times for all 10 realizations of subarea 1 occurred at 2100 yrs. The input file had been modified to set the time required for drift degradation to occur to 2000 yrs and with no seismic drift degradation.

In the TPA code drift degradation begins at the time of repository closure, which was set to 100 yrs for this test. The drift fill time is then the sum of the degradation time and the repository closure time, under these conditions that time is 2100 yrs. This value is consistent with the results recorded in the *driftfail.rlt* files. These results show that criterion 1 of this test was successfully meet.

- criterion 2
Drift degradation should be accelerated by the occurrence of a seismic event prior to complete drift degradation. To evaluate this occurrence, the TPA code was modified in accordance to Table 3 and run for 10 realizations for subarea 1 for 10ky, with the output files option set to append all files. An examination of the file \SVR6\test2b*driftfail.rlt* shows that in realization 8, a seismic event occurred at 1274.8 yrs. Because the drift degradation time was set to 2000 yrs, this event occurred before the drift should have fully degraded. Comparing the height of the drift ceiling in this realization with the same results in test2a shows that drift degradation is accelerated by the seismic event.

The following graph, from the Excel worksheet \SVR6\test2b*comparison.xls* is a plot of the results of realization 8 for subarea 1 for both test2a (without seismicity) and test2b (with seismicity).



In this graph it is evident that at the time of the seismic event (1274.8 yr), the drift degradation is accelerated. Prior to that time both the seismic and non-seismic degradation rates are the same. At the time of the seismic event in test2b, the drift ceiling promptly jumps and the time of the drift fill up is recorded as 1281yr (next TPA code time iteration).

Note: The difference in final height of the ceiling between the two cases is a result of the change in bulking factor which resulted from seismic settling.

The following text is an excerpt from \SVR6\test2a*driftfail.rlt*

```
******************************************************************************
!! REALIZATION    8

!! SECTION: SUBAREA and REALIZATION

                         8   !! Realization

                         1   !! Subarea


!!  SECTION: Drift failure status and times
!!           This section contains data relevant to the failure
!!           status and times of failure for the drifts for
!!           two rock types: rock type 1 (lithophysal) and
!!           rock type 2 (nonlithophysal)

                         1   !! Drift failure Rock type 1 (yes/no:1/0)

               2.10000E+03   !! Drift rock type 1 failure time (yr)

                         1   !! Drift failure Rock type 2 (yes/no:1/0)

               2.10000E+03   !! Drift rock type 2 failure time (yr)
******************************************************************************
```

The following text is an excerpt from \SVR6\test2b*driftfail.rlt*

```
******************************************************************************
!! REALIZATION   8

!! SECTION: SUBAREA and REALIZATION

                         8  !! Realization

                         1  !! Subarea


!! SECTION: Number of seismic events

                         1  !! Number of seismic events


!!  SECTION: Vertical static pressures at the time of the
!!           seismic events for both rock types: rock type 1
!!           is lithophysal rock and rock type 2 is
!!           nonlithophysal rock. These pressures are given in
!!           kiloPascals (kPa).

 Seismic      Event      Vertical Press    Vertical Press
   Event       Time         Rock type 1       Rock type 2
               (yr)               (kPa)             (kPa)
        1     1.27483E+03     1.64838E+02     1.21197E+02

!!  SECTION: Drift failure status and times
!!           This section contains data relevant to the failure
!!           status and times of failure for the drifts for
!!           two rock types: rock type 1 (lithophysal) and
!!           rock type 2 (nonlithophysal)

                         1  !! Drift failure Rock type 1 (yes/no:1/0)

               1.28153E+03  !! Drift rock type 1 failure time (yr)

                         1  !! Drift failure Rock type 2 (yes/no:1/0)

               1.28153E+03  !! Drift rock type 2 failure time (yr)
******************************************************************************
```

The failure time for subarea 1 realization 8 in test2a is recorded at 2100 yr.

These results show that the drift degradation is accelerated by seismicity. These results show that the criterion of this test was successfully tested.

Test 2 Results (PASS/FAIL): **PASS**

Test 3. Vertical pressures for the trapezoidal configuration converge to the values for the chimney configuration.

Path for run directory:

Test case 3a : Manta: D\ValidationTPA\test3a
Test case 3b : Manta: D\ValidationTPA\test3b
Test case 3c : Manta: D\ValidationTPA\test3c
Test case 3d : Manta: D\ValidationTPA\test3d

Environment variable:

Test case 3a, 3b, 3c, 3d : TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Path for archive of results

Test case 3a : [CD: titled P6 Testing]: \SVT6\test3a
Test case 3b : [CD: titled P6 Testing]: \SVT6\test3b
Test case 3c : [CD: titled P6 Testing]: \SVT6\test3c
Test case 3d : [CD: titled P6 Testing]: \SVT6\test3d

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

All test cases were set to append all files, in addition the following parameters were changed in the *tpa.inp* files.

Test case 3a:

Table 3: Test3a

Parameter	Value
FractionDriftDegradationOccursbyChimney	1

Test case 3b

Table 4: Test3b

Parameter	Value
FractionDriftDegradationOccursbyChimney	0
TrapezoidBaseAngle	50.7

Test case 3c :

Table 5: Test3c

Parameter	Value
FractionDriftDegradationOccursbyChimney	0
TrapezoidBaseAngle	75.0

Test case 3d:

Table 6: Test3d

Parameter	Value
FractionDriftDegradationOccursbyChimney	0
TrapezoidBaseAngle	90.0

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify that the drift heights and vertical pressures for the trapezoidal shaped degraded drift approach the heights and pressures from the chimney shaped degraded drift when the trapezoidal base angle is increased to 90 degrees.

Assumptions None, other than those made within the TPA code.

Constraints None

Output files to compare or examine: *driftfail.rlt*

Test Procedure:

1) Execute the TPA code four times using the modified tpa.inp files for tests test3a to test3d, saving the results for examination.
2) Examine the drift ceiling heights and vertical pressures in the output file *driftfail.rlt*.

Pass/Fail criteria:

1) The drift height and vertical pressures for the trapezoidal shaped degraded drift should increase to the chimney values as the trapezoidal angle is increased from 50.7 to 90 degrees.

Test results:
All tests; test3a, test3b, test3c, test3d, successfully executed under the test conditions.

- criterion 1

The final drift height and vertical pressure calculated for the chimney shaped degraded drift from test3a and recorded in the file \SVR6\test3a*driftfail.rlt* are as follows.

Table 7: Test3a Results

Shape	Drift Height (m)	Vertical Pressure (kPa)
Chimney	24.4087	420.770

The final drift heights and vertical pressures calculated for the trapezoidal shaped degraded drifts from test3b, test3c and test3d are recorded in the file \SVR6\test3a...d*driftfail.rlt* and are summarized in the following table, Table 8. The bulking factor which is a sampled parameter which controls the height of the drift has the same sampled value in each of these realizations. (This is because the LHS sampling is unaffected by the adjustment of constant values.)

Table 8: Test3b..d Results

Shape (Degrees)	Drift Height (m)	Vertical Pressure (kPa)
Trapezoidal, 50.7	14.9546	239.125
Trapezoidal, 75.0	19.9699	335.485
Trapezoidal, 90.0	24.4087	420.770

The drift height and vertical pressure of the trapezoidal shape increase as the base angle is changed from 50.7 to 90.0 degrees. At 90 degrees the trapezoidal geometry has the same drift height and vertical pressure. This is the expected behavior since the trapezoidal geometry with a 90 degree base angle is the same shape as the chimney geometry. These results show that criterion 1 of this test has been successfully meet.

Test 3 Results (PASS/FAIL): **PASS**

Test 4. Drift heights, vertical pressures, and equivalent diameters are calculated correctly.

The objective of test 4 is to validate the calculation of drift heights, vertical pressures and equivalent diameters for the eight potential degradation scenarios listed in the following table.

Table 10: Test 4 Degradation Conditions

Test Number	Degraded Drift Shape	Degradation
4a	Chimney	Thermal
4b	Chimney	Thermal and seismic
4c	Chimney	Thermal and Early seismic
4d	Chimney	Seismic only
4e	Trapezoidal	Thermal
4f	Trapezoidal	Thermal and seismic
4g	Trapezoidal	Thermal and Early seismic
4h	Trapezoidal	Seismic only

Testing performed in TPA SCR610 has validated the calculations of the drift heights, vertical pressures and equivalent diameters under the testing conditions identified in Attachment A of Task P-6. Since the testing was completed in TPA SCR610, only two minor changes have been made to the DRIFTFAIL module. These changes include a minor fix to the calculation of the equivalent diameter of the backfill along the vertical axis for thermal mode 2 (TPA SCR627) and a format change was made to the DRIFTFAIL output files *driftfail.ech* and *driftfail.rlt* (TPA SCR664). These changes do not impact the calculations evaluated in SCR610.

Since the testing conditions used in the performance of TPA SCR610 meet the needs of this validation test and no changes have since been made to the calculations tested, the results of SCR610 will be presented to show that the objectives of test4a through test4h have been successfully tested. Documented within these tests is a threshold for agreement between the TPA code results and worksheet results, which specifies that results differ by less than 1%. This level of agreement was established to account for potential rounding errors.

These tests are now sequentially addressed:

Test 4a. **Chimney drift heights, vertical pressures, and equivalent diameters are calculated correctly with non-seismic degradation**.

The validation of drift heights, vertical pressures and equivalent diameters calculations for the chimney shaped degraded drift which occurs by thermal degradation was evaluated by TPA SCR610 P-1. The conditions and results of SCR610 P-1 are presented to show that the objectives of this test have been successfully tested.
The following is a copy of the text and plots from SCR610 P-1

PL-1. Verify drift height, vertical pressures, and equivalent diameters for the chimney failure mechanism (Degradation Only)

1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR610\testresults\pl1

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1

4.0 Special Input Files or Modifications to Input Files Required

4.1 Modify tpa.inp in accordance with the following table:

Parameter	Value
`OutputMode(0=None,1=All,2=UserDefined)`	1
`StopAtSubarea`	1
`MaximumTime[yr]`	1.0e5

`SeismicDisruptiveScenarioF lag(yes=1,no=0)`	0

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used

6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test

None

8.0 Test Description

8.1 Objective: This test is designed to verify that the drift height, vertical pressures, and equivalent diameters generated by the standalone module agree with values generated by spreadsheet calculations.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.inp, driftfail.ech, driftfail.rlt

8.5 Procedure:

1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: “tpa > pl1.out.”

3. Compare the values generated to driftfail.rlt to spreadsheet calculations.

8.6 Pass/Fail Criteria: The drift height versus time values, the vertical pressure versus time values, and the equivalent diameters generated by the DRIFTFAIL module agree with spreadsheet calculations to within 1%.

9.0 Test Results

9.1 Output and Supporting Files: Files are archived to a CD labeled, “TPA SCR #610.”

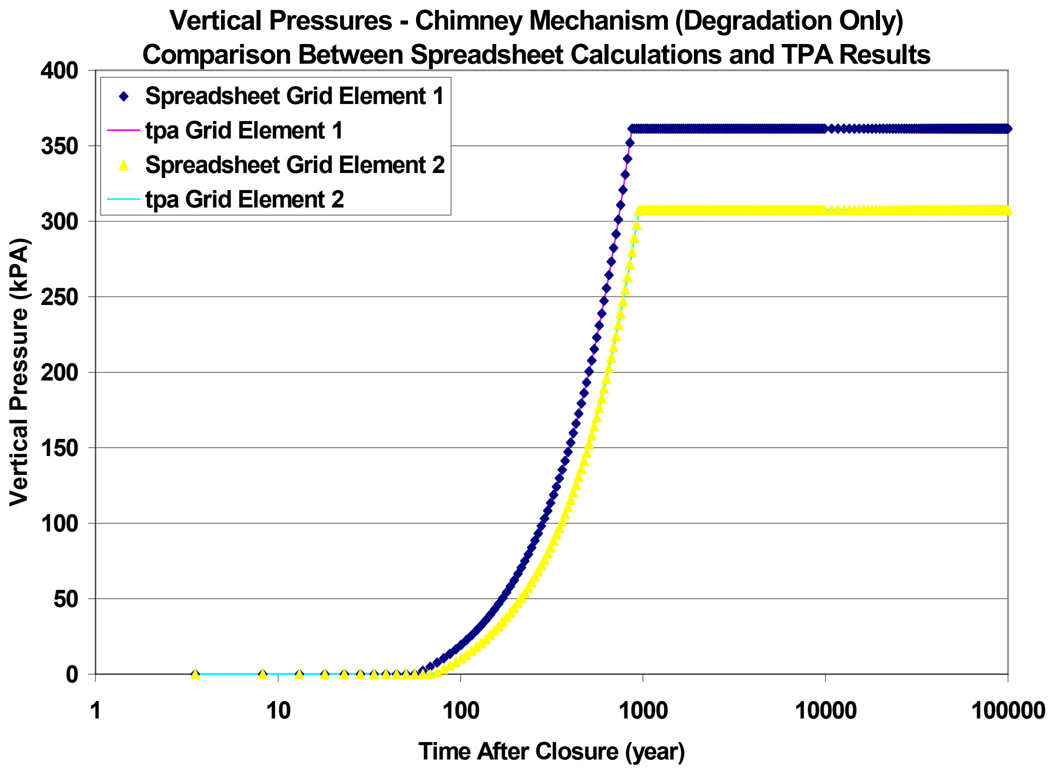
9.2 Criterion 1: Code generated and spreadsheet calculations agree to within 1%.

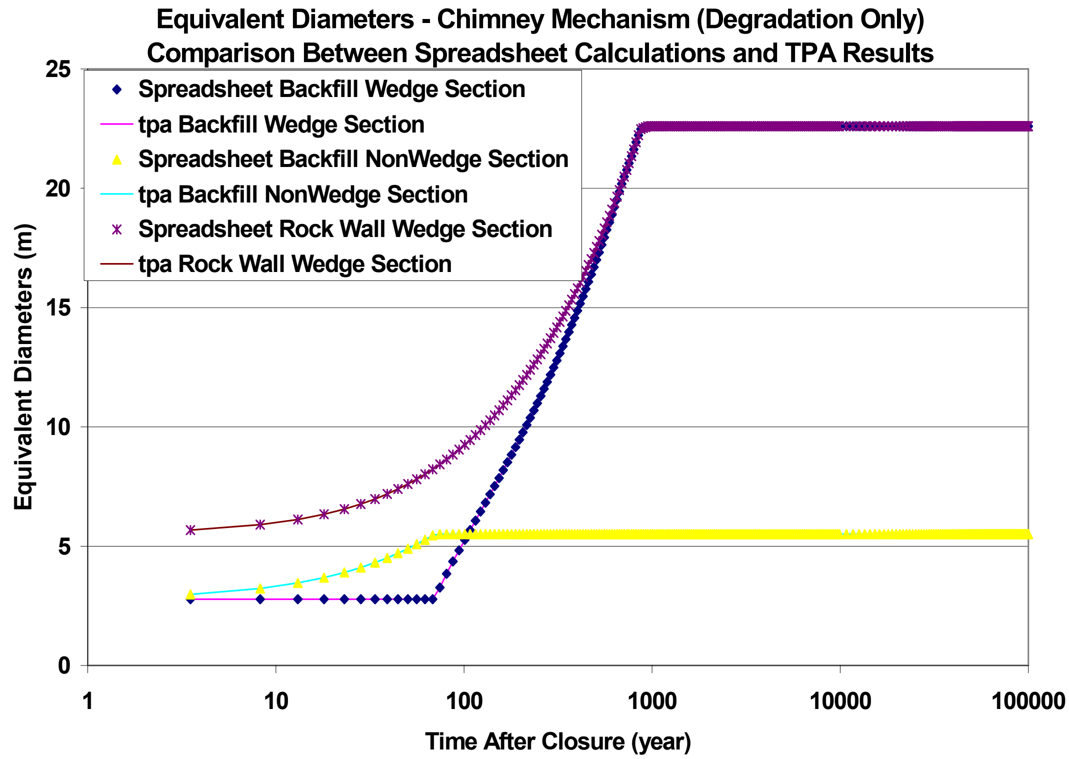
9.3 Overall Test Status:

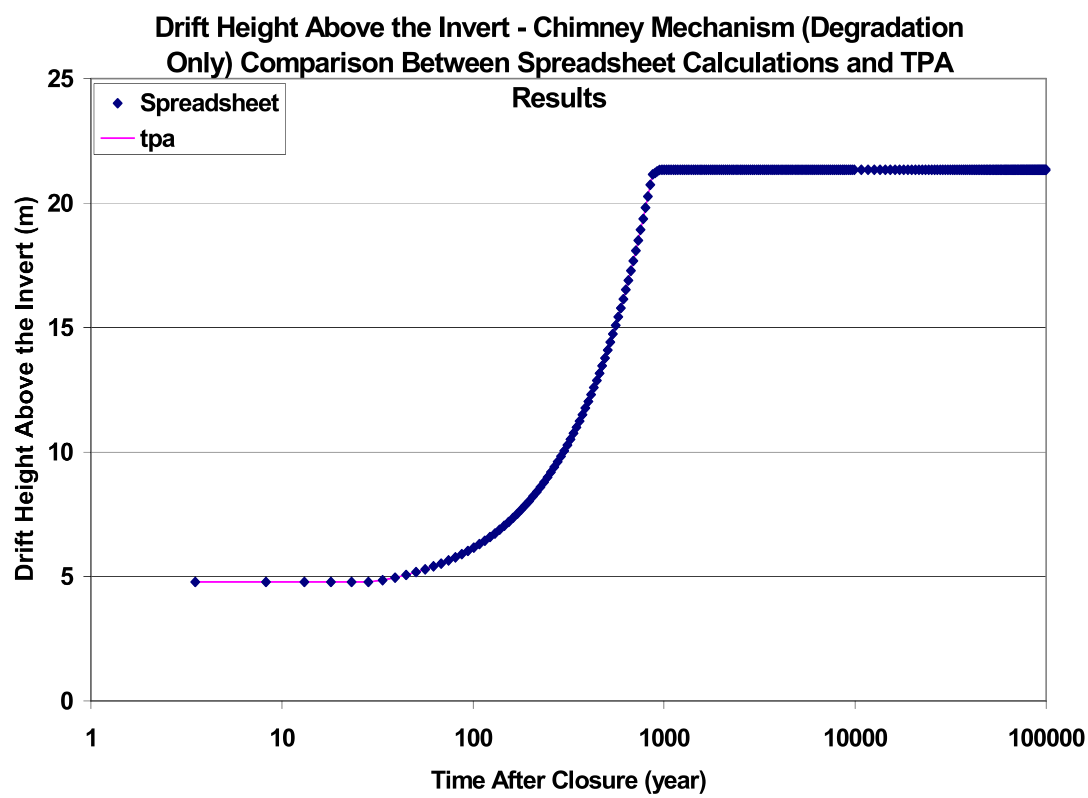
This test **PASSED** the criterion above for test PL-1 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

This test **PASSED** the criterion above for test PL-1 for the UNIX execution because the output files were checked by the diff command with the PC generated output files and they were the same with the exception of the date/time stamp.

Test result from machine tpa agree to within 1% with spreadsheet calculations.







Output files from machine spock checked against output files from machine tpa.

DRIFTFAIL.ECH
3c3
< TPA 5.0.2q, Job started: Thu Apr 6 12:43:14 2006

> TPA 5.0.2q, Job started: Mon Apr 03 16:57:14 2006

DRIFTFAIL.INP
2c2
< DATE/TIMEThu Apr 6 12:43:27 2006

> DATE/TIMEMon Apr 03 16:57:27 2006

DRIFTFAIL.RLT
3c3
< TPA 5.0.2q, Job started: Thu Apr 6 12:43:14 2006

> TPA 5.0.2q, Job started: Mon Apr 03 16:57:14 2006

Test 4a Results (PASS/FAIL): **PASS**

Test 4b. Chimney drift heights, vertical pressures, and equivalent diameters are calculated correctly with seismic and non-seismic degradation.

The validation of drift heights, vertical pressures and equivalent diameters calculations for the chimney shaped degraded drift which occurs by seismic and thermal degradation was evaluated by TPA SCR610 P-3. The conditions and results of SCR610 P-3 are presented to show that the objectives of this test have been successfully tested. The following is a copy of the text and plots from SCR610 P-3

PL-3. Verify drift height, vertical pressures, and equivalent diameters for the chimney failure mechanism (Degradation and Seismicity)
1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR610\testresults\pl3

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1

4.0 Special Input Files or Modifications to Input Files Required
4.1 Modify tpa.inp in accordance with the following table:

Parameter	Value
`OutputMode(0=None,1=All,2=UserDefined)`	1
`StopAtSubarea`	1
`MaximumTime[yr]`	1.0e5

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used
6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test
None

8.0 Test Description
8.1 Objective: This test is designed to verify that the drift height, vertical pressures, and equivalent diameters generated by the standalone module agree with values generated by spreadsheet calculations.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.inp, driftfail.ech, driftfail.rlt

8.5 Procedure:

1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: "tpa > pl3.out."

3. Compare the values generated to driftfail.rlt to spreadsheet calculations.

8.6 Pass/Fail Criteria: The drift height versus time values, the vertical pressure versus time values, and the equivalent diameters generated by the DRIFTFAIL module agree with spreadsheet calculations to within 1%.

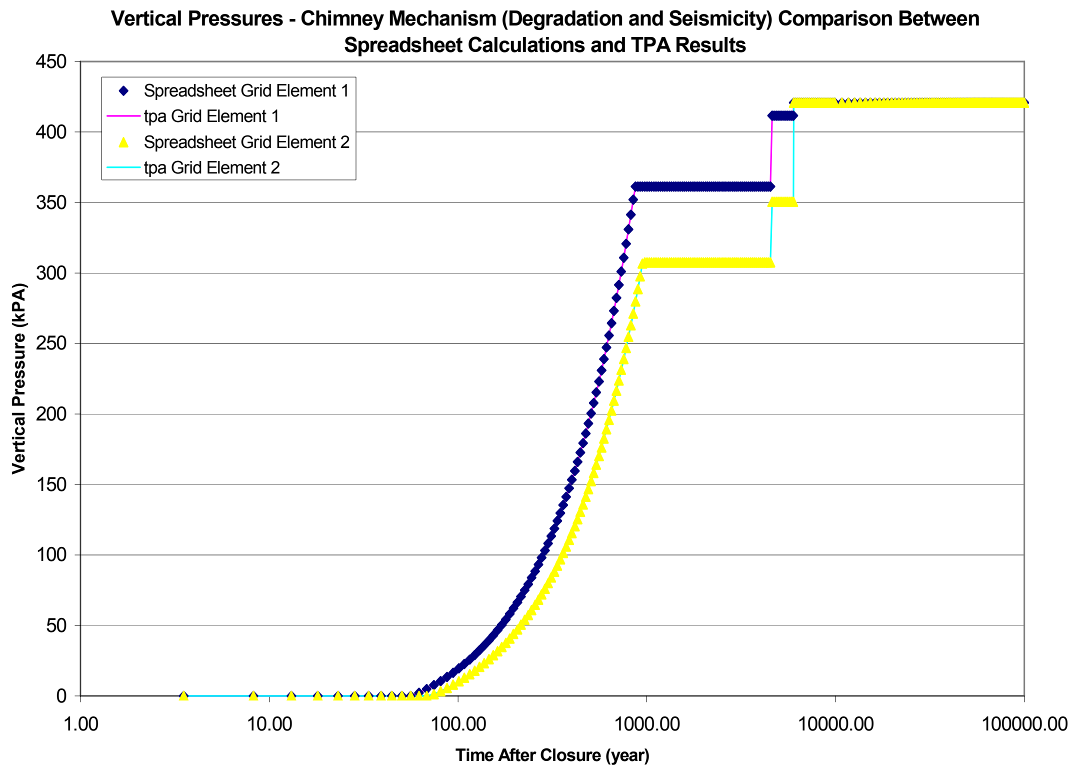
9.0 Test Results
9.1 Output and Supporting Files: Files are archived to a CD labeled, "TPA SCR #610."

9.2 Criterion 1: Code generated and spreadsheet calculations agree to within 1%.

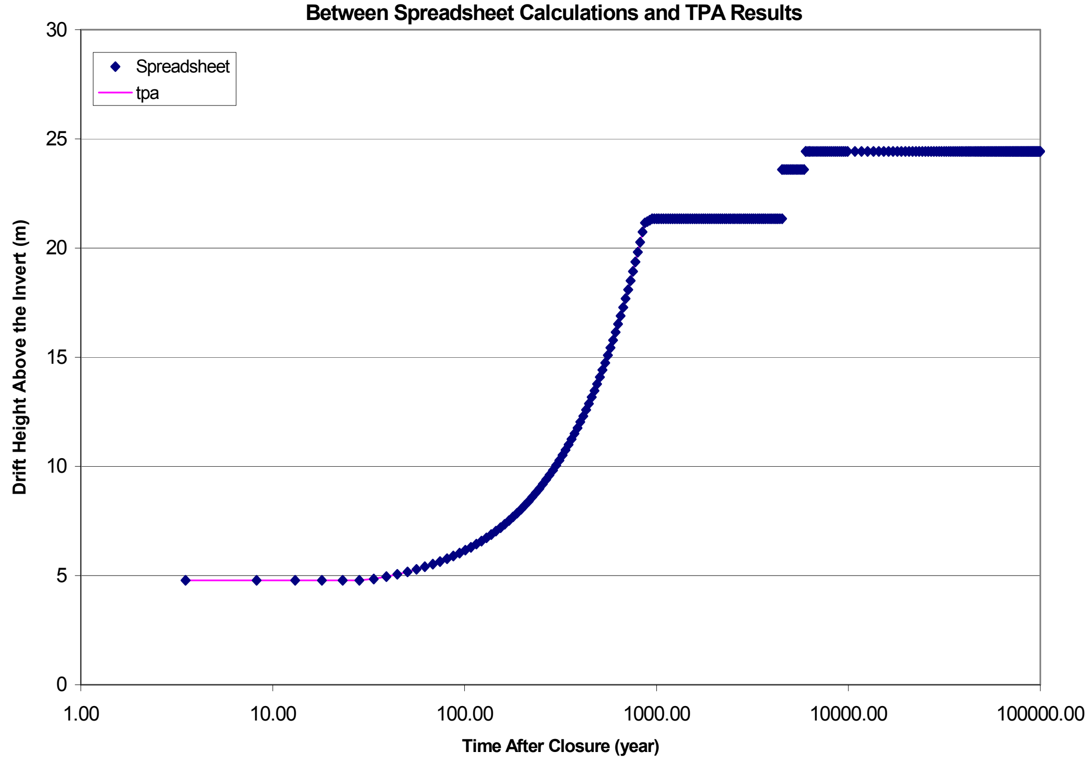
9.3 Overall Test Status:
This test **PASSED** the criterion above for test PL-3 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

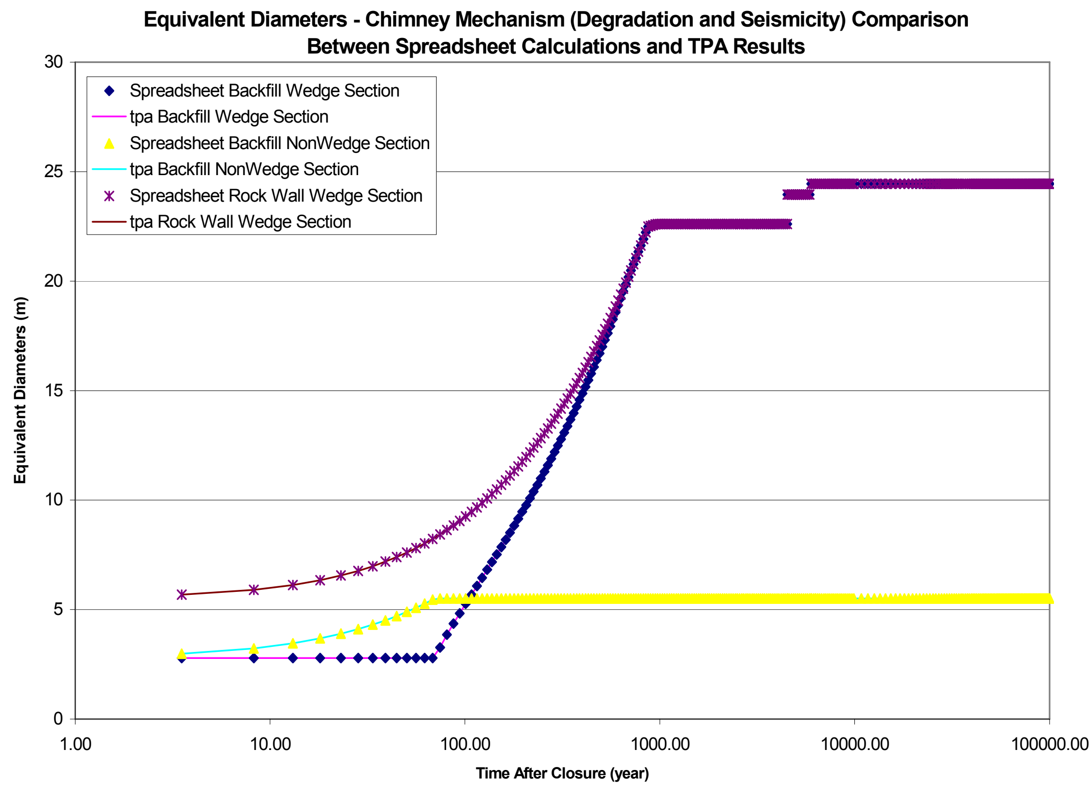
This test **PASSED** the criterion above for test PL-3 for the UNIX execution because the output files were checked by the diff command with the PC generated output files and they were the same with the exception of the date/time stamp.

Test result from machine tpa agree to within 1% with spreadsheet calculations.



Drift Height Above the Invert - Chimney Mechanism (Degradation and Seismicity) Comparison Between Spreadsheet Calculations and TPA Results





Output files from machine spock checked against output files from machine tpa.

DRIFTFAIL.ECH

```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 14:04:03 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 07:57:39 2006
```

DRIFTFAIL.INP

```
2c2
< DATE/TIMEThu Apr  6 14:04:18 2006
---
> DATE/TIMETue Apr 04 07:57:52 2006
```

DRIFTFAIL.RLT

```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 14:04:03 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 07:57:39 2006
```

Test 4b Results (PASS/FAIL): **PASS**

Test 4c. Chimney drift heights, vertical pressures, and equivalent diameters are calculated correctly for early seismic events.

The validation of drift heights, vertical pressures and equivalent diameters calculations for the chimney shaped degraded drift which occurs by early seismic events was evaluated by TPA SCR610 P-5. The conditions and results of SCR610 P-5 are presented to show that the objectives of this test have been successfully tested. The following is a copy of the text and plots from

PL-5. Verify drift height, vertical pressures, and equivalent diameters for the chimney failure mechanism (Degradation and Seismicity with Early Seismic Event)

1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR610\testresults\pl5

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1

4.0 Special Input Files or Modifications to Input Files Required
4.1 Modify driftfail.inp from PL-3 as follows:
Add a seismic event at time 450 years in driftfail.inp which is prior to the time for full drift degradation to be reached.
Set the bulking factor for grid element 1 to 1.19 and for grid element 2 to 1.21.

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used
6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test
None

8.0 Test Description
8.1 Objective: This test is designed to verify that the drift height, vertical pressures, and equivalent diameters generated by the standalone module agree with values generated by spreadsheet calculations.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.inp, driftfail.dat

8.5 Procedure:

1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: “driftfail > pl5.out.”

3. Compare the values generated to driftfail.dat to spreadsheet calculations.

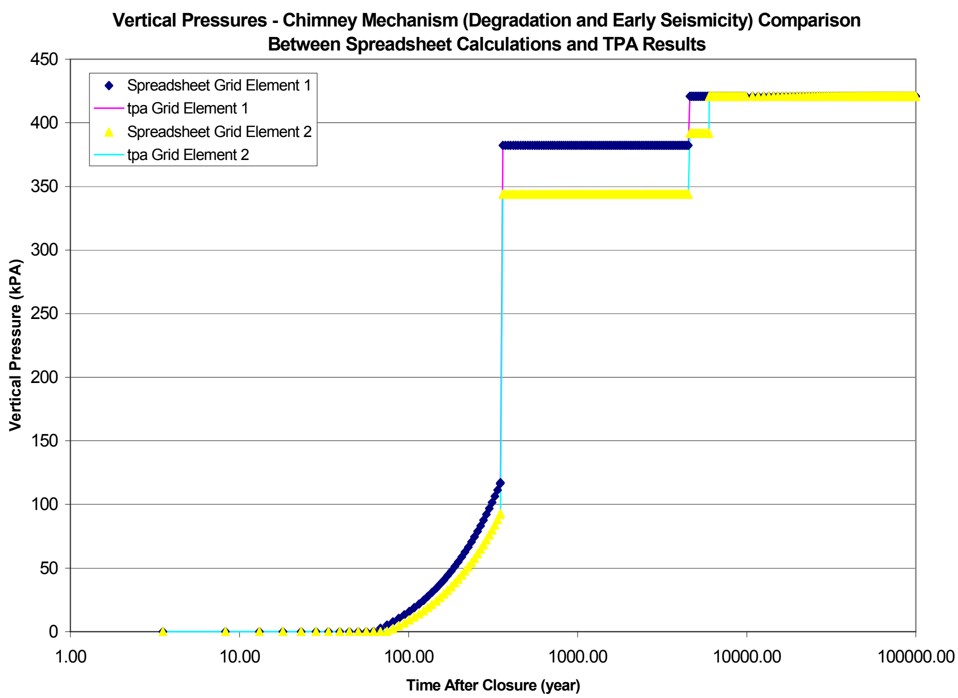
8.6 Pass/Fail Criteria: The drift height versus time values, the vertical pressure versus time values, and the equivalent diameters generated by the DRIFTFAIL module agree with spreadsheet calculations to within 1%.

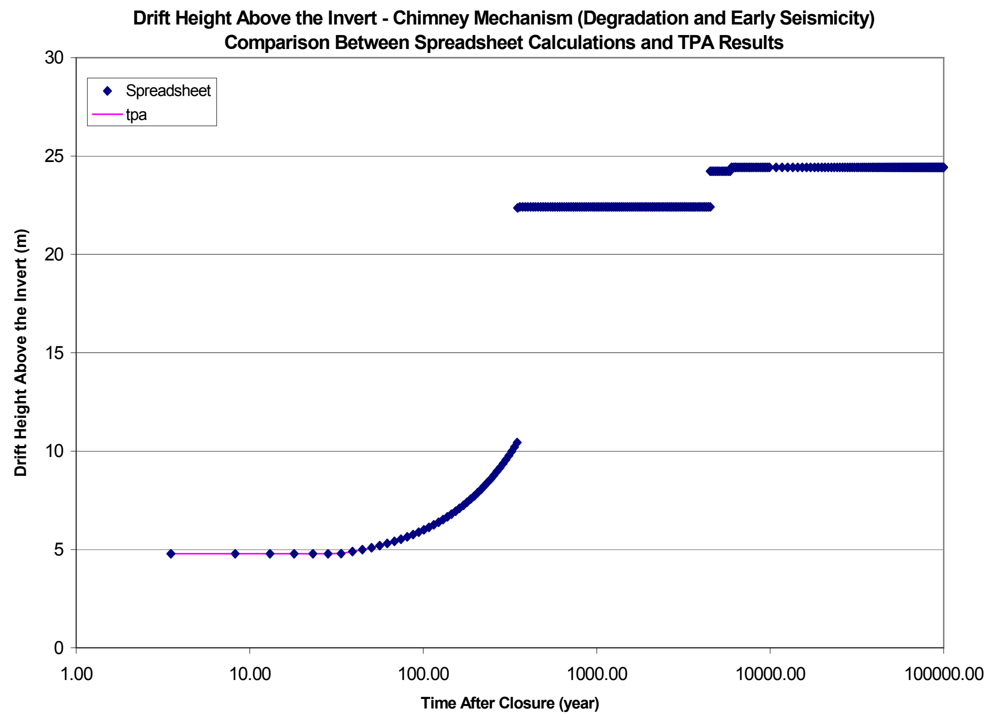
9.0 Test Results
9.1 Output and Supporting Files: Files are archived to a CD labeled, “TPA SCR #610.”

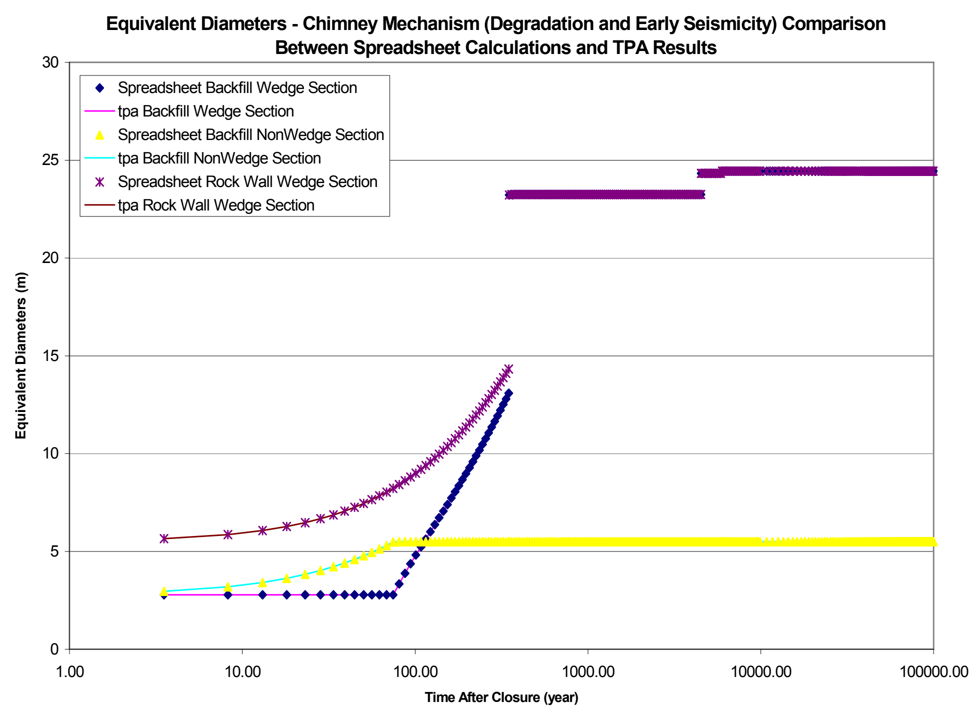
9.2 Criterion 1: Code generated and spreadsheet calculations agree to within 1%.

9.3 Overall Test Status:
This test **PASSED** the criterion above for test PL-5 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.
This test **PASSED** the criterion above for test PL-5 for the UNIX execution because the output files were checked by the diff command with the PC generated output files and they were the same with the exception of the date/time stamp and the headings in the driftfail.dat file. Even though the heading changed in driftfail.dat, the internal values were the same.

Test result from machine tpa agree to within 1% with spreadsheet calculations.







Output files from machine spock checked against output files from machine tpa.

DRIFTFAIL.DAT
```
2c2
< DATE/Time: Thu Apr  6 14:36:30 2006
---
> DATE/Time: Tue Apr 04 11:17:37 2006
8c8
```

```
< : Time           Frac       Press1        Press2          eqRWA         eqRWB
eqBFA        eqBFB       height
---
> : Time            Frac    Press1 kPa    Press2 kPa          eqRWA          eqRWB
      eqBFA          eqBFB        height
```

DRIFTFAIL.INP

```
2c2
< DATE/TIMEThu Apr  6 14:04:18 2006
---
> DATE/TIMETue Apr 04 07:57:52 2006
```

Test 4c Results (PASS/FAIL): **PASS**

Test 4d. Chimney drift heights, vertical pressures, and equivalent diameters are calculated correctly with seismic degradation only.

The validation of drift heights, vertical pressures and equivalent diameters calculations for the chimney shaped degraded drift which occurs by seismic degradation (only) was evaluated by TPA SCR610 P-7. The conditions and results of SCR610 P-7 are presented to show that the objectives of this test have been successfully tested. The following is a copy of the text and plots from SCR610 P-7.

PL-7. Verify drift height, vertical pressures, and equivalent diameters for the chimney failure mechanism (Seismic Only)

1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod2
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod2

<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR610\testresults\pl7

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod2
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod2

4.0 Special Input Files or Modifications to Input Files Required

4.1 Modify driftfail.inp from PL-3 as follows:
Add a seismic event at time 450 years in driftfail.inp which is prior to the time for full drift degradation to be reached.
Set the bulking factor for grid element 1 to 1.19 and for grid element 2 to 1.21.
Turn the drift degradation flag off.

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used

6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test
None

8.0 Test Description

8.1 Objective: This test is designed to verify that the drift height, vertical pressures, and equivalent diameters generated by the standalone module agree with values generated by spreadsheet calculations.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.inp, driftfail.dat

8.5 Procedure:

1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: "driftfail > pl7.out."

3. Compare the values generated to driftfail.dat with spreadsheet calculations.

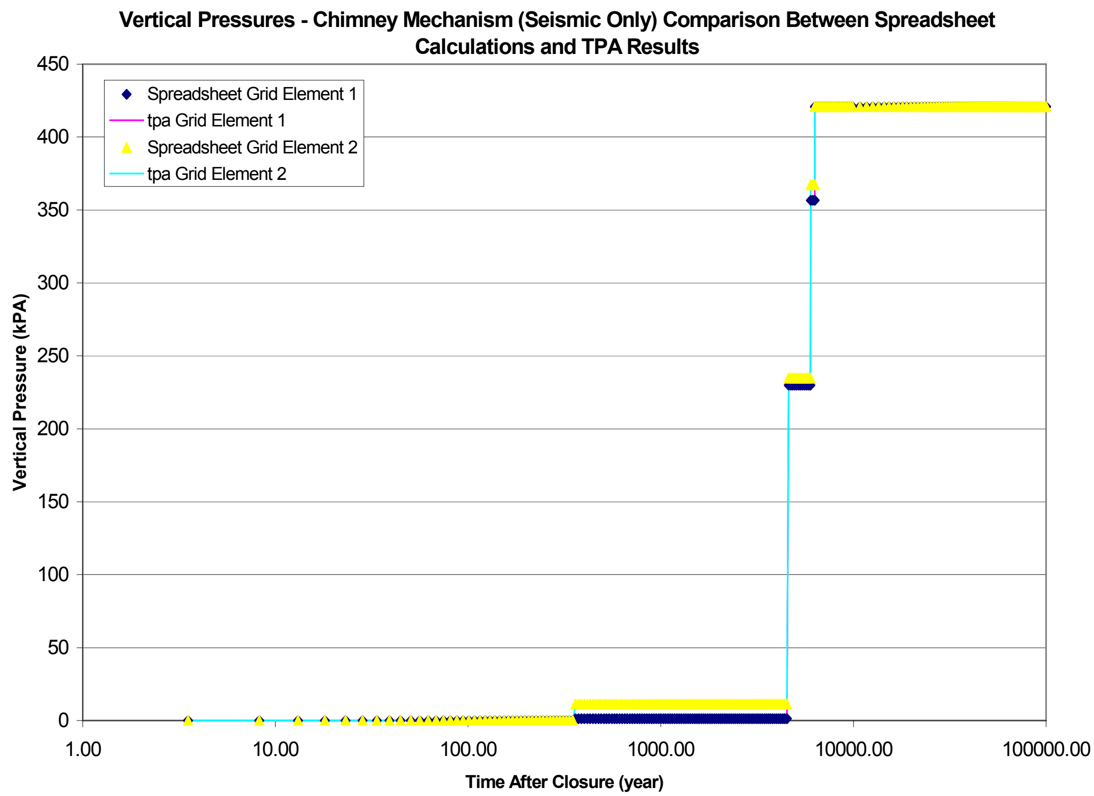
8.6 Pass/Fail Criteria: The drift height versus time values, the vertical pressure versus time values, and the equivalent diameters generated by the DRIFTFAIL module agree with spreadsheet calculations to within 1%.

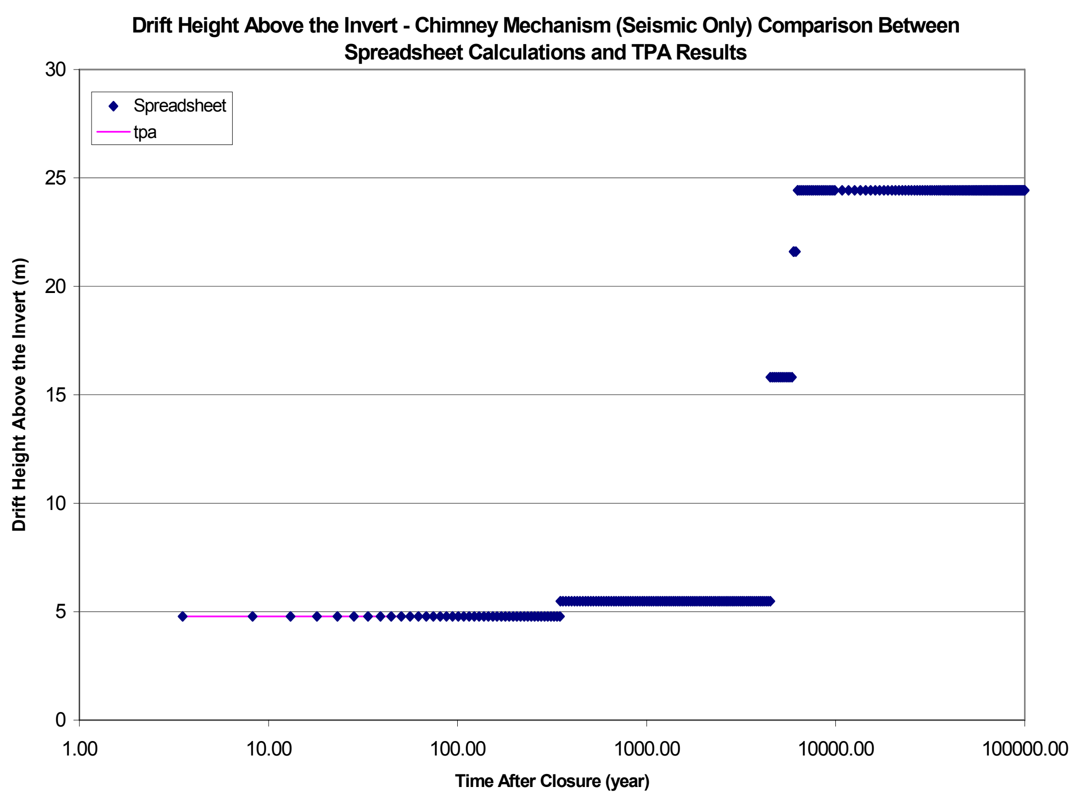
9.0 Test Results

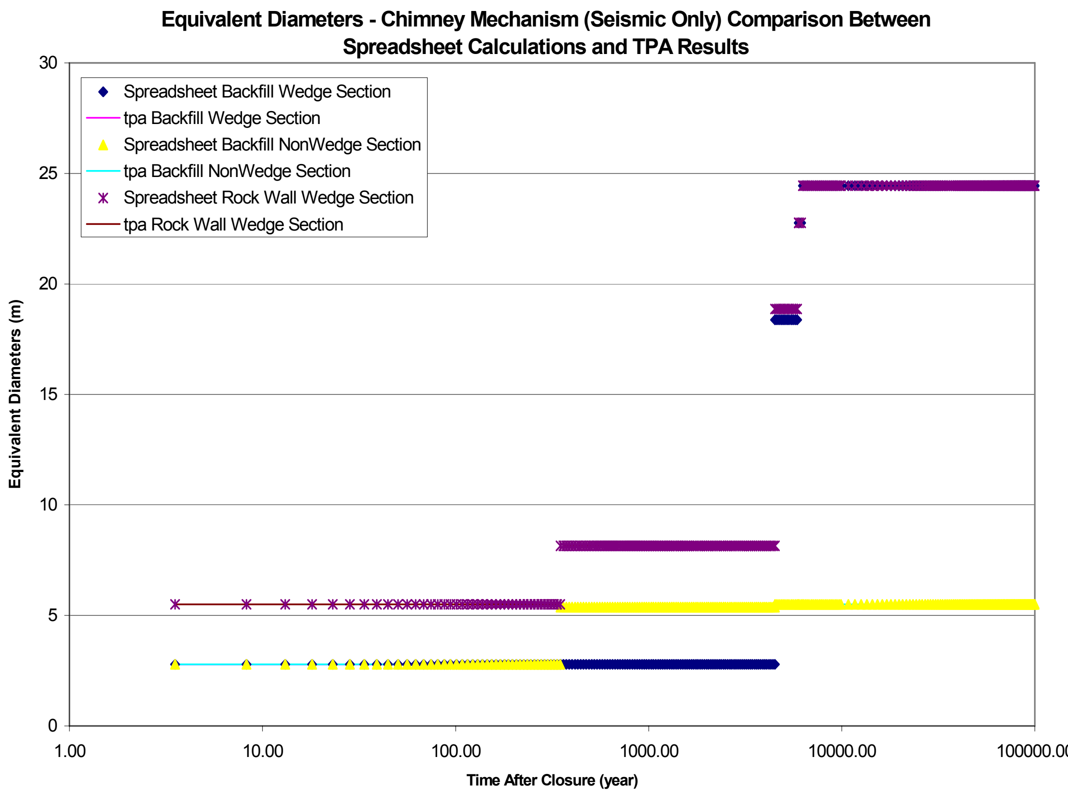
9.1 Output and Supporting Files: Files are archived to a CD labeled, "TPA SCR #610."

9.2 Criterion 1: Code generated and spreadsheet calculations agree to within 1%.

9.3 Overall Test Status:
This test **PASSED** the criterion above for test PL-7 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.
This test **PASSED** the criterion above for test PL-7 for the UNIX execution because the output files were checked by the diff command with the PC generated output files and they were the same with the exception of the date/time stamp.
Test result from machine tpa agree to within 1% with spreadsheet calculations.


Vertical Pressures - Chimney Mechanism (Seismic Only) Comparison Between Spreadsheet Calculations and TPA Results
Spreadsheet Grid Element 1
tpa Grid Element 1
Spreadsheet Grid Element 2
tpa Grid Element 2
Vertical Pressure (kPA)
0
50
100
150
200
250
300
350
400
450
1.00
10.00
100.00
1000.00
10000.00
100000.00
Time After Closure (year)


Drift Height Above the Invert - Chimney Mechanism (Seismic Only) Comparison Between Spreadsheet Calculations and TPA Results
Spreadsheet
tpa
Drift Height Above the Invert (m)
0
5
10
15
20
25
30
1.00
10.00
100.00
1000.00
10000.00
100000.00
Time After Closure (year)



Equivalent Diameters - Chimney Mechanism (Seismic Only) Comparison Between Spreadsheet Calculations and TPA Results
Spreadsheet Backfill Wedge Section
tpa Backfill Wedge Section
Spreadsheet Backfill NonWedge Section
tpa Backfill NonWedge Section
Spreadsheet Rock Wall Wedge Section
tpa Rock Wall Wedge Section
Equivalent Diameters (m)
0
5
10
15
20
25
30
1.00
10.00
100.00
1000.00
10000.00
100000.00
Time After Closure (year)

Output files from machine spock checked against output files from machine tpa.

DRIFTFAIL.DAT
```
2c2
< DATE/Time: Thu Apr  6 15:20:19 2006
---
> DATE/Time: Thu Apr 06 06:43:41 2006
```

DRIFTFAIL.INP
```
2c2
< DATE/TIMEThu Apr  6 14:04:18 2006
---
> DATE/TIMETue Apr 04 07:57:52 2006
```

Test 4d Results (PASS/FAIL): **PASS**

Test 4e. Trapezoid drift heights, vertical pressures, and equivalent diameters are calculated correctly with non-seismic degradation.

The validation of drift heights, vertical pressures and equivalent diameters calculations for the trapezoid shaped degraded drift which occurs by thermal degradation was evaluated by TPA SCR610 P-2. The conditions and results of SCR610 P-2 are presented to show that the objectives of this test have been successfully tested. The following is a copy of the text and plots from SCR610 P-2.

PL-2. Verify drift height, vertical pressures, and equivalent diameters for the trapezoidal failure mechanism (Degradation Only)
1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR610\testresults\pl12

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1

4.0 Special Input Files or Modifications to Input Files Required
4.1 Modify tpa.inp in accordance with the following table:

Parameter	Value
`OutputMode(0=None,1=All,2=UserDefined)`	1
`StopAtSubarea`	1
`MaximumTime[yr]`	1.0e5

SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DriftDegradationMethodSelectionValue	Uniform 0.8, 1.0

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used
6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test
None

8.0 Test Description
8.1 Objective: This test is designed to verify that the drift height, vertical pressures and equivalent diameters generated by the standalone module agree with values generated by spreadsheet calculations.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.inp, driftfail.ech, driftfail.rlt

8.5 Procedure:

1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: "tpa > pl2.out."

3. Compare the values generated to driftfail.rlt to spreadsheet calculations.

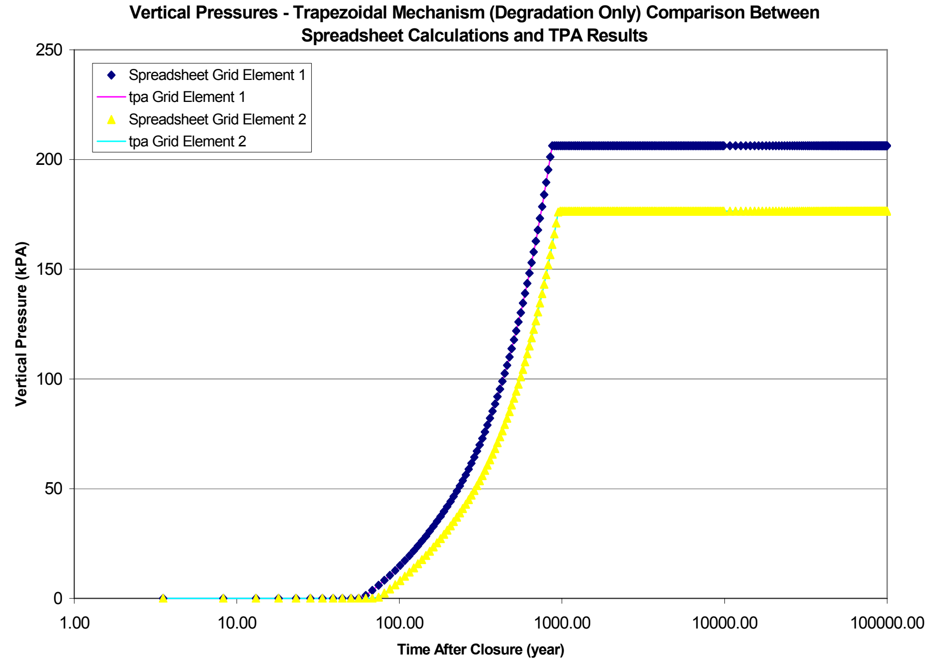
8.6 Pass/Fail Criteria: The drift height versus time values, the vertical pressure versus time values, and the equivalent diameters generated by the DRIFTFAIL module agree with spreadsheet calculations to within 1%.

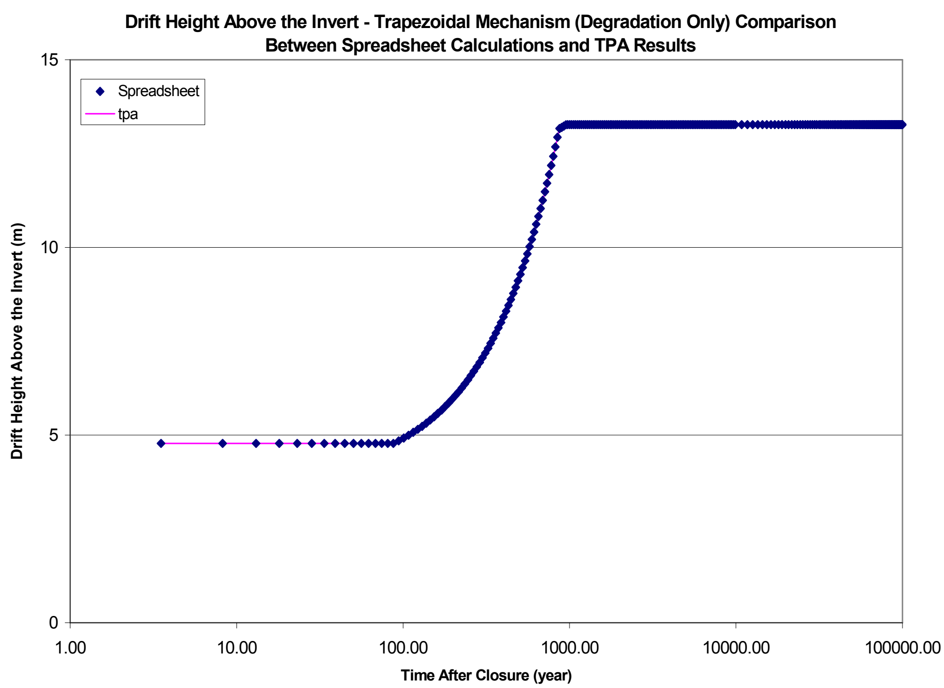
9.0 Test Results
9.1 Output and Supporting Files: Files are archived to a CD labeled, "TPA SCR #610."

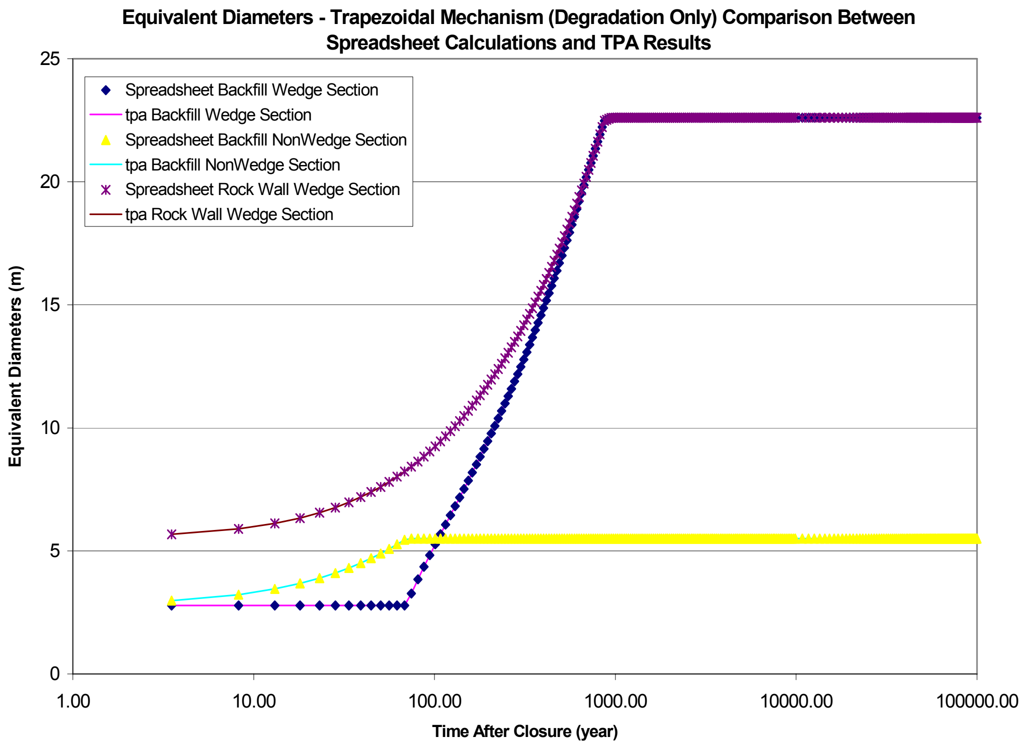
9.2 Criterion 1: Code generated and spreadsheet calculations agree to within 1%.

9.3 Overall Test Status:
This test **PASSED** the criterion above for test PL-2 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.
This test **PASSED** the criterion above for test PL-2 for the UNIX execution because the output files were checked by the diff command with the PC generated output files and they were the same with the exception of the date/time stamp.

Test result from machine tpa agree to within 1% with spreadsheet calculations.







Output files from machine spock checked against output files from machine tpa.

DRIFTFAIL.ECH
```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 13:34:53 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 07:25:45 2006
```

DRIFTFAIL.INP
```
2c2
< DATE/TIMEThu Apr  6 13:35:07 2006
---
> DATE/TIMETue Apr 04 07:25:58 2006
```

DRIFTFAIL.RLT
```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 13:34:53 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 07:25:45 2006
```

Test 4e Results (PASS/FAIL): **PASS**

Test 4f. Trapezoidal drift heights, vertical pressures, and equivalent diameters are calculated correctly with seismic and non-seismic degradation.

The validation drift heights, vertical pressures and equivalent diameters calculations for the trapezoid shaped degraded drift which occurs by seismic and thermal degradation was evaluated by TPA SCR610 P-4. The conditions and results of SCR610 P-4 are presented to show that the objectives of this test have been successfully tested. The following is a copy of the text and plots from SCR610 P-4.

PL-4. Verify drift height, vertical pressures, and equivalent diameters for the trapezoidal failure mechanism (Degradation and Seismicity)

1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR610\testresults\pl4

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod1

4.0 Special Input Files or Modifications to Input Files Required
4.1 Modify tpa.inp in accordance with the following table:

Parameter	**Value**
`OutputMode(0=None,1=All,2=UserDefined)`	1
`StopAtSubarea`	1
`MaximumTime[yr]`	1.0e5
`DriftDegradationMethodSelectionValue`	Uniform 0.8, 1.0

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used
6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test
None

8.0 Test Description
8.1 Objective: This test is designed to verify that the drift height, vertical pressures, and equivalent diameters generated by the standalone module agree with values generated by spreadsheet calculations.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.inp, driftfail.ech, driftfail.rlt

8.5 Procedure:

1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: "tpa > pl4.out."

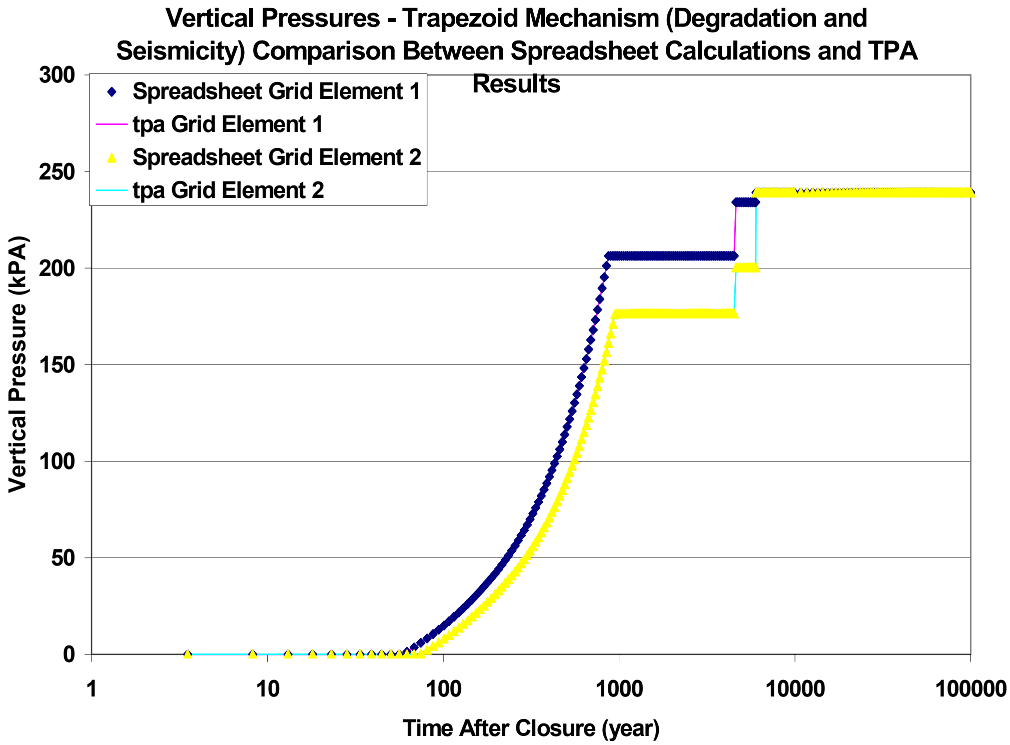
3. Compare the values generated to driftfail.rlt to spreadsheet calculations.

8.6 Pass/Fail Criteria: The drift height versus time values, the vertical pressure versus time values, and the equivalent diameters generated by the DRIFTFAIL module agree with spreadsheet calculations to within 1%.

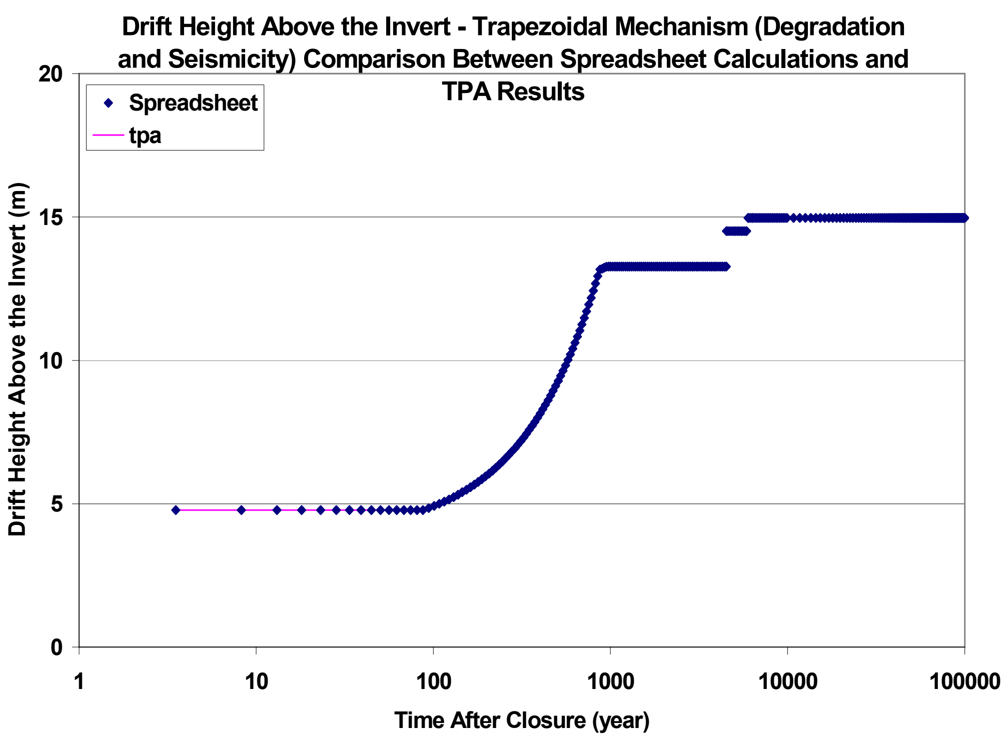
9.0 Test Results
9.1 Output and Supporting Files: Files are archived to a CD labeled, "TPA SCR #610."

9.2 Criterion 1: Code generated and spreadsheet calculations agree to within 1%.

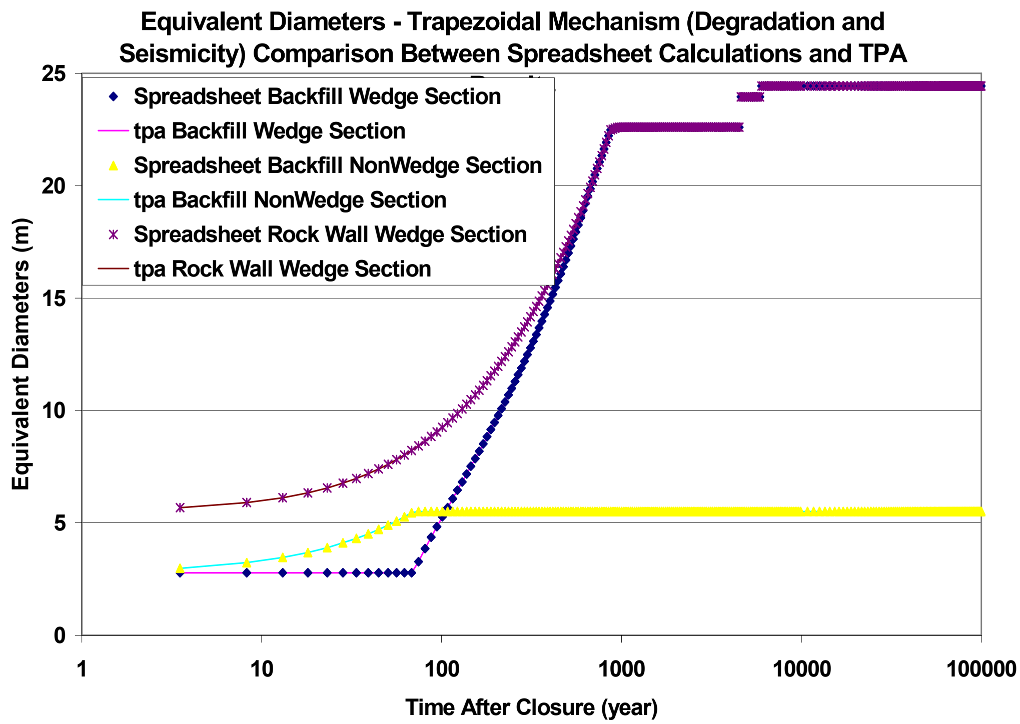
9.3 Overall Test Status:
This test **PASSED** the criterion above for test PL-4 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.
This test **PASSED** the criterion above for test PL-4 for the UNIX execution because the output files were checked by the diff command with the PC generated output files and they were the same with the exception of the date/time stamp.
Test result from machine tpa agree to within 1% with spreadsheet calculations.



Vertical Pressures - Trapezoid Mechanism (Degradation and Seismicity) Comparison Between Spreadsheet Calculations and TPA Results
Spreadsheet Grid Element 1
tpa Grid Element 1
Spreadsheet Grid Element 2
tpa Grid Element 2
Vertical Pressure (kPA)
300
250
200
150
100
50
0
1
10
100
1000
10000
100000
Time After Closure (year)



Drift Height Above the Invert - Trapezoidal Mechanism (Degradation and Seismicity) Comparison Between Spreadsheet Calculations and TPA Results
Spreadsheet
tpa
Drift Height Above the Invert (m)
20
15
10
5
0
1
10
100
1000
10000
100000
Time After Closure (year)


Equivalent Diameters - Trapezoidal Mechanism (Degradation and Seismicity) Comparison Between Spreadsheet Calculations and TPA Results
Spreadsheet Backfill Wedge Section
tpa Backfill Wedge Section
Spreadsheet Backfill NonWedge Section
tpa Backfill NonWedge Section
Spreadsheet Rock Wall Wedge Section
tpa Rock Wall Wedge Section
Equivalent Diameters (m)
Time After Closure (year)
0
5
10
15
20
25
1
10
100
1000
10000
100000

Output files from machine spock checked against output files from machine tpa.

DRIFTFAIL.ECH
```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 14:14:10 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 10:09:59 2006
```

DRIFTFAIL.INP
```
2c2
< DATE/TIMEThu Apr  6 14:14:23 2006
---
> DATE/TIMETue Apr 04 10:10:12 2006
```

DRIFTFAIL.RLT
```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 14:14:10 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 10:09:59 2006
```

Test 4f Results (PASS/FAIL): **PASS**

Test 4g. **Trapezoid drift heights, vertical pressures, and equivalent diameters are calculated correctly for early seismic events.**

The validation drift heights, vertical pressures and equivalent diameters calculations for the trapezoid shaped degraded drift which occurs by early seismic events was evaluated by TPA SCR610 P-6. The conditions and results of SCR610 P-6 are presented to show that the objectives of this test have been successfully tested. The following is a copy of the text and plots from SCR610 P-6.

PL-6. Verify drift height, vertical pressures, and equivalent diameters for the trapezoidal failure mechanism (Degradation and Seismicity with Early Seismic Event)
1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod
<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR610\testresults\pl6

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod

4.0 Special Input Files or Modifications to Input Files Required
4.1 Modify driftfail.inp from PL-4 as follows:

Add a seismic event at time 450 years in driftfail.inp which is prior to the time for full drift degradation to be reached.
Set the bulking factor for grid element 1 to 1.19 and for grid element 2 to 1.21.

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used
6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test
None

8.0 Test Description
8.1 Objective: This test is designed to verify that the drift height, vertical pressures, and equivalent diameters generated by the standalone module agree with values generated by spreadsheet calculations.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.inp, driftfail.dat

8.5 Procedure:
1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: “driftfail > pl6.out.”

3. Compare the values generated to driftfail.dat to spreadsheet calculations.

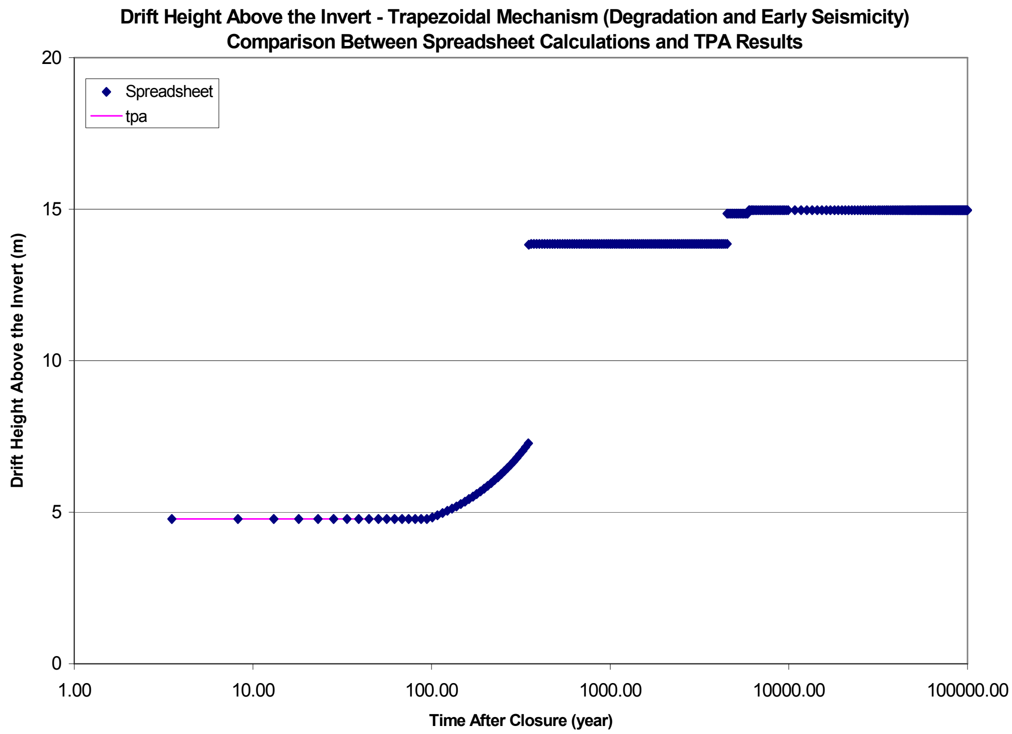
8.6 Pass/Fail Criteria: The drift height versus time values, the vertical pressure versus time values, and the equivalent diameters generated by the DRIFTFAIL module agree with spreadsheet calculations to within 1%.

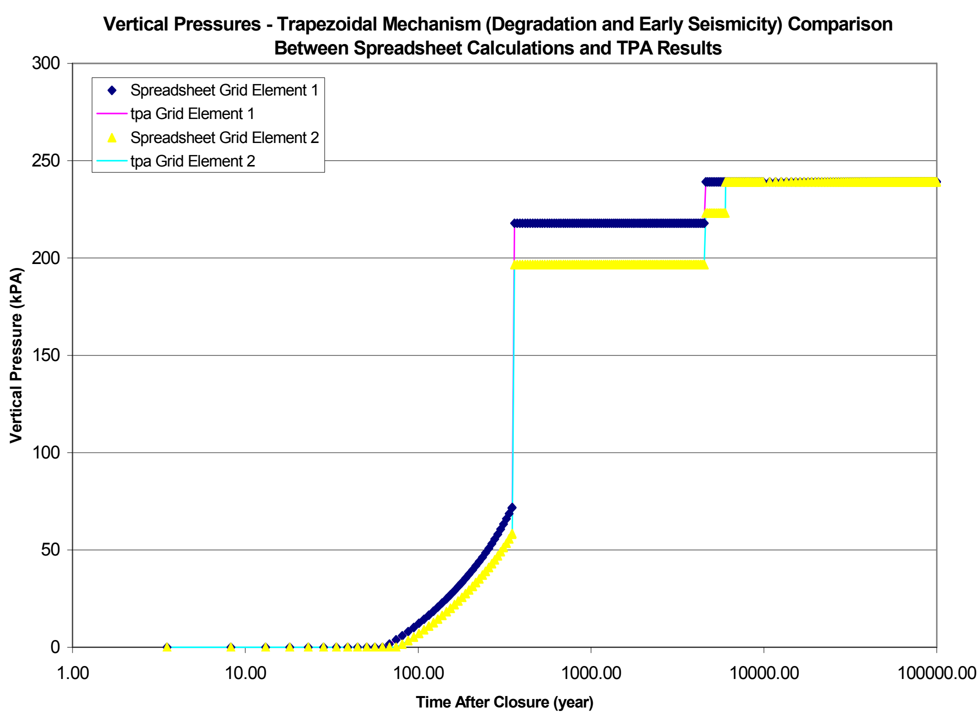
9.0 Test Results
9.1 Output and Supporting Files: Files are archived to a CD labeled, “TPA SCR #610.”

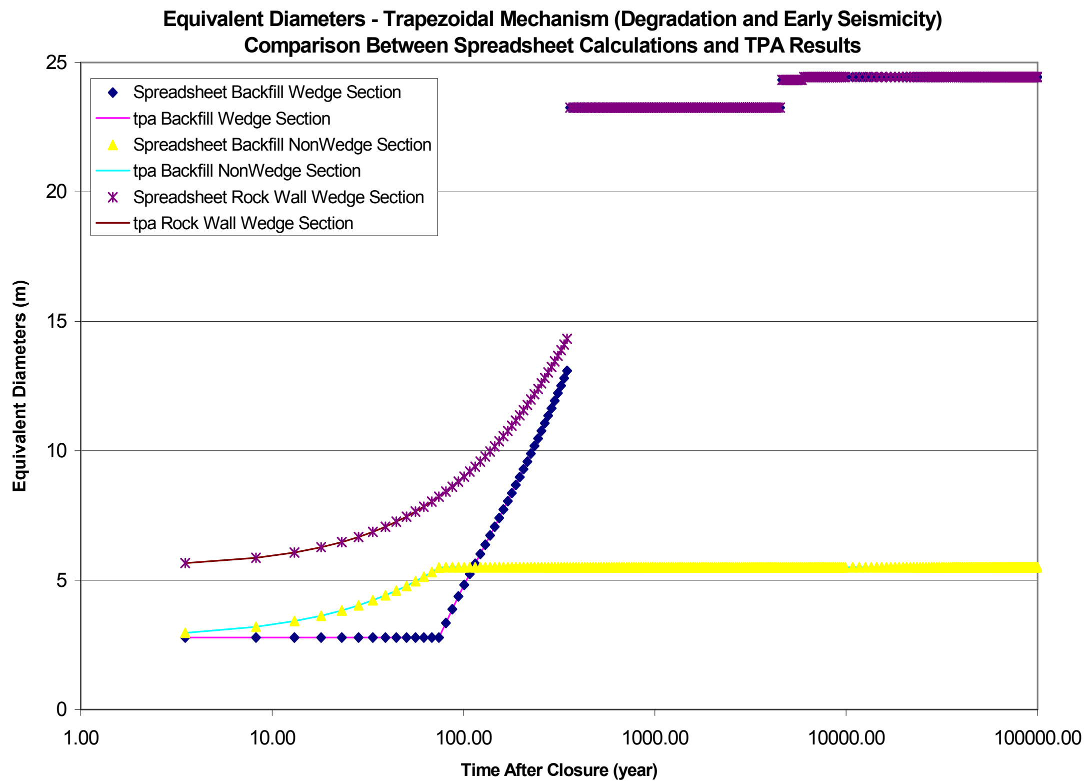
9.2 Criterion 1: Code generated and spreadsheet calculations agree to within 1%.

9.3 Overall Test Status:
This test **PASSED** the criterion above for test PL-6 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.
This test **PASSED** the criterion above for test PL-6 for the UNIX execution because the output files were checked by the diff command with the PC generated output files and they were the same with the exception of the date/time stamp and the headings in the driftfail.dat file. Even though the heading changed in driftfail.dat, the internal values were the same.

Test result from machine tpa agree to within 1% with spreadsheet calculations.







Output files from machine spock checked against output files from machine tpa.

DRIFTFAIL.DAT

```
2c2
< DATE/Time: Thu Apr  6 14:49:20 2006
---
> DATE/Time: Tue Apr 04 14:38:33 2006
8c8
< : Time          Frac       Press1       Press2          eqRWA
eqRWB        eqBFA        eqBFB       height
---
> : Time           Frac      Press1 kPa    Press2 kPa          eqRWA
eqRWB         eqBFA         eqBFB        height
```

DRIFTFAIL.INP

```
2c2
< DATE/TIMEThu Apr  6 14:14:23 2006
---
> DATE/TIMETue Apr 04 10:10:12 2006
```

Test 4g Results (PASS/FAIL): **PASS**

Test 4h. Trapezoidal drift heights, vertical pressures, and equivalent diameters are calculated correctly with seismic degradation only.

The validation drift heights, vertical pressures and equivalent diameters calculations for the trapezoid shaped degraded drift which occurs by seismic degradation (only) was evaluated by TPA SCR610 P-8. The conditions and results of SCR610 P-8 are presented to show that the objectives of this test have been successfully tested. The following is a copy of the text and plots from SCR610 P-8.

PL-8. Verify drift height, vertical pressures, and equivalent diameters for the trapezoidal failure mechanism (Seismic Only)

1.0 Path for Run Directory
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod2
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod2
<<Run Directory>> = $TPA_TEST\test

2.0 Path for Archived Results
\SCR610\testresults\pl8

3.0 Environment Variables
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod2
$TPA_TEST and $TPA_DATA = \SCR610\tpa502qmod2

4.0 Special Input Files or Modifications to Input Files Required
4.1 Modify driftfail.inp from PL-4 as follows:
Add a seismic event at time 450 years in driftfail.inp which is prior to the time for full drift degradation to be reached.
Set the bulking factor for grid element 1 to 1.19 and for grid element 2 to 1.21.
Turn the drift degradation flag off.

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used
6.1 No change is required for input files.

7.0 Utility Scripts Needed to Perform the Test
None

8.0 Test Description
8.1 Objective: This test is designed to verify that the drift height, vertical pressures, and equivalent diameters generated by the standalone module agree with values generated by spreadsheet calculations.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.inp, driftfail.dat

8.5 Procedure:

1. Set the environment variables in accordance with Section 3.0.

2. At the command prompt from the <<Run Directory>>, type the following: "driftfail > pl8.out."

3. Compare the values generated to driftfail.dat to spreadsheet calculations.

8.6 Pass/Fail Criteria: The drift height versus time values, the vertical pressure versus time values, and the equivalent diameters generated by the DRIFTFAIL module agree with spreadsheet calculations to within 1%.

9.0 Test Results

9.1 Output and Supporting Files: Files are archived to a CD labeled, "TPA SCR #610."

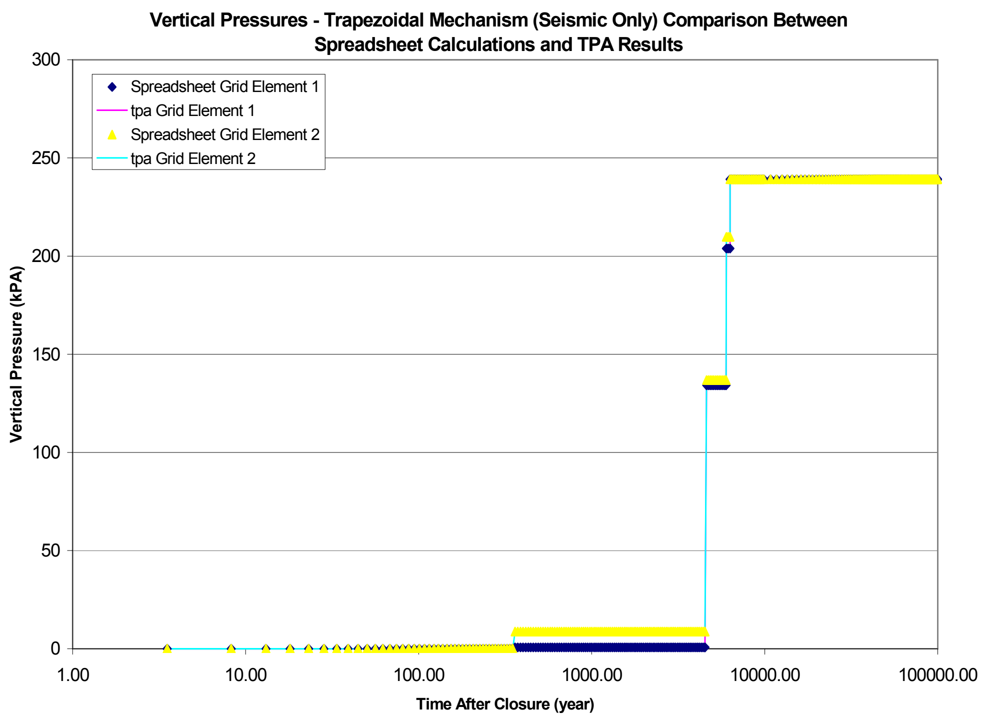
9.2 Criterion 1: Code generated and spreadsheet calculations agree to within 1%.

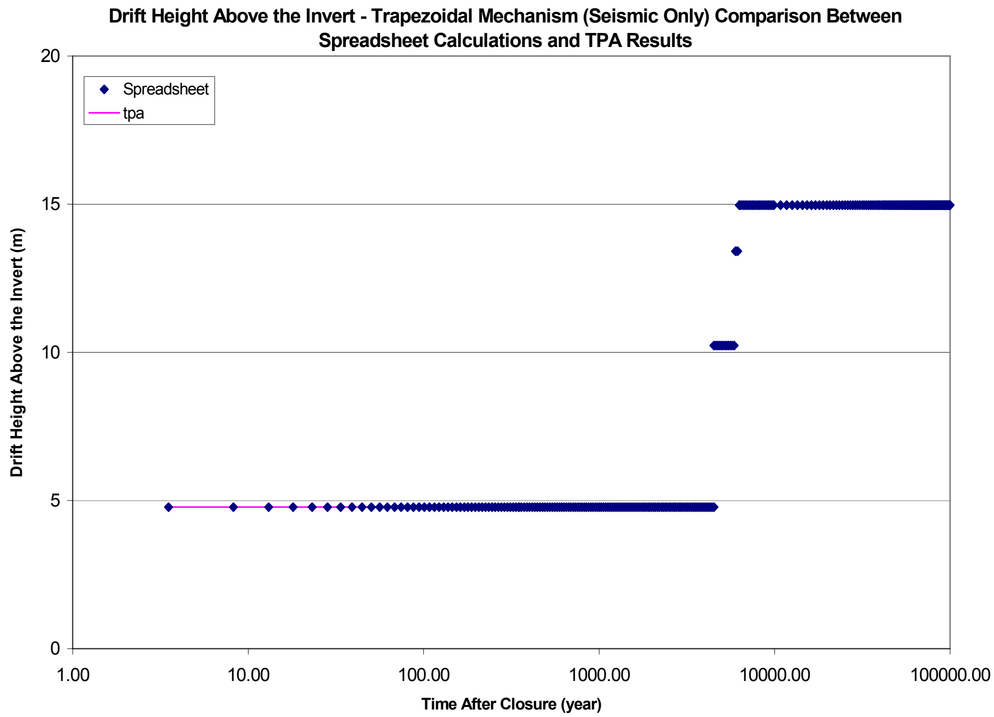
9.3 Overall Test Status:

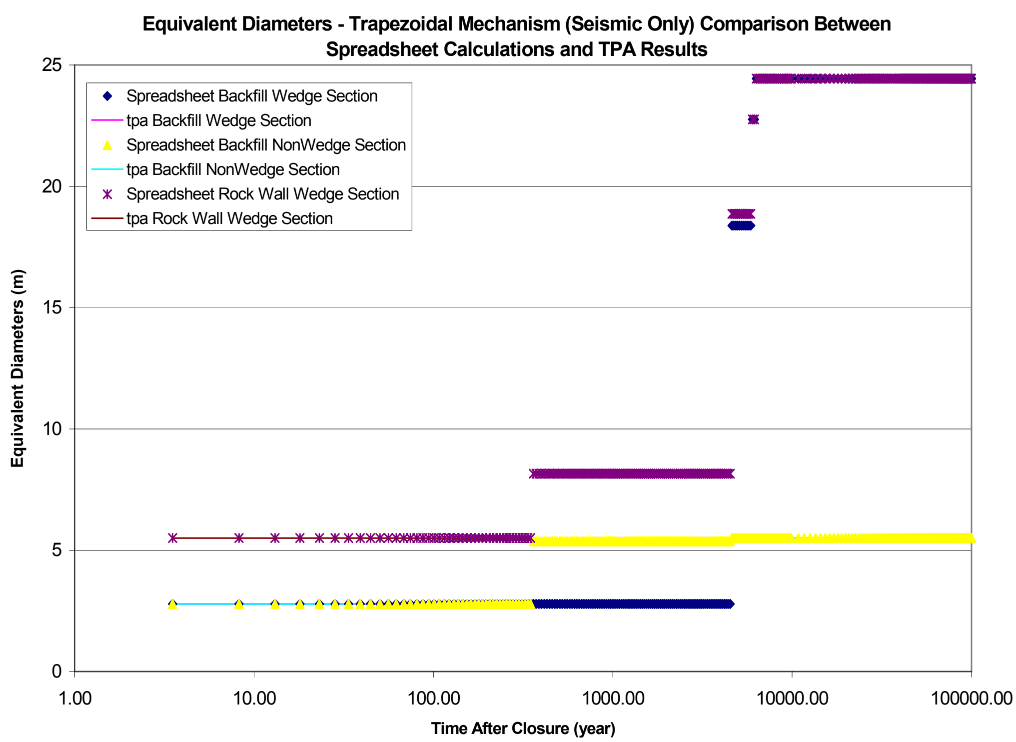
This test **PASSED** the criterion above for test PL-8 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

This test **PASSED** the criterion above for test PL-8 for the UNIX execution because the output files were checked by the diff command with the PC generated output files and they were the same with the exception of the date/time stamp.

Test result from machine tpa agree to within 1% with spreadsheet calculations.







Output files from machine spock checked against output files from machine tpa.

DRIFTFAIL.DAT

```
2c2
< DATE/Time: Thu Apr  6 15:33:24 2006
---
> DATE/Time: Thu Apr 06 10:22:30 2006
```

DRIFTFAIL.INP

```
2c2
< DATE/TIMEThu Apr  6 14:14:23 2006
---
> DATE/TIMETue Apr 04 10:10:12 2006
```

Test 4h Results (PASS/FAIL): **PASS**

Test 5. Sesimically induced mechanical failure do not occur prior to repository closure.

Version of TPA code

Test case : tpa51betaT

Path for run directory:

Test case : Manta: D\ValidationTPA\SVR6\test5

Environment variable:

Test case : TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Path for archive of results

Test case : [CD: Folder titled P7]=\Validation_test\SVR6\test5

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

The reference case was run for 500 realizations of 10kys, for subarea 1, with the append option set to append files 4.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify that seismically induced mechanical failures do not occur prior to repository closure.

Assumptions: None, other than those made within the TPA code.

Constraints None

Test Procedure:

1. Execute 500 realizations of the reference case for 10ky, for subarea 1.
2. Examine the data files *driftfail.ech* and *driftfail.rlt*

Pass/Fail criteria:

1. Seismic events which occur prior to repository closure should result in no drift degradation.

Test results:

An examination of the append file *driftfail.ech* shows that of the 500 realizations four realizations had seismic events within the pre-closure period; realizations 103, 120, 301, and 487. For each of these events the MAFE, PGV, PGA and CF are all recorded as having values of zero.

The following is a excerpt from SVR5\test5*driftfail.ech* shows the results for realization 103. The first event at a time of 80.6 yrs has a value of 0.0 for all of its characteristics.

```
****************************************************************************
                    103 !! Realization

!! ALL SUBAREAS

!! SECTION: Number of Seismic Events

                        3  !! Number of seismic events


!! SECTION: Seismic events descriptive data
!!        This section contains data describing seismic events
!!        Descriptive data includes the following items
!!        The time of the seismic event (yr)
!!        The Mean Annual Probability of Exceedance (MAPE)
!!        The Peak Ground Velocity (PGV) of the event (m/sec)
!!        The Peak Ground Acceleration (PGA) of the event (g)

           Time[yr]          MAPE        PGV[m/s]        PGA[g]            CF
    1    8.06538E+01    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    2    1.77244E+02    8.46744E-05    5.11904E-01    2.50850E-01    1.97466E-01
    3    8.32744E+03    1.69147E-05    9.17606E-01    1.93585E+00    1.46390E-01
****************************************************************************
```

An examination of the append file *driftfail.rlt* shows that for the realizations which had seismic events prior to repository closure no drift degradation occurred.

The following excerpt from SVR6\test5*driftfail.rlt* shows the results for realization 103. The first event is at time 80.6 yrs, while no drift degradation occurs and the drift height remains constant.

SVR7\test3*driftfail.rlt*

```
***********************************************************************
    TIME      Avg Drift
              Height Above
              Invert
    (yr)      (m)
     0.00E+00         4.78E+00
     2.31E+00         4.78E+00
     4.67E+00         4.78E+00
```

7.09E+00	4.78E+00
9.57E+00	4.78E+00
1.21E+01	4.78E+00
1.47E+01	4.78E+00
1.74E+01	4.78E+00
2.01E+01	4.78E+00
2.28E+01	4.78E+00
2.57E+01	4.78E+00
2.86E+01	4.78E+00
3.16E+01	4.78E+00
3.46E+01	4.78E+00
3.78E+01	4.78E+00
4.09E+01	4.78E+00
4.42E+01	4.78E+00
4.76E+01	4.78E+00
5.10E+01	4.78E+00
5.45E+01	4.78E+00
5.81E+01	4.78E+00
6.17E+01	4.78E+00
6.55E+01	4.78E+00
6.93E+01	4.78E+00
7.33E+01	4.78E+00
7.73E+01	4.78E+00
8.14E+01	4.78E+00
8.56E+01	4.78E+00
9.00E+01	4.78E+00
9.44E+01	4.78E+00
9.89E+01	4.78E+00

****

These results show that the objectives of this test have been successfully tested.

Test Results (PASS/FAIL): **PASS**

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: **20.06002.01.354**
Software Name: **TPA**	Version: **TPA51BetaT**
Test ID: **P-7**	Test Series Name: **Mechanical Failure of Drip Shields and Waste Packages**

Test Method

- ■ code inspection
- ■ output inspection
- □ hand calculation
- ■ spreadsheet
- ■ graphical
- □ comparison with external code results

Test Objective: See Attachment A : TPA Version 5.1 Software Validation Task P-7 Objectives, Assumptions, Planned Tests

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): WindowsXP (SP2)

Input Data (files, data base, mode settings): See Attachment A TPA Version 5.1 Software Validation Task P-7 Objectives, Assumptions, Planned Tests

Assumptions, constraints, and/or scope of test:

See Attachment A: TPA Version 5.1 Software Validation Task P-7 Objectives, Assumptions, Planned Tests

Test Procedure: See Attachment A: TPA Version 5.1 Software Validation Task P-7 Objectives, Assumptions, Planned Tests

Test Results

Location: See attached CD labeled "TPA Version 5.1 Validation Task P-7

Test Criterion and Analysis of Results:
See Attachment B : TPA5.1 Software Validation Task P-7 Test Results

Test Evaluation (Pass/Fail): **PASS**

Notes:

Tester: J. Mancillas	Date: 4/25/2007

Attachment A

TPA Version 5.1 Software Validation Task P-7
Objectives, Assumptions, Planned Tests

The following describes the objectives, assumptions, and planned tests for Task P-7 of the TPA Version 5.1 code Software Validation. Test results, including descriptions of deviations from the planned tests, are described in Attachment B of Task P-7.

OBJECTIVES
TPA Version 5.1 Software Validation Task P-7 verifies the process level calculations performed by the TPA module MECHFAIL. Tests performed in Task P-7 are the following:

1. Ensure that the input data provided to the *mechfail.f* code by *mechdrive.f* is correctly interpreted.
2. Seismic frequency and magnitude distributions are correctly generated and correlated to peak ground velocities, peak ground accelerations, and compaction factors.
3. Seismically induced mechanical failure does not occur prior to repository closure.
4. Verify the calculation of drip shield vertical load carrying capacity, including the effects of corrosion, temperature and creep in accordance with Drip Shield- Waste Package Mechanical Interaction Report by L. Ibarra et al, 2007. This test will also verify the waste package capacity calculations which account for corrosion effects. These calculations will be verified under static and dynamic loading conditions.
5. The number of calculated waste packages failures within 10,000 and 100,000 years are consistent with failure trends determined by independent calculations.
6. Waste mechanical package failures cease to occur after the drip shield fails by corrosion, due to the lack of a drip shield-waste package interaction.
7. Test the ability to deactivate temperature and creep effects on drip shield calculations.

ASSUMPTIONS
For the purposes of this validation test, it is assumed:

- The input parameters and their distributions supplied by *tpa.inp* are consistent with the abstractions of the modeled processes.
- Previous validation testing of this module and testing of subsequent SCRs affecting this module have been properly performed, and may be used as confirmation of TPA code performance.

TESTS
The following planned tests sequentially address the objectives of validation task P-7. During the validation testing the validation teams may modify the planned tests or conduct additional testing, to be documented in Attachment B of Task P-7, as necessary to understand and verify software performance related to the MECHFAIL module.

1. Execute the TPA code for a single reference case realization of 10,000 years for one

subarea, appending all files. Compare the files *mechfail_ds.inp* and *mechfail_wp.inp*, which contain the barrier time dependent values; thickness, temperatures, and vertical pressures, with the following data files: *driftfail.rlt* (vertical pressures), *gencorrfail.out* (WP thickness), *dsfail.rlt* (DS thickness), and *nfenv.rlt* (DS temperature).

2. Execute the TPA code for three reference case realizations of 10,000 years for one subarea. By un-commenting out and using a print statement in the subroutine SAMPLEHAZARDCURVE (line 1835), the TPA code will be modified to print out all seismic events and their properties. This will result in the reporting of 30,000 seismic events which can be statistically evaluated (Note: 10,000 seismic events are evaluated for each realization. Typically only the first few events which occur during a simulation are used.). Examining the seismic data an analysis of the distribution of seismic properties will be performed and compared to values cited in Ibarra et. al., 2007.

3. Execute the TPA code for 500 realizations of the reference case for one subarea, with the append option set to 4, to append *driftfail.ech*. After completion of the simulations, examine *driftfail.ech*. This file contains data for all the seismic events which were generated. Events which occurred before closure (100 years) should have Mean Anual frequencey of Exceedance (MAFE), Peak Ground Acceleration (PGA), Peak Ground Velocity (PGV) and Compaction Factor (CF) values of zero. (Note it is expected that of the 500 realizations, only 5 events will occur before closure).

4. After the evaluation of test #1, the files *mechfail_ds.inp* and *mechfail_wp.inp* will be copied into separate directories. A copy of the file *mechfail.exe* will also be placed into each of those directories. In the files *mechfail_ds.inp* and *mechfail_wp.inp* the debug flag will be turned on and the *mechfail.exe* code will be executed in a standalone manner. The screen output of time dependent load and capacity data will be captured and compared against MS Excel calculations of DS and WP capacity. Static and dynamic loading scenarios will be evaluated.

5. Execute the TPA code for 100 reference cases of one million year simulation times with the append option selected to 7, to append the file *ebsrel.rlt*. An examination of the *ebsrel.rlt* file will indicate the number of waste packages mechanically failed. The fraction failed should as the time increases from 10,000 to 100,000 years. The increase in failure fraction should increase by roughly an order of magnitude, because of the number of seismic events which occur in 100,000 years should be about 10 times the number which occurs in 10,000 years. Performing an off line calculation using GoldSim the fraction of mechanical failures should be determined and compared to the TPA results.

6. Execute the TPA code for 20 reference case realizations of 100ky simulation times, with the append option selected to All. The drip shield corrosion rate will be changed to a value of 2.98e-5 m/yr. This results in a dripshield corrosion failure at 503 yr. An examination of the failure times recorded in *ebsrel.rlt* will be compared with the time of drip shield corrosion failure times in *dsfail.rlt*. The comparison of these results should show that waste package mechanical failures do not occur after drip shield corrosion failure.

7. Execute the TPA code reference case for subarea one with the parameters

CalculateTemperatureMultiplierFlag(yes=1,no=0) and CalculateCreepMultiplierFlag(yes=1,no=0) both set to 1 (one) and 0 (zero). Then compare the results of the *mechfail_ds.dat* to hand calculations to verify the proper calculation of drip shield capacity without the inclusion of temperature and creep effects.

Attachment B

TPA 5.1 Software Validation Task P-7 Test Results

Following are test results for the validation test cases described in Attachment A for TPA Version 5.1 code Software Validation Task P-7. Additional details related to test procedures are also provided.

Test 1. **Ensure the input data provided to the *mechfail.f* code by *mechdrive.f* is correctly interpreted.**

Version of TPA code

Test case : tpa51betaT

Path for run directory:

Test case : Manta: D\ValidationTPA\SVR7\test1

Environment variable:

Test case : TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Path for archive of results

Test case : [CD: Folder titled P7]=\Validation_test\SVR7\test1

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

Test1 will be run for one realization of 10,000 years, for subarea 1, with the file output option set to append all.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Ensure the input data provide to the *mechfail.f* code by *mechdrive.f* is correctly interpreted.

Assumptions: None, other than those made within the TPA code.

Constraints None

Output files to compare or examine: *mechfail_ds.inp*, *mechfail_wp.inp* and *driftfail.rlt*, *gencorrfail.out*, *dsfail.rlt*, *nfenv.rlt* *mechfail_ds.def* and *mechfail_wp.def*, and *tpa.inp*

Test Procedure:

1. Execute a single reference case realization of 10,000 years for one subarea
2. Compare the files *mechfail_ds.inp* and *mechfail_wp.inp* with *driftafil.rlt*, *gencorrfail.out*, *dsfail.rlt* and *nfenv.rlt*.

Pass/Fail criteria:

1) The data contained in *mechfail_ds.inp* should be consistent with the data contained in the files *driftafil.rlt*, *dsfail.rlt* and *nfenv.rlt*.

2)The data contained in *mechfail_wp.inp* should be consistent with the data contained in the files *driftafil.rlt*, *gencorrfail.out* and *nfenv.rlt*.

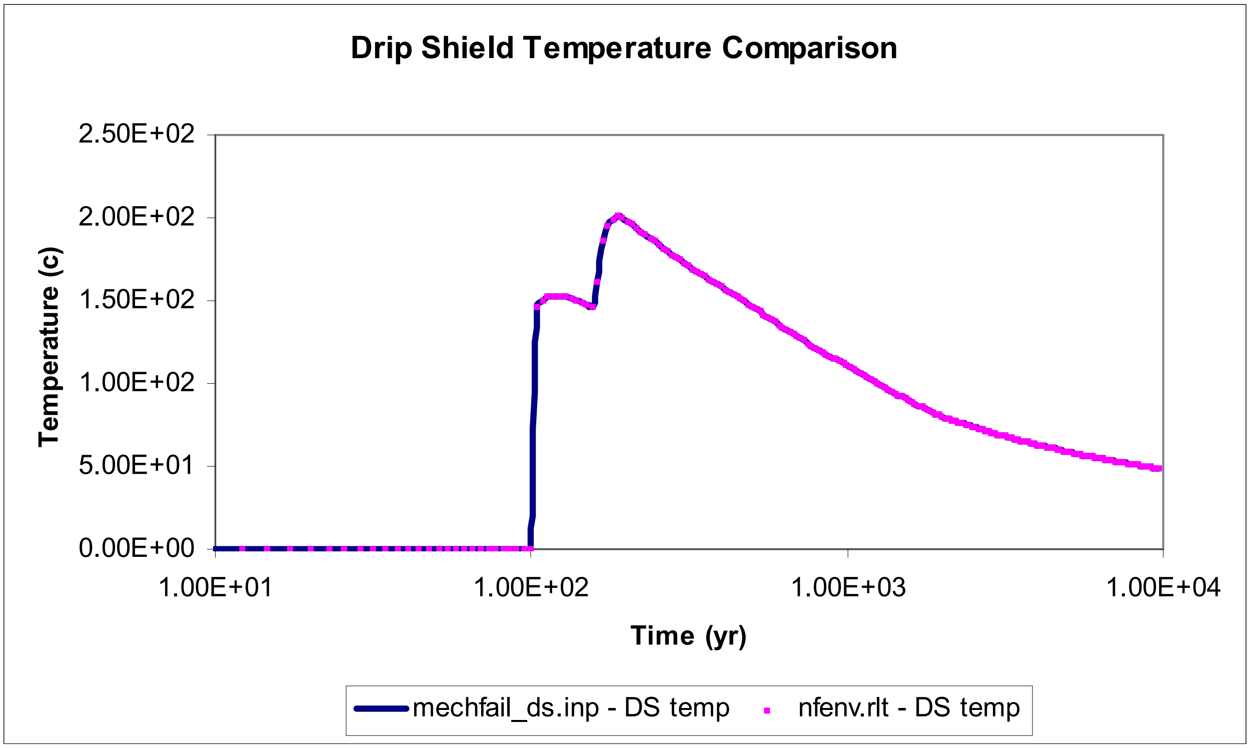
Test results:

The TPA code successfully executed under the testing conditions.

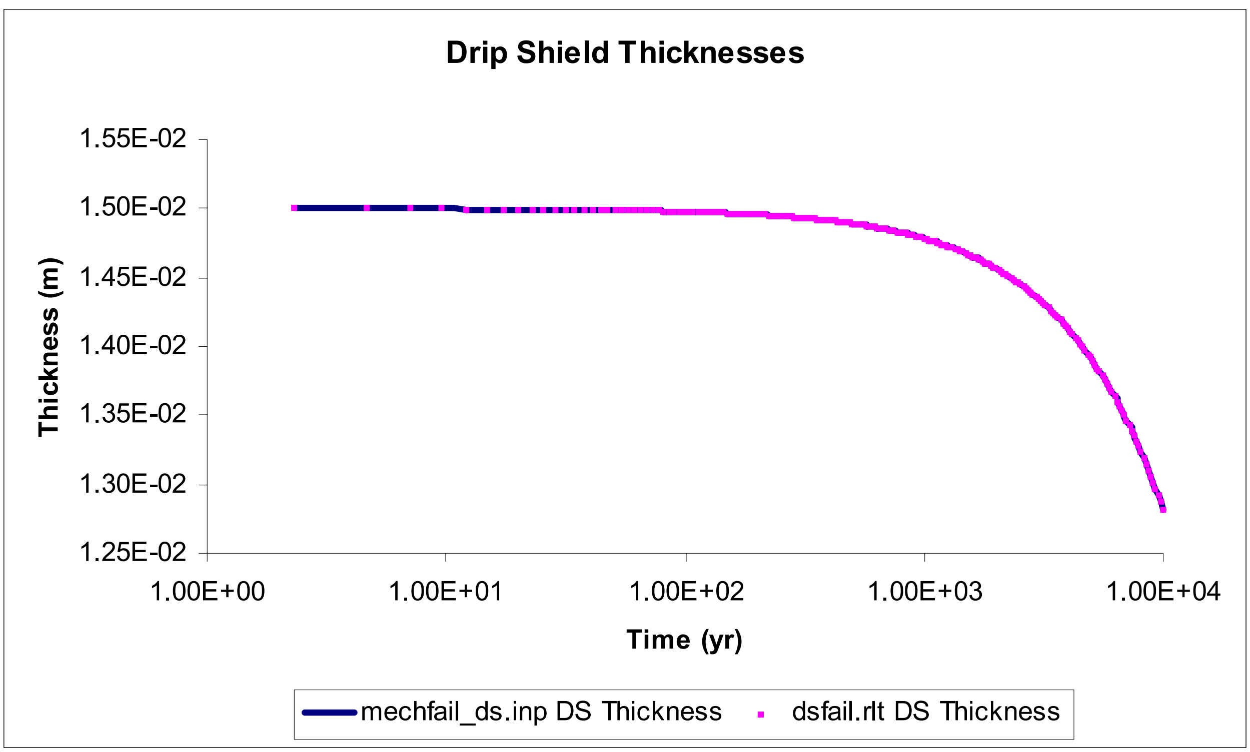
- criterion 1

The following three plots compare the values of drip shield thickness, drip shield temperature and vertical pressures exerted on the drip shield by rock types one and two for values used by *mechfail_ds.inp* and a secondary data file to verify the values.

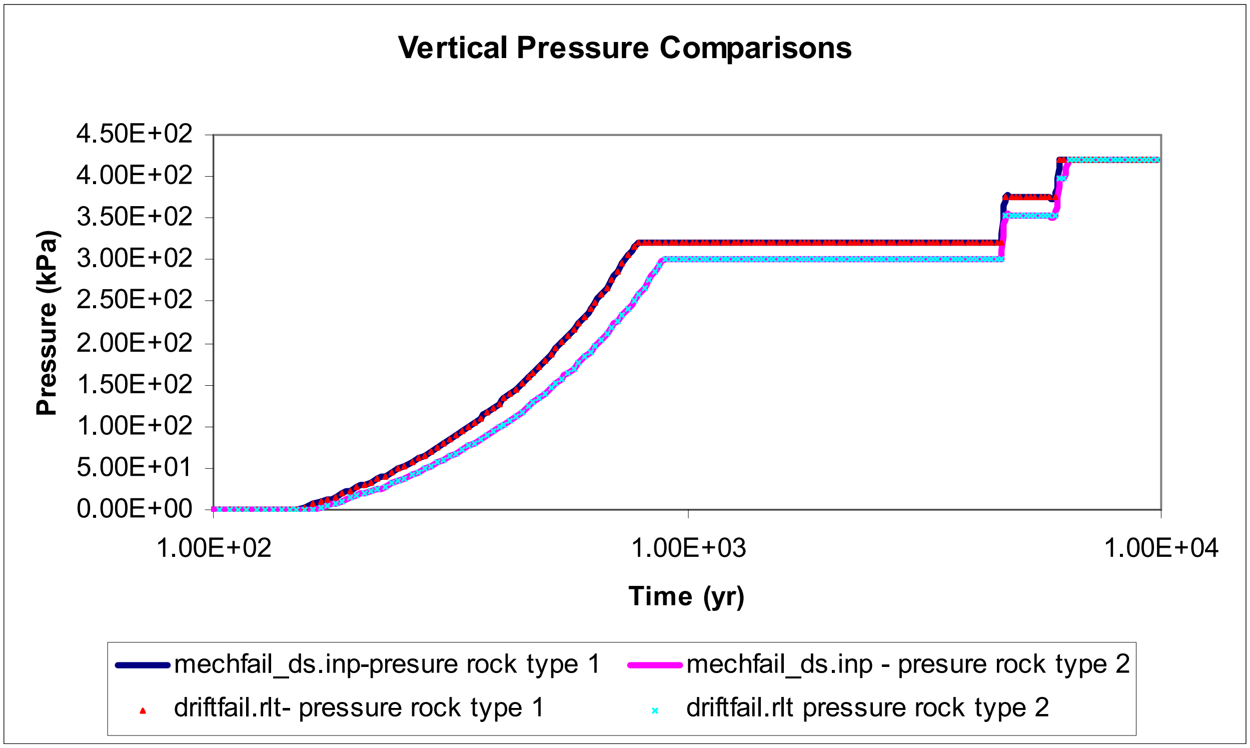
The following plot compares the drip shield temperatures reported in \SVR7\test1\ *mechfail_ds.inp* and SVR7\test1\ *nfenv.rlt*



The following plot compares the drip shield thickness reported in SVR7\test1\ *mechfail_ds.inp* and SVR7\test1*dsfail.rlt*. (Note: Time is plotted on a log scale, and that the drip shield corrosion rate is constant value.)



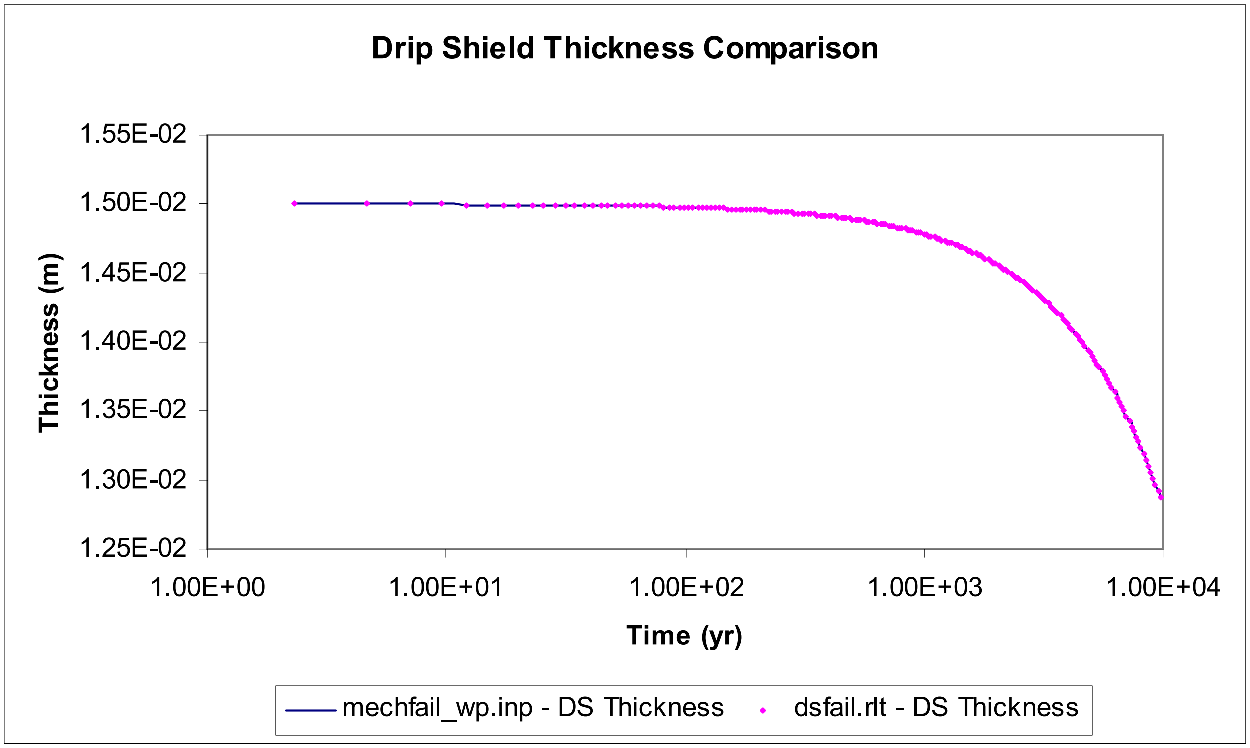
The following plot compares the vertical pressures reported in \SVR7\test1\ *mechfail_ds.inp* and SVR7\test1*driftfail.rlt* for rock type one and two.



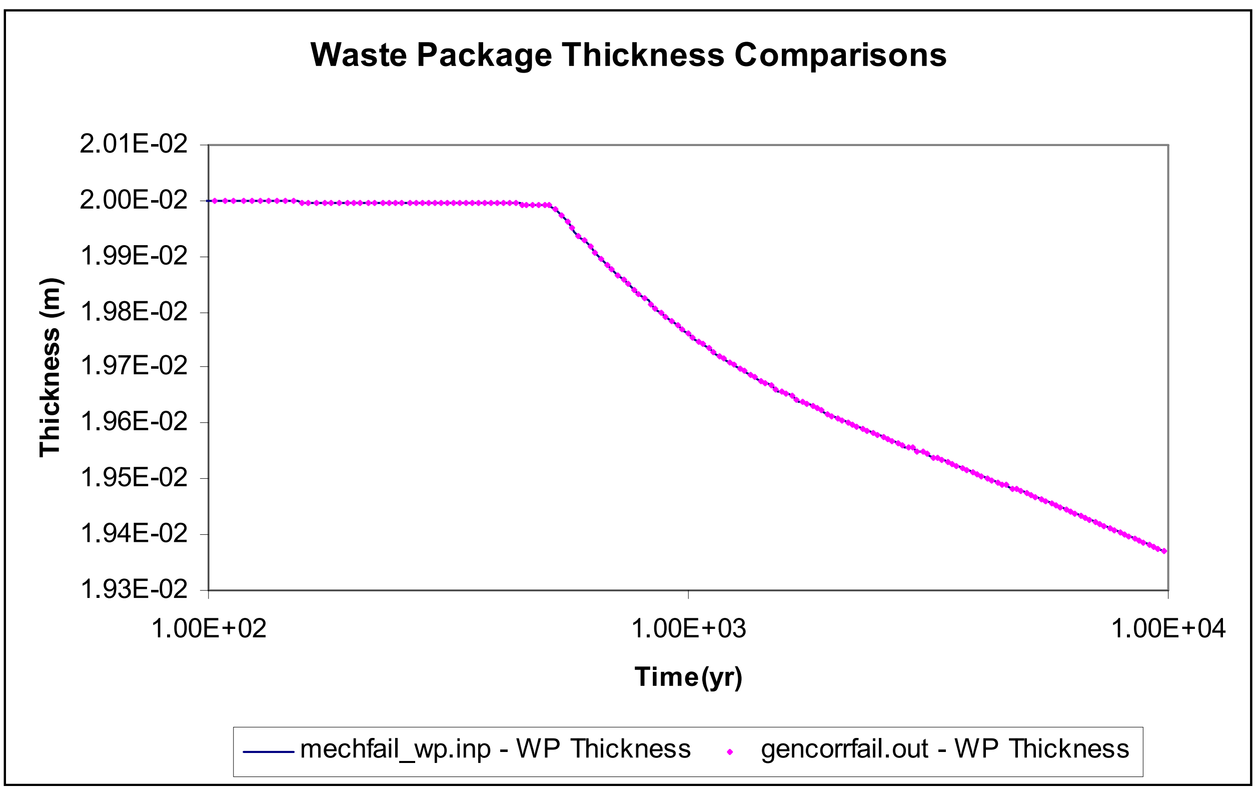
- criterion 2

The following three plots compare the values of drip shield thickness, waste package thickness and vertical pressures exerted on the drip shield by rock types one and two for values used by *mechfail_ws.inp* and a second file to verify the values.

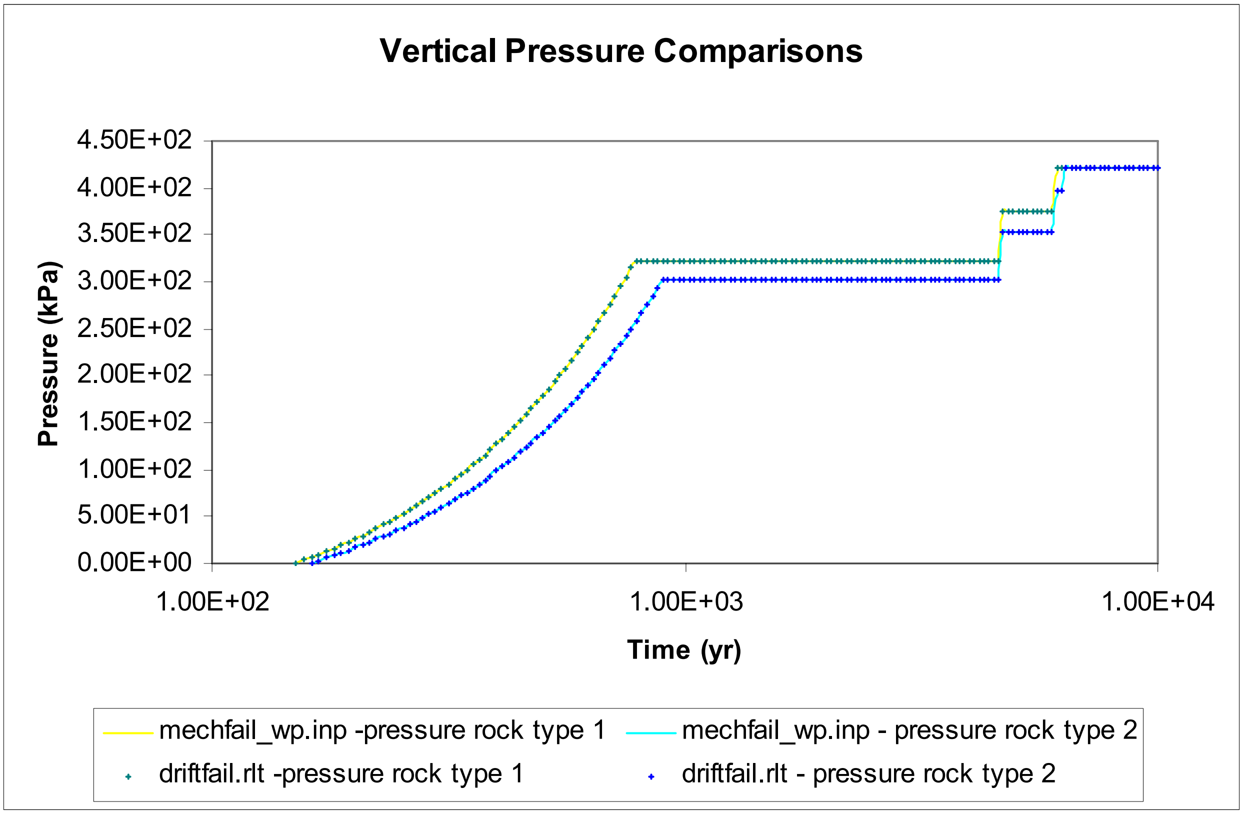
The following plot compares the drip shield thickness reported in SVR7\test1\ *mechfail_ws.inp* and SVR7\test1*dsfail.rlt*.



The following plot compares the waste package thickness reported in SVR7\test1\ *mechfail_wp.inp* and SVR7\test1*gencorrfail.out*, which is the waste package thickness as a result of general corrosion.



The following plot compares the vertical pressures reported in \SVR7\test1\ *mechfail_wp.inp* and SVR7\test1*driftfail.rlt* for rock type one and two.



Other input data including; number of seismic events, time of seismic events, number of time steps, load capacity parameters, have been verified by comparison with other data files (*mechfail_ds.def, mechfail_wp.def, driftfail.inp, driftfail.rlt*, *tpa.inp*).

These result show that the data contained in *mechfail_wp.inp* and *mechfail_ds.inp* are properly interpreted and that the objectives of this test have be successfully evaluated.

The MS Excel worksheet \SVR7\test1\SVR#7_worksheet.xls contains the calculations used to generate the graphs presented in this test.

Test Results (PASS/FAIL): **PASS**

Test 2 Seismic frequency and magnitude distribution area correctly generated.

Version of TPA code

Test case : tpa51betaT

Path for run directory:

Test case : Manta: D\ValidationTPA\SVR7\test2

Environment variable:

Test case : TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Path for archive of results

Test case : [CD: Folder titled P7]=\Validation_test\SVR7\test2

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): reference case

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify the seismic frequency and magnitude distributions are correctly generated and correlated to peak ground velocities, peak ground accelerations and compaction factors.

Assumptions: None, other than those made within the TPA code.

Constraints None

Test Procedure:

1. Modify the TPA code to screen print all the seismic events sampled in each realization
2. Recompile the TPA code with the print statement included.
3. Execute three realizations of the TPA code for subarea 1, for 10,000 years, capturing the screen print (*tpa.exe>screen_capture*).
4. Examine the seismic data for consistency with L. Ibarra et al., 2007.

Pass/Fail criteria:

1. The seismic frequency and magnitude distributions are in agreement with L. Ibarra et al., 2007.
2. The PGV distributions are in agreement with the L. Ibarra et al., 2007.
3. The PGA distributions are in agreement with the L. Ibarra et al., 2007.
4. The CF distributions are in agreement with the L. Ibarra et al., 2007.

Test results:

The TPA code successfully executed under the testing conditions. The code was modified to screen print all the seismic events generated by the seismic sampling subroutine *samplehazardcurve* in the sampler.f module. The following text is an excerpt from that module depicting the print statement.

SVR7\test2\tpa51betaT2\sampler.f

```
************************************************************************
c  test location for printing all seismic events
c  either used or not used
       print*, timeofevents(kkj),dmape(kkj),pgv(kkj),pga(kkj),cf(kkj)
c        print*, dinterpfact
************************************************************************
```

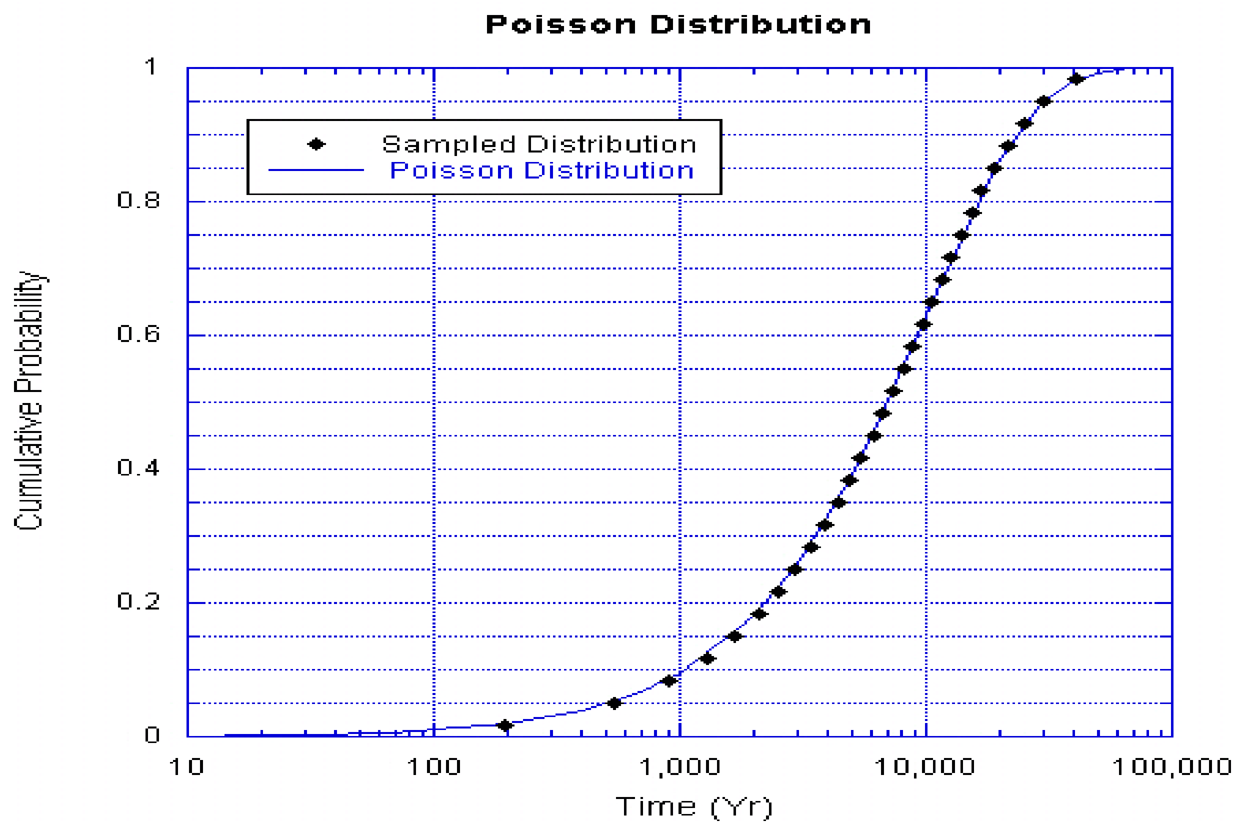
The modified TPA code and executable were save in the directory SVR7\test2\tpa51betaT2.

The data for the following analyses was performed in a MS Excel workbook,

SVR7\test2\ *seismic_analysis.xls*

- criterion 1

An examination of the time distribution and magnitude distribution of the generated seismic events was performed. The cumulative distribution function (CDF) of the inter arrival times of the seismic events was compared to the CDF of a Poisson distribution with a recurrence period of 10,000 years. The sampled distribution matched with the analytic CDF of the Poisson distribution. The following plot shows the correlation between the two, with the square dots depicting the sampled distribution and the solid line showing the analytic CDF of the Poisson distribution. These results agree with the expected values and show that this objective has been successfully tested.



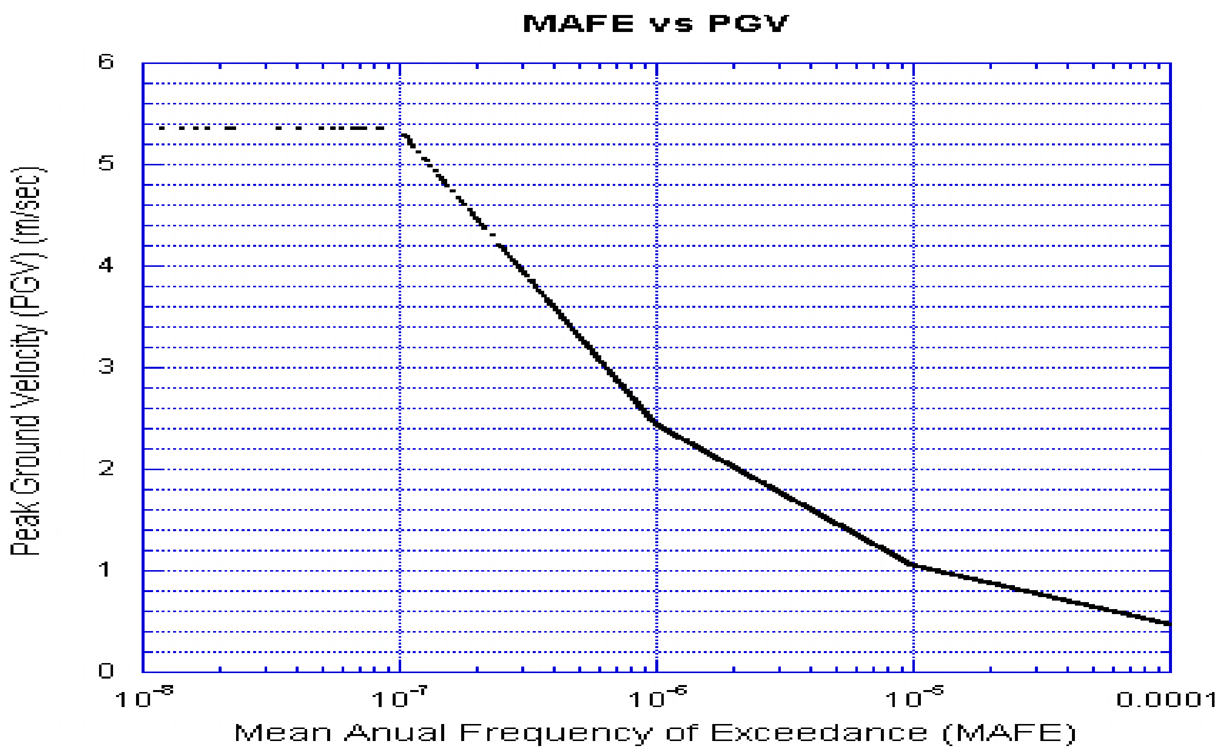
The statistical distribution of seismic event Mean Annual Frequency of Exceedance (MAFE) are described by L. Ibarra et al., 2007. A comparison between the sampled distribution of MAFE values and the distribution described by L Ibarra et al. is shown in Table 2.1. These results agree with the expected values and show that this criterion has been successfully evaluated.

Table 2.1. MAFE Distributions

	L .Ibarra Values	Sampled Values
MAFE<10^{-4}	100.00 %	100.00 %
$10^{-5<}$ MAFE<10^{-4}	90.1 %	90.097 %
$10^{-6<}$ MAFE<10^{-5}	9.2 %	8.913 %
$10^{-7<}$ MAFE<10^{-6}	0.7 %	0.9266 %
MAFE<10^{-7}	0.08 %	0.0633 %

- criterion 2

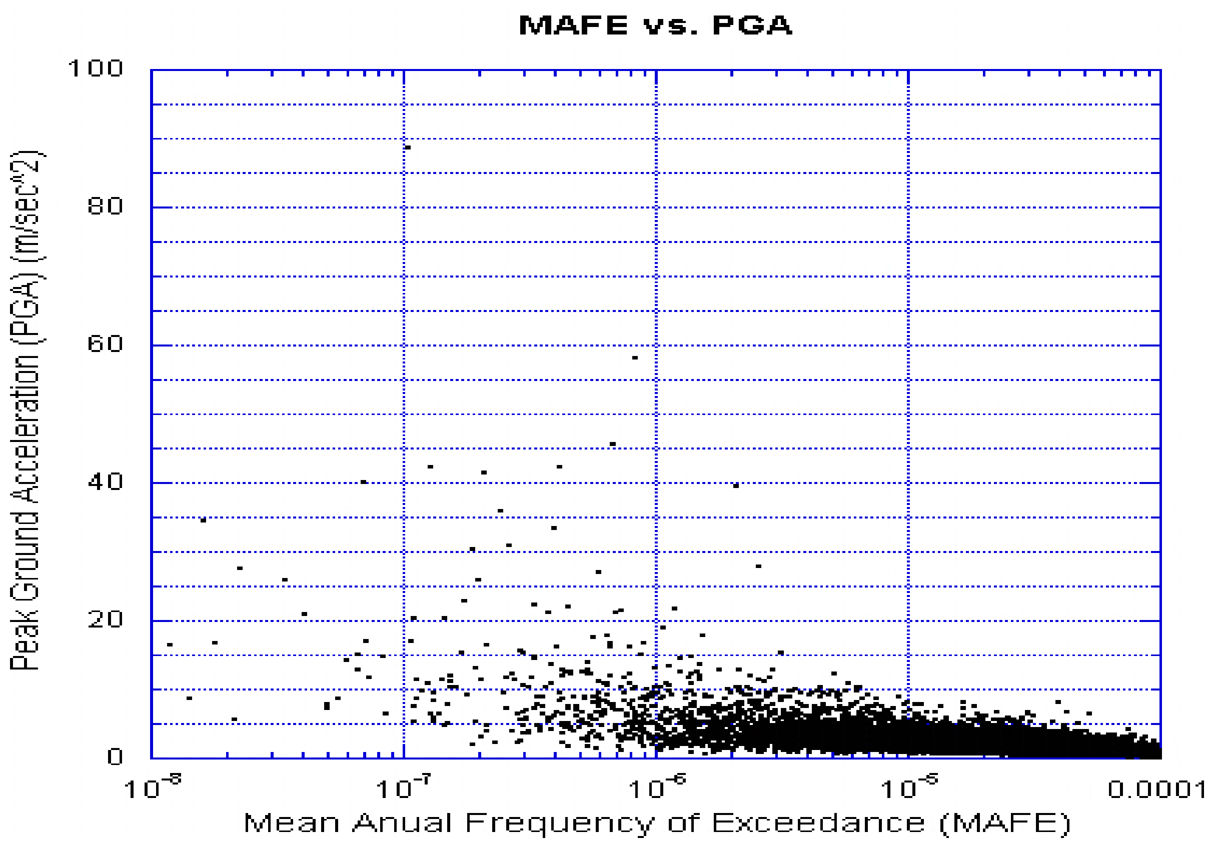
The distribution of Peak Ground Velocity (PGV) for seismic events is described by L. Ibarra et al., 2007, Table 5-1. The PGV is dependent on the MAFE of the seismic event, were the velocity is 0.47, 1.05, 2.44 and 5.35 m/s for -log(MAFE) values of 4, 5, 6 and 7, with the values being interpolated between the defined points. The following plot shows MAFE vs PGV for 30,000 seismic events.



These results are consistent with the expected results and show that this criterion has been successfully evaluated.

-criterion 3

The distribution of Peak Ground Acceleration (PGA) for seismic events is described by L. Ibarra, et al. 2006, Table 5-3. The PGA increases in magnitude as the MAFE of the event decreases. The following plot shows the MAFE vs. PGA for 30,000 seismic events.



These results are consistent with the expected results and show that this criterion has been successfully evaluated.

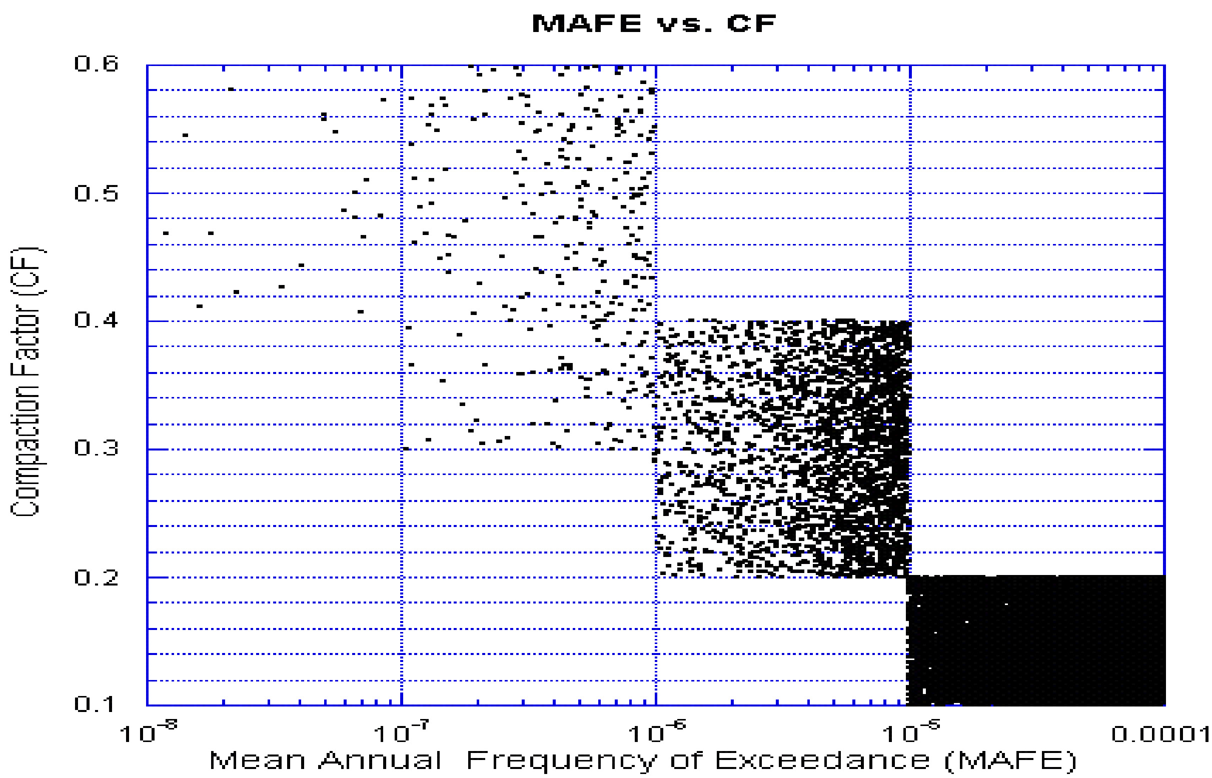
-criterion 4

The distribution of Peak Ground Acceleration (PGA) for seismic events is described by L. Ibarra et al., 2007, Table 5-4. The values are listed here in Table 2.2

Table 2.2 Compaction Factors from L. Ibarra et al., 2007

MAFE	Compaction Factor (CF)
10^{-4}	10-20 %
10^{-5}	20-40 %
10^{-6}	30-60 %
10^{-7}	40-60%

The following plot shows the MAFE vs. CF for 30,000 seismic events.



These results are consistent with the expected results and show that this criterion has been successfully evaluated.

Test Results (PASS/FAIL): **PASS**

Test 3. **Seismically induced mechanical failure does not occur prior to repository closure.**

Version of TPA code

Test case : tpa51betaT

Path for run directory:

Test case : Manta: D\ValidationTPA\SVR7\test3

Environment variable:

Test case : TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT

Path for archive of results

Test case : [CD: Folder titled P7]=\Validation_test\SVR7\test3

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

The reference case was run for 500 realizations of 10,000 years, for subarea 1, with the append option set to append files 4 to append the files *driftfail.ech* and *driftfail.rlt*.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify that seismically induced mechanical failures do not occur prior to repository closure.

Assumptions: None, other than those made within the TPA code.

Constraints None

Test Procedure:

1. Execute 500 realizations of the reference case for 10,000 years, for subarea 1.
2. Examine the data files *driftfail.ech* and *driftfail.rlt*

Pass/Fail criteria:

1. Seismic events which occur prior to repository closure should result in no drift degradation and no drip shield or WP failures occur.

Test results:

An examination of the append file *driftfail.ech* shows that of the 500 realizations four realizations had seismic events within the pre-closure period; realizations 103, 120, 301, and 487. For each of these events the MAFE, PGV, PGA and CF are all recorded as having values of zero.

The following is a excerpt from SVR7\test3*driftfail.ech* shows the results for realization 103. The first event at a time of 80.6 years has a value of 0.0 for all of its characteristics.

```
***************************************************************************
                    103 !! Realization

!! ALL SUBAREAS

!! SECTION: Number of Seismic Events

                        3  !! Number of seismic events


!! SECTION: Seismic events descriptive data
!!         This section contains data describing seismic events
!!         Descriptive data includes the following items
!!         The time of the seismic event (yr)
!!         The Mean Annual Probability of Exceedance (MAPE)
!!         The Peak Ground Velocity (PGV) of the event (m/sec)
!!         The Peak Ground Acceleration (PGA) of the event (g)

          Time[yr]          MAPE        PGV[m/s]          PGA[g]              CF
    1     8.06538E+01    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    2     1.77244E+02    8.46744E-05    5.11904E-01    2.50850E-01    1.97466E-01
    3     8.32744E+03    1.69147E-05    9.17606E-01    1.93585E+00    1.46390E-01
***************************************************************************
```

An examination of the append file *driftfail.rlt* shows that for the realizations which had seismic events prior to repository closure no drift degradation occurred.

The following excerpt from SVR7\test3*driftfail.rlt* shows the results for realization 103.

The first event is at time 80.6 years, has no drift degradation and the drift height remains constant.

SVR7\test3*driftfail.rlt*

```
***********************************************************************
   TIME      Avg Drift
             Height Above
             Invert
   (yr)      (m)
    0.00E+00        4.78E+00
    2.31E+00        4.78E+00
    4.67E+00        4.78E+00
    7.09E+00        4.78E+00
    9.57E+00        4.78E+00
    1.21E+01        4.78E+00
    1.47E+01        4.78E+00
    1.74E+01        4.78E+00
    2.01E+01        4.78E+00
    2.28E+01        4.78E+00
    2.57E+01        4.78E+00
    2.86E+01        4.78E+00
    3.16E+01        4.78E+00
    3.46E+01        4.78E+00
    3.78E+01        4.78E+00
    4.09E+01        4.78E+00
    4.42E+01        4.78E+00
    4.76E+01        4.78E+00
    5.10E+01        4.78E+00
    5.45E+01        4.78E+00
    5.81E+01        4.78E+00
    6.17E+01        4.78E+00
    6.55E+01        4.78E+00
    6.93E+01        4.78E+00
    7.33E+01        4.78E+00
    7.73E+01        4.78E+00
    8.14E+01        4.78E+00
    8.56E+01        4.78E+00
    9.00E+01        4.78E+00
    9.44E+01        4.78E+00
    9.89E+01        4.78E+00
*****************************************************************************
```

The following excerpt from SVR7\test3*mechfail.rlt* shows the results for realization 103.

The first event is at time 80.6 years, no drip shield failure or waste package failure occurs.

****

Step	TPA Time (year)	DS Total Fraction (unitless)	DS Corrosion Fraction (unitless)	DS Static Fraction (unitless)	DS Dynamic Fraction (unitless)	WP Total Fraction (unitless)	WP Static Fraction (unitless)	WP Dynamic Fraction (unitless)
1	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2	2.31016E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
3	4.67440E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4	7.09399E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5	9.57023E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
6	1.21044E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
7	1.46980E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
8	1.73522E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
9	2.00686E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
10	2.28486E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
11	2.56937E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
12	2.86054E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
13	3.15852E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
14	3.46349E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
15	3.77559E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
16	4.09499E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
17	4.42188E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
18	4.75642E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
19	5.09879E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
20	5.44917E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
21	5.80776E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
22	6.17474E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
23	6.55032E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
24	6.93469E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
25	7.32805E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

```
    26   7.73063E+01   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
0.00000E+00   0.00000E+00   0.00000E+00
    27   8.14263E+01   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
0.00000E+00   0.00000E+00   0.00000E+00


    28   8.56428E+01   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
0.00000E+00   0.00000E+00   0.00000E+00
    29   8.99579E+01   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
0.00000E+00   0.00000E+00   0.00000E+00
    30   9.43741E+01   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
0.00000E+00   0.00000E+00   0.00000E+00
    31   9.88937E+01   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
0.00000E+00   0.00000E+00   0.00000E+00
    32   1.03519E+02   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
0.00000E+00   0.00000E+00   0.00000E+00
    33   1.08253E+02   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
0.00000E+00   0.00000E+00   0.00000E+00
*****************************************************************************
```

These results show that no drip shields or waste packages are mechanically failed prior to repository closure.

Test Results (PASS/FAIL): **PASS**

Test 4. Verify drip shield and waste package load capacity calculations.

The objective of this test is to verify the calculation of drip shield load capacity, including the effects of corrosion, temperature and creep in accordance with the L. Ibarra et al., 2006. This test will also verify the waste package capacity calculations which account for corrosion effects. These calculations will be verified under static and dynamic loading conditions.

The current implementation of the MECHFAIL module, in TPA code version 51betaT, originated in TPA SCR609. The MECHFAIL module was implemented in TPA code version TPA502s. Since then this module has been modified by TPA SCRs 627, 659, 660, and 669.

SCR627 corrected the content of an error printing statement, and did not affect the MECHFAIL calculations. SCR659 introduced the ability to negate temperature and creep effects on drip shield vertical load carrying capacity; this does not affect the MECHFAIL calculations under reference case conditions. SCR660 changed the corrosion thickness of the waste package from the localized thickness to the general corrosion thickness. This code change did not alter the MECHFAIL module, it only changed the data submitted to the MECHFAIL module. SCR669 changed the format of data files to increase transparency, this change did not affect any MECHFAIL calculations. Because the MECHFAIL module has been only minimally changed the results testing performed in TPA SCR609 will be used to show that the objectives of this test have been successfully tested.

4a Drip shield static load capacity and failure status calculations.

The verification of drip shield capacity as a function of thickness, temperature, and creep was performed by TPA SCR609 SL-1. This testing involved the comparison of calculations performed in MS Excel with the results of the MECHFAIL module. In addition drip shield mechanical failure time was also verified in this testing. The results of SCR609 SL-1 are presented to show that the objectives of this test have been successfully tested. The following text and plots are excerpted from SCR609 SL-1.

SL-1. Name :Test drip shield and waste package failure flags with no seismic events.

Path for run directory:

Testcase: [TPA]:Public\SCR609\mech_fail\run1

Path for archive of results:

Testcase: SCR609\mech_fail\run1

Archived to CD titled :SCR609 Testing

Environment variables:

Testcase : TPA_DATA=[TPA]:Public\SCR609\tpa502s
TPA_TEST =[TPA]:Public\SCR609\tpa502s

Special input files or modification to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Seismic flag turned off

Utility scripts needed to perform the test: none

Utility codes needed in the analysis of the test data: MS Excel

Test description: The mechfail.f module evaluates the failure status of the dripshield (DS) and waste package outer barrier (WP). The status of the DS and WP is determined by a comparison of the vertical pressure and the capacity of the DS and WP. This test evaluates if the status of the DS and WP is properly evaluated by the mechfail module under static conditions.

-Objective Determine if the status of the DS and WP is properly returned during static conditions

-Assumptions None other than those made within the TPA code

-Constraints None

-Output files to compare or examine mechfail_ds.dat, mechfail_wp.dat debug output file from mechfail module

-Step-by-step test procedure to be used

1) Perform a single subarea realization.

2) save the mechfail_ds.inp and mechfail_wp.inp files into two subdirectories

SCR609\mech_fail\run1\DS_failure

SCR609\mech_fail\run1\WP_failure

3) Place a copy of the stand alone code mecfail.e into each of those directories.

4) The mechfail_ds.inp and mechfail_wp.inp file are then renamed mechfail.inp in their respective directories and the debug flag option is turned on.

5) The mechfail.e is then executed in each directory and the screen output is captured. The screen output is a result of the debug flag being set to on.

6) The DS and WP capacities will then be compared to MS Excel calculations.

7) The DS and WP failure status will then be compared to MS Excel status calculations for comparison.

-pass fail criteria

1) The DS and WP capacities calculated by mechfail.e should be the same as those generated by the MS Excel Worksheet using the same input parameters.

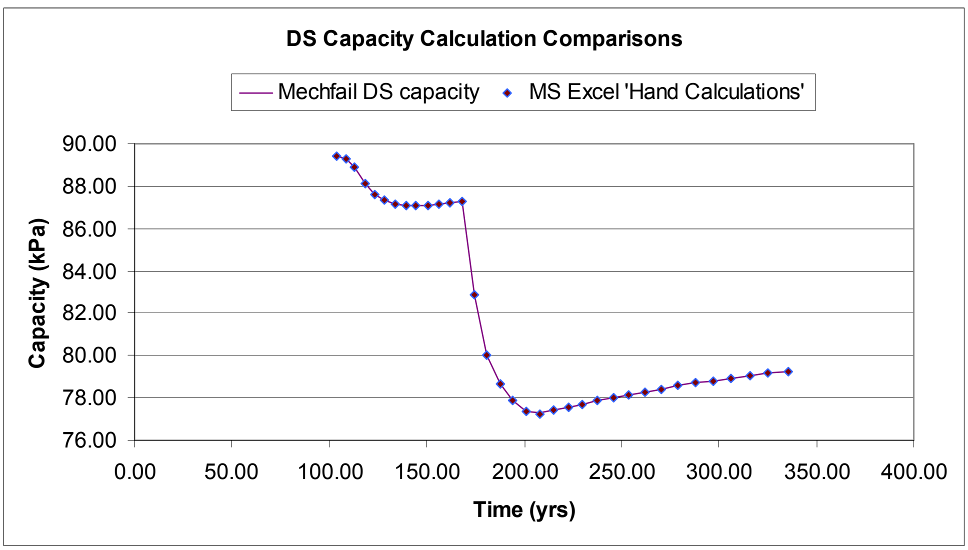
2) The failure status of the DS and WP should be the same as that calculated by the MS Excel Worksheet using the same applied vertical pressures.

Test Results

-criterion 1

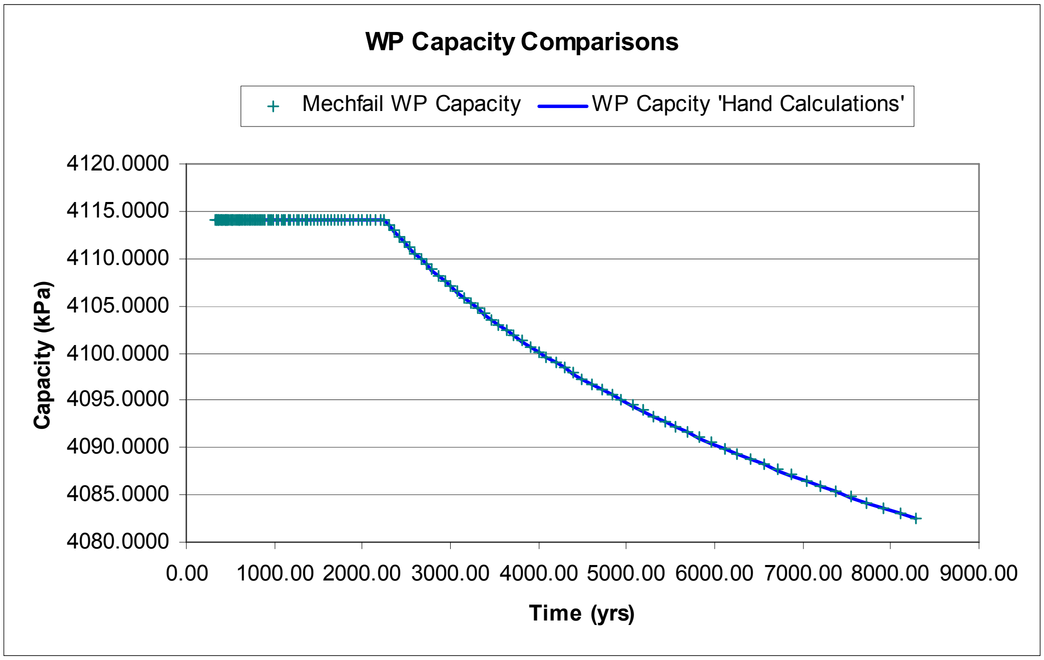
The following plot shows the comparison of DS capacity for rock type one, as determined by the mechfail module to that calculated in the Excel Worksheet titled:

SCR609\mech_fail\run1\DS_failure\DS_failure no Seismic.



The following plot show the comparison of the WP capacity for rock type one as determined by the mechfail module to that calculated by hand using a MS Excel Worksheet titled:

SCR609\mech_fail\run1\WP_failure\WP_failure no Seismic



In both the DS and WP capacities the hand calculations agree with the *mechfail.e* results. In the mechfail module the calculations are repeated for rock type two using the same algorithms, so the testing of the first rock type should be a sufficient test of the capacity calculations. This results are presented to show that criterion 1 of SCR609 has been successfully meet.

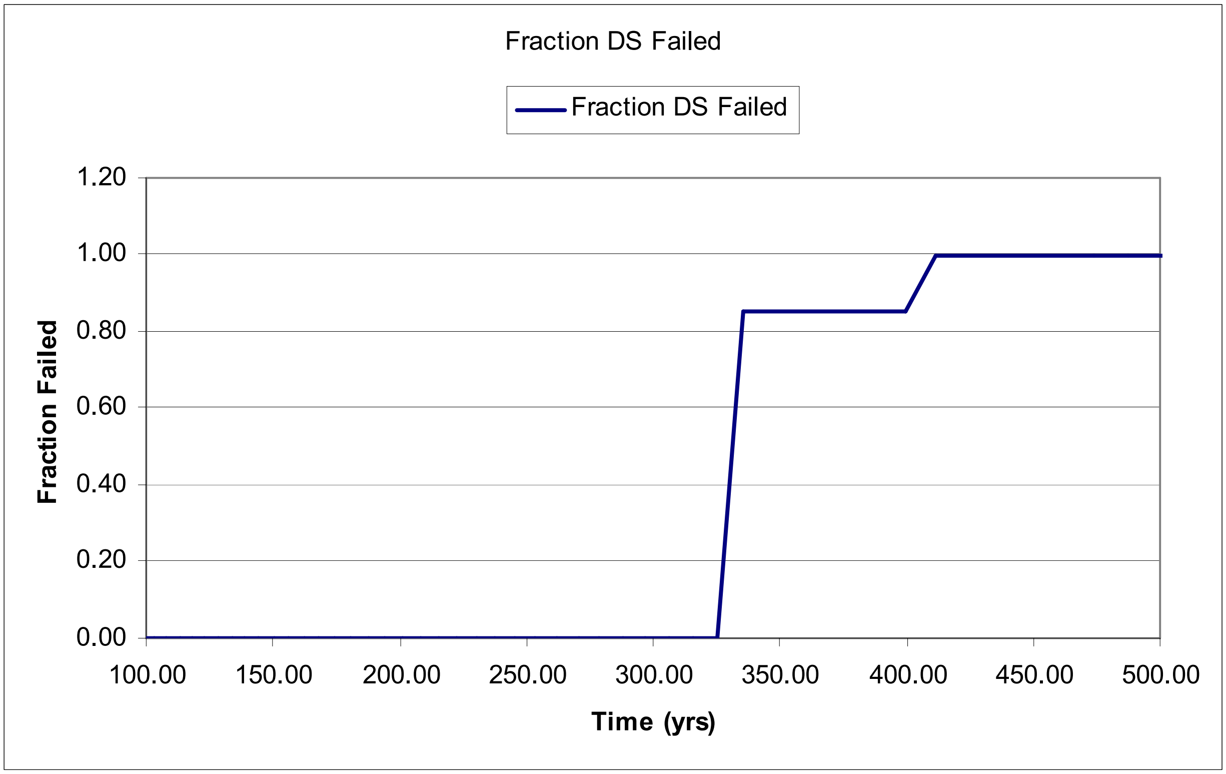
It is pointed out that the WP capacity is determined only for the period from which DS failure occurs to the time at which the DS has been completely corroded away and can no longer interact with the WP. After that time the DS WP interaction no longer exists and can not fail the WP.

-criterion 2

The failure status of the DS and WP s are compared between the mechfail module and hand calculations using MS Excel.

The DS is failed when the vertical pressure on the DS exceeds the DS capacity. The following plot shows the DS capacity and vertical pressures as a function of time.

In this plot the failure of DS 1 occurs at a time of 335 yrs and DS 2 fails at a time of 412 yrs.
The following plot shows the fraction of DS failure as determined by the mechfail module.



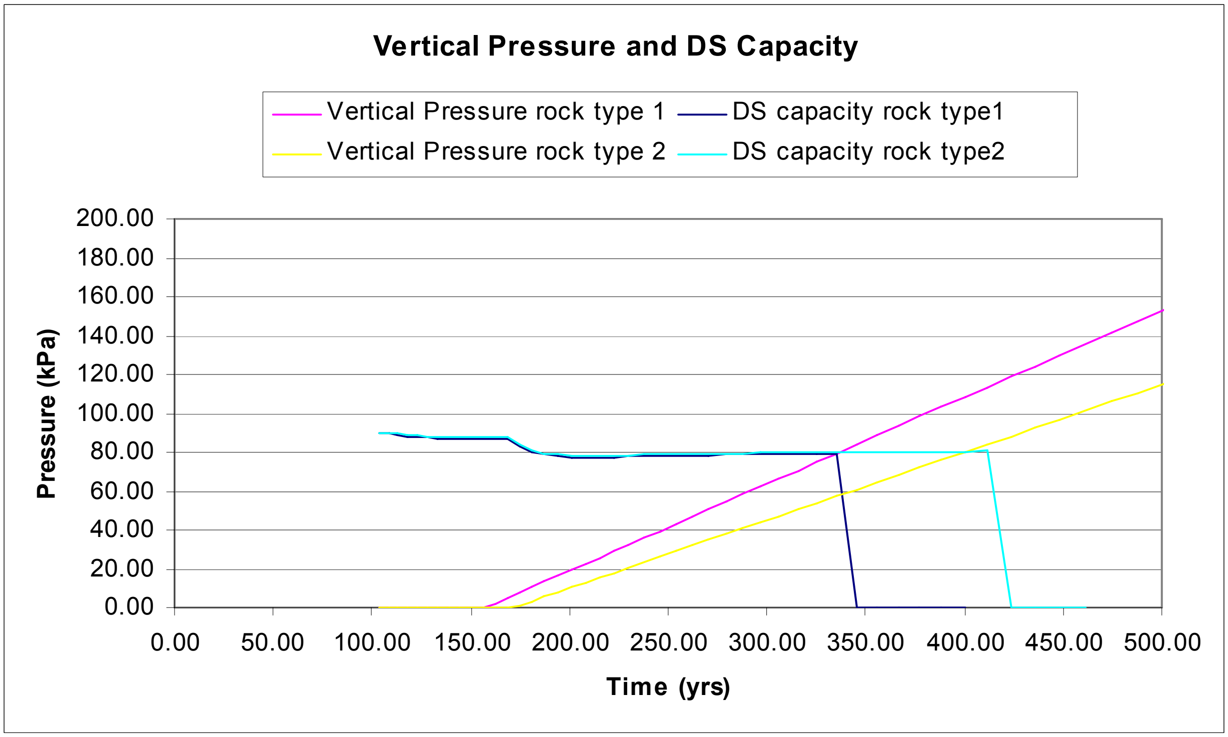
The failure time of the DS as reported by the mechfail module corresponds to the same time as that determined by hand calculations in the MS Excel Worksheet.

SCR609\mech_fail\run1\DS_failure\DS_failure no Seismic.

The failure of the WP under static conditions is not achievable under normal simulation conditions and was not tested. The fraction of WP failed during this testing was returned by the mechfail module as being zero. This is fully consistent with the WP design.

The non failure of the WP as reported by the mechfail module corresponds to that determined by hand calculations in the MS Excel Worksheet.

SCR609\mech_fail\run1\WP_failure\WP_failure no Seismic



The capacities and failure status of the DS and WP are consistent with hand calculations and are presented to show that criterion 2 of SCR609 was successfully meet.

-overall test status: **PASS**

End of excerpt.

Test Results (PASS/FAIL): **PASS**

4b. Waste Package static load capacity and failure status calculations

The verification of waste package capacity as a function of thickness and the evaluation of WP failure status was performed by TPA SCR609 SL-1, which is documented in test 4a.

Test Results (PASS/FAIL): **PASS**

4c. Drip shield dynamic loading and failure status calculation

The verification of drip shield failure under dynamic loading was performed by TPA SCR609 SL-2. This test involved the evaluation of the static loading and the dynamic loading resulting from seismic shaking. The results of SCR609 SL-2 are presented to show that the objectives of this test have been successfully tested. The following text is excerpted from SCR609 SL-2.

SL-2. Name :Test drip shield and waste package failures during seismic events.

Path for run directory:

Testcase: [TPA]:Public\SCR609\mech_fail\run2

Path for archive of results:

Testcase: SCR609\mech_fail\run2

Archived to CD titled :SCR609 Testing

Environment variables:

Testcase : TPA_DATA=[TPA]:Public\SCR609\tpa502s
TPA_TEST =[TPA]:Public\SCR609\tpa502s

Special input files or modification to input files required: None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): Drift degradation flag is disabled

Utility scripts needed to perform the test: none

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

Test description: The DS and WP can fail due to seismic induced pressures in which the ground shaking will magnify the static pressure applied on the DS or WP

-Objective Execute the *mechfail.e* module under conditions which will result in DS and WP failure due to Seismic activity

-Assumptions None other than those contained within the TPA code

-Constraints None

-Output files to compare or examine debug screen capture of the *mechfail.e* module

-Step-by-step test procedure to be used

1) Perform a single subarea realization.

2) save the mechfail_ds.inp and mechfail_wp.inp files into two subdirectories

SCR609\mech_fail\run2\DS_failure

SCR609\mech_fail\run2\WP_failure

3) Place a copy of the stand alone code mecfail.e into each of those directories.

4) The mechfail_ds.inp and mechfail_wp.inp file are then renamed mechfail.inp in their respective directories and the debug flag option is turned on.

5) Modify the mechfail.inp file as necessary to induce a discernable seismically induced failure.

6) The mechfail.e is then executed in each directory and the screen output is captured. The screen output is a result of the debug flag being set to on.

7) The Dynamic vertical pressures generated by the mechfail.e module will then be compared to hand calculated dynamic vertical pressures.

8) The DS and WP failure status will then be compared to MS Excel status calculations for comparison.

-pass fail criteria

1) The dynamic pressure of the seismic events and the status of the DS returned by the *mechfail.e* module should match hand calculations.

2)The dynamic pressure of the seismic events and the status of the WP returned by the *mechfail.e* module should match hand calculations.

Test Results

-criterion 1

To test the DS capacity under seismic conditions the drift degradation flag was deactivated. The TPA code was run for one realization and for one subarea. The mech_fail_ds.inp file was then saved to the directory SCR609\mech_fail\run2\DS_failure\. The sampled parameters were such that the DS failed immediately after a seismic event because of the resultant static load from accumulated rubble. The failure occurred after the first seismic event, but not during the seismic event.

To test for failures during seismic events these files (*mechfail.inp* and *mechfail.e*) were copied to the directory

SCR609\mech_fail\run2\DS_failure\test\.

The mechfail.inp file was then modified to have a static vertical pressure for the first seismic event. The pressure was changed from 0.00 (no rubble) to 50 kPa and the time of the first seismic event was moved to 461.1 yrs

This resulted in a dynamic vertical pressure of (1+.752)*50*1.5=131.4 kPa,(where 1.5 is the dynamic amplification factor and 0.752 is the PGA of the first seismic event, which is greater than the DS capacities for rock types 1 and 2, which were respectively 83.5 and 84.3 kPa.

Under these conditions the mechfail.e module returned the corect Seismic dynamic pressures DS failure times and DS failure cause.

These results are recorded in the files

SCR609\mech_fail\run2\DS_failure\test\mechfail.dat

SCR609\mech_fail\run2\DS_failure\test\out (debug screen capture)

and summarized on an MS Excel Worksheet

SCR609\mech_fail\run2\DS_failure\test\DS_failures Seismic

These results show that SCR609 has been properly implemented.

- Criterion 2

To test the WP capacity under seismic conditions the drift degradation flag was deactivated. The TPA code was run for one realization and for one subarea. The mechfail_ds.inp file was then saved to the directory SCR609\mechfail\run2\WP_failure. Under the sampled conditions the WP did not fail.

To test for failures during seismic events these files (*mechfail.inp* and *mechfail.e*) were copied to the directory SCR609\mech_fail\run2\WP_failure\test\. The *mechfail.inp* file was then modified to have an exaggerated PGA of 7.32 (gs)for the third seismic event (of thirteen). Under these conditions the WP experienced Dynamic pressures of 4378.79 kPa and 4449.63 kPa in grid elements one and two. The WP capacities for both grid elements at the time of the third seismic event were 4093.86 kPa. The mechfail module correctly calculated the dynamic vertical pressures and returned the correct failed status (failed)of the WP at the correct time.

These calculations and results are summarized in the MS Excel Worksheet titled WP_failures Seismic in the directory *SCR609\mech_fail\run2\WP_failure\test\WP_failures Seismic.*

These results show that SCR609 was properly implemented

-overall test status: **PASS**

End of excerpt.

Test Results (PASS/FAIL): **PASS**

4d. Waste Package dynamic loading and failure status calculation

The verification of waste package failure under dynamic loading was performed by TPA SCR609 SL-2. This test involved the evaluation of the static loading and the dynamic loading resulting from seismic shaking. The results of SCR609 SL-2 show that the objectives of this test have been successfully tested. An excerpt of the test results of SCR609 SL-2 are presented in the testing and results of test 4c.

Test Results (PASS/FAIL): **PASS**

Test 5. **Number of mechanical failures increases as the length of the simulation increases**.

Version of TPA code

Test case1 : tpa51betaT

Path for run directory:

Test case 1 : Manta: D\ValidationTPA\SVR7\test5

Environment variable:

Test case : TPA_DATA=..\tpa51betaT

TPA_TEST=..\tpa51betaT

Path for archive of results

Test case : [CD: Folder titled P7]=\Validation_test\SVR7\test5

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

Test1 will be run for 100 realizations of one million years , with the file output option set to append all

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Ensure the TPA code generates a rate of waste packages failure which is consistent with the behavior expected for the abstraction described by L. Ibarra et al., 2007.

Assumptions: None, other than those made within the TPA code.

Constraints None

Test Procedure:

1. Execute 100 realizations of the reference case for one million years

4. Perform an off line calculation to evaluate the waste package failure rate to compare with the values generated by the TPA code results.

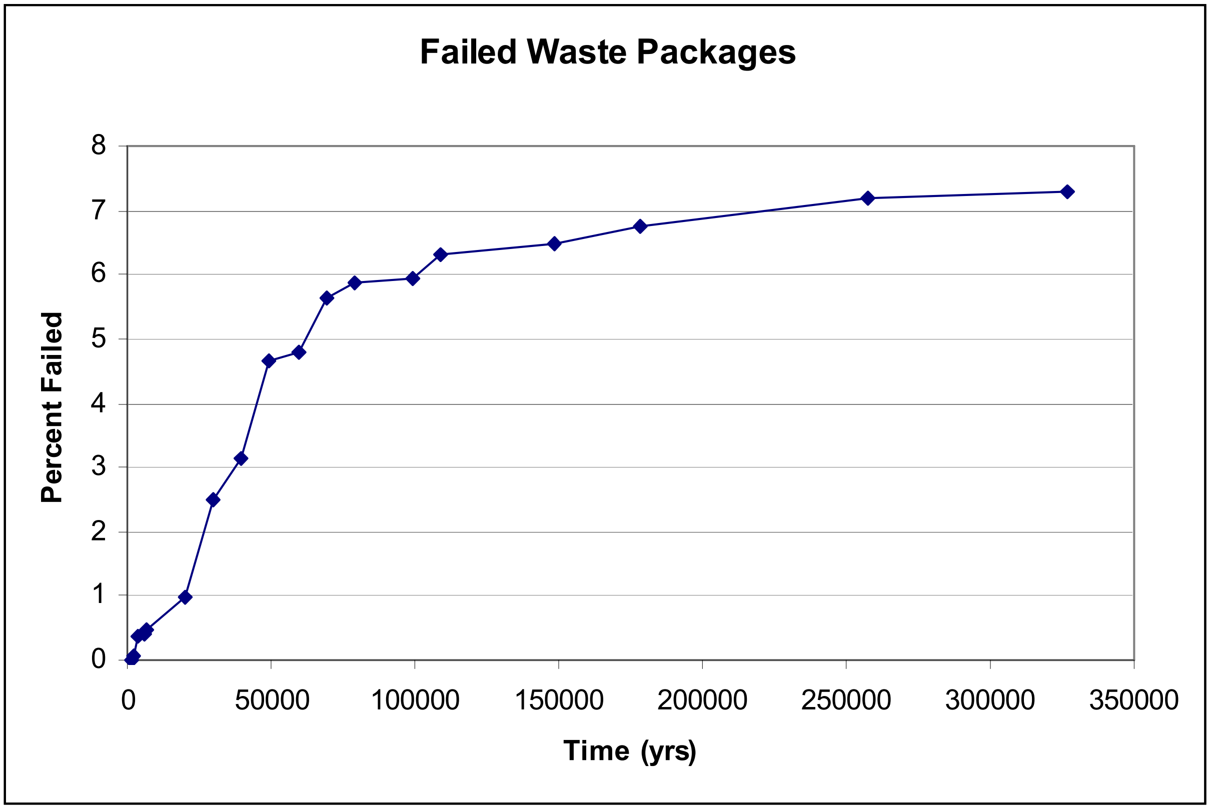
Pass/Fail criteria:

1. The trend of mechanical failure increases as the simulation time increases from 10,000 to 100,000 years. The failure trend then levels off.

Test Results

The TPA code version 51betaT was executed for 100 realizations of one million years. The screen output was captured to the file SVR7\test5*out*. This output was examined for the time distribution of waste package mechanical failures.

The following graph shows the fractional failure of waste packages.



From this plot it is seen that the failure of waste packages increases at a rate of slightly less than 1.0 %/10,000yrs in the first 50,000 years. After that time the rate of failure decreases and the total fraction of failures plateaus after about 300,000 years. Results generated by a simplified mechanical failure analysis performed using GoldSim confirm these results. The GoldSim model, saved in SVR7*Mechfail_simplifed_rlt.gsm,* used seismic distributions of events and magnitudes and mechanical properties for waste package capacity calculations described in the Ibarra 2007 report*,* generated a waste package failure probability of 0.7% in 10,000 years. These results compare well with the results generated by 100 realizations of the TPA code.

The plateau of the WP failures results from the removal of the DS-WP interaction by corrosion failure of the DS. The mean failure time of the DS, by corrosion, occurs at 50,335.57 y, based on the *tpa.inp* drip shield corrosion rate. The DS corrosion rate is described by a log triangular distribution; 2.0e-8, 2.98e-7 and 6.4e-7 m/yr. This corrosion rate distribution results in a maximum lifetime of 750,000 yr for the DS (with a DS thickness of 0.015m). Thus the DS-WP interaction can persist till 750,000 yr.

These results show that the objectives of this test have been successfully tested.

Test Results (PASS/FAIL): **PASS**

Test 6. Waste package failures do not occur after drip shield corrosion failure.

Version of TPA code

Test case1 : tpa51betaT

Path for run directory:

Test case 1 : Manta: D\ValidationTPA\SVR7\test6

Environment variable:

Test case : TPA_DATA=..\tpa51betaT

TPA_TEST=..\tpa51betaT

Path for archive of results

Test case : [CD: Folder titled P7]=\Validation_test\SVR7\test6

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

Test1 will be run for 20 realizations of 100,000 years , with the file output option set to append all, and with the drip shield corrosion rate set to a high value of 2.98e-5 m/y.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify the drip shield waste package interaction does not occur after the drip shield has been failed by corrosion.

Assumptions: None, other than those made within the TPA code.

Constraints None

Test Procedure:

1. Execute the TPA code for 20 realizations for 100,000 years, with the corrosion rate set to 2.98e-5 m/yr.
2. Examine the file *dsfail.rlt*.
3. Examine the file *ebsrel.rlt* and the screen output of the TPA code.
4. Examine *driftfail.ech*.

Pass/Fail criteria:

1. Waste package failures should not occur after the drip shield has failed by corrosion.

Test Results

- criterion 1

An examination of the *dsfail.rlt* file and the TPA screen output shows that under these input conditions the drip shield fails by corrosion at 503 yr. An examination of *ebsrel.rlt* and *wpsfail.rlt* shows that no waste packages were failed in any of the 20 realizations after the drip shield was failed by corrosion. An examination of *driftfail.ech* shows that each realization had on average 10 seismic events, and several events were sufficiently large enough to cause WP failures (specifically in realization 11, event 6 – time= 97,437 yr, MAFE =8.45 e-8, PGA =11.9). These files are saved in the directory [CD]:\SVR7\test6.

These results are consistent with the expected behavior of the drip shield waste package mechanical interaction abstraction. When the DS fails by corrosion very early in the simulation time; no mechanical failures are expected after that time. The very large seismic event in realization 11 would have resulted in mechanical failure if the DS-WP interaction had existed. These results are presented to show that criterion 1 of this test have been successfully meet.

Test Results (PASS/FAIL): **PASS**

Test 7. Test the flags CalculateTemperatureMultiplierFlag(yes=1,no=0) and CalculateCreepMultiplierFlag(yes=1,no=0)

Version of TPA code
Test case : tpa51betaT
Path for run directory:
Test case : Manta: D\ValidationTPA\SVR7\test7
Environment variable:
Test case : TPA_DATA=..\tpa51betaT
TPA_TEST=..\tpa51betaT
Path for archive of results
Test case : [CD: Folder titled P7]=\Validation_test\SVR7\test7
Test case A : [CD: Folder titled P7]=\Validation_test\SVR7\test7a

Test case B : [CD: Folder titled P7]=\Validation_test\SVR7\test7b

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

The flags **CalculateTemperatureMultiplierFlag(yes=1,no=0)** and **CalculateCreepMultiplierFlag(yes=1,no=0)** will be changed from 1 to 0.

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify that the control flags **CalculateTemperatureMultiplierFlag(yes=1,no=0)** and **CalculateCreepMultiplierFlag(yes=1,no=0)** properly function.

Assumptions: None, other than those made within the TPA code.

Constraints None

Test Procedure:

1. Execute a reference case of 10,000 years for subarea 1 in the directory test7.
2. Copy the files *mechfail.exe* and *mechfail_ds.inp* into a directory named test7a.
3. In directory test7a, copy the file *mechfail_dp.inp* to a file named *mechfail.inp*.
4. Modify the *mechfail.inp* file in test7a to generated the debug output.
5. Execute the *mechfail.exe* and capture the screen output (*mechfail.exe>out*) in test7a
6. Perform a second reference case of 10,000 years for subarea 1 in directory test7, altering the control flag values for **CalculateTemperatureMultiplierFlag(yes=1,no=0)** and **CalculateCreepMultiplierFlag(yes=1,no=0)** to both be 0 in the *tpa.inp* file.
7. Copy the files *mechfail.exe* and *mechfail_ds.inp* into a directory named test7b.
8. In directory test7b, copy the file *mechfail_dp.inp* to a file named *mechfail.inp*.
9. Modify the *mechfail.inp* file in test7b to generated the debug output.
10. Execute the *mechfail.exe* and capture the screen output (*mechfail.exe>out*) in test7b.

Pass/Fail criteria:

1. The correct values for the control flags are recorded in the *mechfail.inp* files.
2. The *mechfail.exe* debug output, which records the time dependent values used and generated by the MECHFAIL module, records creep and temperature values which are consistent with the control flags.

Test Results

The TPA code executed successfully under these test conditions.

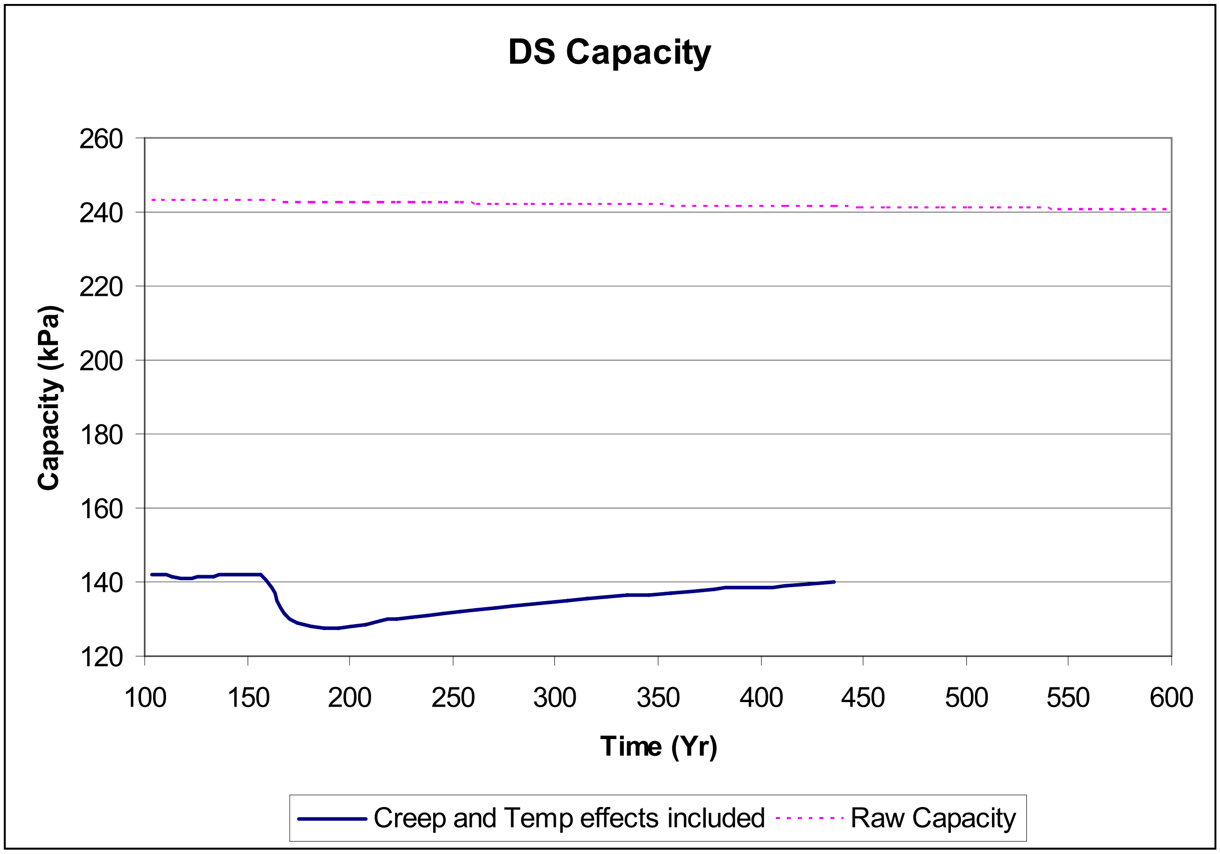
- criterion 1.

The *mechfail.inp* file records the value of the **CalculateTemperatureMultiplierFlag(yes=1,no=0)** and **CalculateCreepMultiplierFlag(yes=1,no=0)** in section four. In directory test7a the values for these flags were both 1. In directory test7b the values for these flags were both 0. These were the expected values based on the tpa.inp input parameters used to generate these input files. These results verifies that the proper values for these control flags are passed to the MECHFAIL module. The results of this test show that the criterion 1 of this test has been successfully met

- criterion 2.

An examination of the debug data generated by the MECHFAIL module shows; i) when both control flags are set to 1, temperature and creep effects are used when determining the capacity of the drip shield, ii) when both the control flags are set to 0, temperature and creep effects are negated when determining the capacity of the drip shield. The debug files SVR7\test7a\out and SVR7\test7b\out are presented to support these conclusions. The results of this test show that criterion 2 of this test has been successfully meet.

The following plot shows the impact of creep and temperature effect of DS vertical load carrying capacity.



Test Results (PASS/FAIL): **PASS**

References : L. Ibarra et al., Drip Shield- Waste Package Mechanical Interaction Report, 2007

Additional Testing 1.

Version of TPA code

Test case : tpa51betaT

Path for run directory:

Test case : Manta: D\ValidationTPA\SVR7\test_add1

Environment variable:

Test case : TPA_DATA=..\tpa51betaT

TPA_TEST=..\tpa51betaT

Path for archive of results

Test case : [CD: Folder titled P7]=\Validation_test\SVR7\test_add1

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Confirm that WP failures can occur under static conditions.

Assumptions: None, other than those made within the TPA code.

Constraints None

Test Procedure:

1) Place a copy of *mechfail.exe* from TPA51betaT into the directory D:\ValidationTPA\SVR7\test_add1.

2) Place a copy of the reference case run *mechfail_wp.inp* into the directory D:\ValidationTPA\SVR7\test_add1.

3) Rename the D:\ValidationTPA\SVR7\test_add1\ *mechfail_wp.inp* to D:\ValidationTPA\SVR7\test_add1\ *mechfail.inp*

4) Edit D:\ValidationTPA\SVR7\test_add1\ *mechfail.inp*, changing the vertical pressure at time 501 yr from 1.59091e2 kPa to 1.5091e6 kPa for rock type 1

5) Execute the standalone *mechfail.exe*

Pass/Fail criteria:

1) The output generated by the standalone code *mechfail.exe* should generate WP failure, which occurs at 5.2971e2 yr.

Test Results

The standalone module MECHFAIL *(mechfail.exe)* evaluates the mechanical failure of DS and WP. In the TPA code this module is executed twice. On the first call MECHFAIL evaluates the failure of DS by comparing the vertical load against a calculated DS load capacity. On the second call MECHFAIL evaluates the failure of WP by comparing vertical load against a calculated WP load capacity and the failure status of the DS. If the drip shield is not failed no DS-WP interaction is evaluated.

In this test, the file D:\ValidationTPA\SVR7\test_add1\ *mechfail_wp.inp* is the intermediate input to the MECHFAIL module (DS status has already been evaluated). And the vertical load has been modified to an artificially high value of 1.5091e6 kPa at a time of 501 years. This time was selected because it was after the time of DS failure but prior to any seismic events which could cause WP failures, and the high value vertical load was selected to ensure that the WP capacity is exceeded (The WP capacity can range between ~900kPa to 20,000kPa).

An examination of the results of MECHFAIL using the modified input file shows that WP static failure is reported at time 501 yr. The fraction of WP failed is reported at 0.85, which is the fraction of rock type 1.

The following text is an excerpt from the output file generated by mechfail.exe

D:\ValidationTPA\SVR7\test_add1\ *mechfail_wp.dat*

```
*****************************************************************************
TITLE - mechfail_wp.dat
DATE/Time: Mon Jun 18 15:54:51 2007
:
:Mechanical Failure Data versus Time
:  Fraction Failed - Subarea Analysis
:Subarea   10
:          Time      WP Total     WP Static    WP Dynamic
    0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
    2.31016E+00   0.00000E+00   0.00000E+00   0.00000E+00
...
...
   3.88495E+02   0.00000E+00   0.00000E+00   0.00000E+00
    3.99900E+02   0.00000E+00   0.00000E+00   0.00000E+00
    4.11572E+02   0.00000E+00   0.00000E+00   0.00000E+00
    4.23518E+02   0.00000E+00   0.00000E+00   0.00000E+00
    4.35743E+02   0.00000E+00   0.00000E+00   0.00000E+00
    4.48255E+02   0.00000E+00   0.00000E+00   0.00000E+00
    4.61059E+02   0.00000E+00   0.00000E+00   0.00000E+00
    4.74163E+02   0.00000E+00   0.00000E+00   0.00000E+00
```

```
    4.87574E+02   0.00000E+00   0.00000E+00   0.00000E+00
    5.01299E+02   8.50000E-01   8.50000E-01   0.00000E+00
    5.15346E+02   8.50000E-01   8.50000E-01   0.00000E+00
    5.29721E+02   8.50000E-01   8.50000E-01   0.00000E+00
    5.44432E+02   8.50000E-01   8.50000E-01   0.00000E+00
...
****************************************************************************
```

These results confirm that MECHFAIL will return failed WP status when the static vertical load applied to a WP exceeds the WP load capacity.

Test Results (PASS/FAIL): **PASS**

SOFTWARE VALIDATION REPORT (SVR)

SVR#: P-8	Project#: 06002.01.354
Software Name: TPA	Version: TPA51betaU
Test ID: Drip Shield Corrosion	Test Series Name:

Test Method

x code inspection	☐ spreadsheet
x output inspection	☐ graphical
x hand calculation	☐ comparison with external code results

Test Objective: See Attachment A

Test Environment Setup

Hardware (platform, peripherals): *Desktop PC* with Intel Pentium 4 processor.

Software (OS, compiler, libraries, auxiliary codes or scripts): *Microsoft Windows XP*

Input Data (files, data base, mode settings):

Assumptions, constraints, and/or scope of test:
See Attachment A—TPA Version 5.1 Validation Task P-8
Objectives, Assumptions, Scope of Tests

Test Procedure and Pass/Fail Criteria:
See Attachment A—TPA Version 5.1 Validation Task P-8
Objectives, Assumptions, Scope of Tests

Test Results

Location: See attached CD labeled "TPA Version 5.1 Validation Task P-8"

Analysis of Results: See Attachment B, TPA Version 5.1 Validation Task P-8 Test Results

Test Evaluation (Pass/Fail): Pass

Notes:

Tester: X. He, and P. Shukla	Date: 4/27/2007

Attachment A

SVR#8 Test Plan

Objectives, Assumptions, Scope of Tests

OBJECTIVES

The objective of Software Validation Report (SVR) #8 is to verify process level calculations performed by the TPA module DSFAIL (drip shield failure). The specific issues to be addressed by SVR #8 are the following:

1. The dsfail.f module provide correct values of input parameters to dsfailt.f code, and parameters -corrosion rate, initial thickness -are correctly passed to standalone code dsfailt.f..
2. The time of drip shield failure is correctly calculated by dsfailt.f.
3. Changes to specific failure depth thresholds (specified by parameter DSFractionThicknessPenetratedForFailureByCorrosion[] in tpa.inp) result in proportional changes to calculated corrosion failure time.

ASSUMPTIONS

For the purposes of this validation test, it is assumed:

- The input parameters and their distributions supplied by *tpa.inp* are consistent with the abstractions of the modeled processes.

TEST PROCEDURE AND PASS/FAIL CRITERIA

The following tests sequentially address the objectives of this SVR. During validation testing the validation teams may conduct additional testing, to be documented in the SVR, as necessary to understand and verify software performance related to the DSFAIL module.

For all the tests copy the tpa.inp file from TPA Version 5.1BetaU and use it as tpa.inp file after changing the OutputMode from 0 to 1 and the SelectAppendFiles from 0 to 21.

Test 1. Modify the input value of DripShieldThickness[m] and change the DripShieldCorrosionRate[m/yr] to a constant value from logtriangular in tpa.inp in accordance with the following table:

Parameter	Value
DripShieldCorrosionRate[m/yr]	2.0e-6
DripShieldThickness[m]	0.020

Then, execute the TPA code for one reference case realization for all subareas.

Pass/Fail Criterion: The TPA code should reproduce the values specified in the above table.

Test 2. Modify the DripShieldThickness and DripShieldCorrosionRate separately in accordance with the following table.

	Parameter	Value
Test 2a	DripShieldThickness[m]	0.002
Test 2b	DripShieldCorrosionRate[m/yr]	1.0e-5 m/yr

In Test 2a, change the input value of the DripShieldThickness[m] from 0.015 to 0.002. With this thickness, the drip shield should fail at 9163 years after its emplacement by hand calculation. In Test 2b, change the input parameter of DripShieldCorrosionRate[m/yr] to a constant value of 1.0e-5 m/year. With this corrosion rate, the drip shield should fail in 1500 years. Then execute the TPA code for one reference case realization separately for the two cases.

Pass/Fail Criterion: The TPA code should reproduce the hand-calculated values specified in the above table.

Test 3. Modify the input values of parameters DripShieldCorrosionRate[m/yr] and DSFractionThicknessPenetratedForFailureByCorrosion[] in accordance with the following table:

Parameter	Value
DripShieldCorrosionRate[m/yr]	1.0e-5 m/yr
DSFractionThicknessPenetratedForFailureByCorrosion[]	0.75

The hand calculation indicates that the drip shield should fail in 1125 years. Execute the TPA code for one reference case realization for all subareas.

Pass/Fail Criterion: The TPA code should reproduce the hand-calculated values specified in the above table.

Overall Pass/Fail Criteria: If all the three test criteria are met, then the overall test will be considered as PASS.

Attachment B
TPA Version 5.1 Software Validation Task P-8 Test Results

Following are test results for the validation test cases described in Attachment A for TPA Version 5.1 code Software Validation Task P-8. Additional details related to test procedures are also provided.

Test 1. Objective 1: The dsfail.f module provide correct values of input parameters to dsfailt.f code, and parameters -corrosion rate, initial thickness -are correctly passed to standalone code dsfailt.f..

Environment variable:
Reference case: TPA_DATA=..\tpa51betaU
TPA_TEST=..\tpa51betaU

Test case: TPA_DATA=..\tpa51betaU
TPA_TEST=..\tpa51betaU

Path for archive of results
Reference case: Smurf: D\P8\P8-Reference_case
Test case : Smurf: D\P8\P8-Test1

Special input files or modifications to input files required : None

Special diagnostic code modifications required: None

Program modes to be used (append flags, scenario/model switches, etc.):
Reference case : append 21 (dsfail.ech and dsfail.rlt only)
Test case : append 21 (dsfail.ech and dsfail.rlt only)

Table 1. Original and Modified Values of Input Parameters for Test 1

Parameter	Original (reference case)	Modified (test case)
DripShieldCorrosionRate[m/yr]	logtriangular 2.0e-8, 2.98e-7, 6.4e-7	constant 2.0e-6
DripShieldThickness[m]	constant 0.015	constant 0.020

Test Procedure, Pass/Fail criteria, and other details are in **Attachment A**.

Analysis of Results—Reference Case and Test Case:

In the reference case, the original values of DripShieldCorrosionRate[m/yr] and DripShieldThickness[m] as listed in Table 1 in the first column are appeared in the *tpa.inp*. The following is a copy of part of the *tpa.inp* file related to these parameters and *the dsfailt.inp* file for the reference case. The corresponding values are highlighted.

Reference Case

```
******************************************************************************
constant
EmplacementBackfillThickness[m]
0.0
**
constant
DripShieldThickness[m]
0.015
**
constant
DripShieldEqvIntDia[m]
2.75
**
** rwr 4/24/06; SCR626; remove unused parameters
** constant
** LengthOfRefluxZone[m]
** 20.0
******************************************************************
**          ***>>>  DSFAIL   <<<***
**
** rwr 12/29/06; SCR663; Task 1 - Drift Degradation Scenario Module
Integration
**                           (modify the following parameter distribution)
**                           (the parameter name, distribution, and
justification were
**                            contained in two files attached by an email that
was sent from
**                            O. Pensado to R. Rice on 12/18/06; the file names
**                            were "parameters.wpd" and
"DriftDeg_recommendation_03.ppt")
** triangular
** DripShieldCorrosionRate[m/yr]
** 8.6e-8, 1.72e-7, 2.6e-7
**(use a different distribution based on 2/15/07 email from O. Pensado
** titled "Revised value of DripShieldCorrosionRate[m/yr]"
**uniform
**DripShieldCorrosionRate[m/yr]
**7.6d-8, 1.32d-6
** rwr 2/26/07; SCR673; Reformat Input/Output/Intermediate Files
**                       (modify the following parameter distribution)
**                       (contained in an email that was sent from O. Pensado
to)
**                       (R. Rice on 3/7/07 with a subject line
"DripShieldCorrosionRate)
**                       (and wpflow.def")
** triangular
** DripShieldCorrosionRate[m/yr]
** 2.0e-8, 2.98e-7, 6.4e-7
logtriangular
DripShieldCorrosionRate[m/yr]
2.0e-8, 2.98e-7, 6.4e-7
**
*************************************************
! TITLE - dsfailt.inp
! DATE/TIME Tue Mar 20 11:53:58 2007
! Input file for module DSfailt and is rewritten for each realization

! This file contains the file names for the fluoride concentration data and DS
thickness vs. time
```

```
! data and parameters relevant to DS corrosion

! SECTION 1


 'fluoride.dat'   ! fileIn, Input data file, fluoride concentration versus
time
  'dsfailt.dat'   ! fileOut, Output data file 1, tracking thickness of the
drip shield vs time
    2.18270E-07   ! CorrRate, m/yr, drip shield corrosion rate :
DSCorrRate[m/yr]
    1.50000E-02   ! DSThick, m, drip shield thickness : DripShieldThickness[m]

           2.84   ! slope, dimensionless, slope of drip shield enhancing
factor
        1.0e-04   ! minF, M, minimum fluoride concentration affecting the DS
corrosion rate
        2.0e-03   ! maxF, M, maximum fluoride concentration affecting the DS
corrosion rate
              0   ! FluorideEnh, (0 or 1). 0 : no fluoride enhancing, 1:
fluoride enhancing.
********************************************************************************
```

In the test case, the values of DripShieldCorrosionRate[m/yr] and DripShieldThickness[m] are modified as listed in Table 1 in the second column in the *tpa.inp*. The following is a copy of part of the *tpa.inp* file with the modified parameter values and the *dsfailt.inp* file for the test case. The corresponding values are highlighted.

Test Case

```
********************************************************************************
constant
EmplacementBackfillThickness[m]
0.0
**
constant
DripShieldThickness[m]
0.020
**
constant
DripShieldEqvIntDia[m]
2.75
**
** rwr 4/24/06; SCR626; remove unused parameters
** constant
** LengthOfRefluxZone[m]
** 20.0
**********************************************************
**          ***>>>  DSFAIL   <<<***
**
** rwr 12/29/06; SCR663; Task 1 - Drift Degradation Scenario Module
Integration
**                           (modify the following parameter distribution)
**                           (the parameter name, distribution, and
justification were
**                            contained in two files attached by an email that
was sent from
**                            O. Pensado to R. Rice on 12/18/06; the file names
**                            were "parameters.wpd" and
"DriftDeg_recommendation_03.ppt")
** triangular
** DripShieldCorrosionRate[m/yr]
```

```
** 8.6e-8, 1.72e-7, 2.6e-7
**(use a different distribution based on 2/15/07 email from O. Pensado
** titled "Revised value of DripShieldCorrosionRate[m/yr]"
**uniform
**DripShieldCorrosionRate[m/yr]
**7.6d-8, 1.32d-6
** rwr 2/26/07; SCR673; Reformat Input/Output/Intermediate Files
**                        (modify the following parameter distribution)
**                        (contained in an email that was sent from O. Pensado
to)
**                        (R. Rice on 3/7/07 with a subject line
"DripShieldCorrosionRate)
**                        (and wpflow.def")
** triangular
** DripShieldCorrosionRate[m/yr]
** 2.0e-8, 2.98e-7, 6.4e-7
constant
DripShieldCorrosionRate[m/yr]
2.0e-6
**
****************************************
! TITLE - dsfailt.inp
! DATE/TIME Thu Mar 22 17:28:16 2007
! Input file for module DSfailt and is rewritten for each realization

! This file contains the file names for the fluoride concentration data and DS
thickness vs. time
! data and parameters relevant to DS corrosion

! SECTION 1



 'fluoride.dat'   ! fileIn, Input data file, fluoride concentration versus
time
  'dsfailt.dat'   ! fileOut, Output data file 1, tracking thickness of the
drip shield vs time
    2.00000E-06   ! CorrRate, m/yr, drip shield corrosion rate :
DSCorrRate[m/yr]
    2.00000E-02   ! DSThick, m, drip shield thickness : DripShieldThickness[m]

           2.84   ! slope, dimensionless, slope of drip shield enhancing
factor
        1.0e-04   ! minF, M, minimum fluoride concentration affecting the DS
corrosion rate
        2.0e-03   ! maxF, M, maximum fluoride concentration affecting the DS
corrosion rate
              0   ! FluorideEnh, (0 or 1). 0 : no fluoride enhancing, 1:
fluoride enhancing.

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

Test Results (PASS/FAIL): Both the reference case and the test case realization successfully executed under the test conditions. Both cases demonstrate that correct inputs are provided from the *dsfail.f* module to the ds*failt.f* code. These results demonstrate that objective 1 of SVR8 has been successfully tested. It meets the criterion specified in Test 1 in Attachment A, so the test result is **PASS.**

Test 2. Objective 2: The time of drip shield failure is correctly calculated by dsfailt.f..

Environment variable:

Reference case: TPA_DATA=..\tpa51betaU
TPA_TEST=..\tpa51betaU

Test case: TPA_DATA=..\tpa51betaU
TPA_TEST=..\tpa51betaU

Path for archive of results
Reference case: Smurf: D\P8\P8-Reference_case
Test case : Smurf: D\P8\P8-Test2

Special input files or modifications to input files required : None

Special diagnostic code modifications required: None

Program modes to be used (append flags, scenario/model switches, etc.):
Reference case : append 21 (dsfail.ech and dsfail.rlt only)
Test case : append 21 (dsfail.ech and dsfail.rlt only)

Table 2. Original and Modified Values of Input Parameters for Test 2

	Parameter	Original (reference case)	Modified (test case)
Test 2a	DripShieldThickness[m]	constant 0.015	constant 0.002
Test 2b	DripShieldCorrosionRate[m/yr]	logtriangular 2.0e-8, 2.98e-7, 6.4e-7	constant 1.0e-5

Test Procedure, Pass/Fail criteria, and other relevant details are in **Attachment A**.

Analysis of Results—Reference Case and Test Case:

The reference case realization successfully executed in Test 1 under the test conditions. In the reference case, no failure of the drip shield in 10K years. The following is a copy of the *dsfailt.dat* file for the reference case. The failure status of the drip shield is highlighted.

```
******************************************************************************
GENERATING MODULE: dsfailt
 Uniform corrosion of drip shield
 Thickness of drip shield vs time
 0  Failure Flag (=1 if failed, 0 otherwise)
 No failure of DS in  10000  years
 201  Number of time steps in this file
  Time[yr]       Thickness[m]
  0.0000E+00     1.5000E-02
  2.3102E+00     1.4999E-02
  4.6744E+00     1.4999E-02
  7.0940E+00     1.4998E-02
  9.5702E+00     1.4998E-02
  1.2104E+01     1.4997E-02
  1.4698E+01     1.4997E-02
  1.7352E+01     1.4996E-02
  2.0069E+01     1.4996E-02
```

2.2849E+01	1.4995E-02
2.5694E+01	1.4994E-02
2.8605E+01	1.4994E-02
3.1585E+01	1.4993E-02
3.4635E+01	1.4992E-02
3.7756E+01	1.4992E-02
4.0950E+01	1.4991E-02
4.4219E+01	1.4990E-02
4.7564E+01	1.4990E-02
5.0988E+01	1.4989E-02
5.4492E+01	1.4988E-02
5.8078E+01	1.4987E-02
6.1747E+01	1.4987E-02
6.5503E+01	1.4986E-02
6.9347E+01	1.4985E-02
7.3281E+01	1.4984E-02
7.7306E+01	1.4983E-02
8.1426E+01	1.4982E-02
8.5643E+01	1.4981E-02
8.9958E+01	1.4980E-02
9.4374E+01	1.4979E-02
9.8894E+01	1.4978E-02
1.0352E+02	1.4977E-02
1.0825E+02	1.4976E-02
1.1310E+02	1.4975E-02
1.1806E+02	1.4974E-02
1.2313E+02	1.4973E-02
1.2832E+02	1.4972E-02
1.3364E+02	1.4971E-02
1.3908E+02	1.4970E-02
1.4464E+02	1.4968E-02
1.5034E+02	1.4967E-02
1.5617E+02	1.4966E-02
1.6213E+02	1.4965E-02
1.6824E+02	1.4963E-02
1.7449E+02	1.4962E-02
1.8088E+02	1.4961E-02
1.8743E+02	1.4959E-02
1.9413E+02	1.4958E-02
2.0098E+02	1.4956E-02
2.0800E+02	1.4955E-02
2.1518E+02	1.4953E-02
2.2252E+02	1.4951E-02
2.3004E+02	1.4950E-02
2.3774E+02	1.4948E-02
2.4562E+02	1.4946E-02
2.5368E+02	1.4945E-02
2.6193E+02	1.4943E-02
2.7037E+02	1.4941E-02
2.7901E+02	1.4939E-02
2.8785E+02	1.4937E-02
2.9690E+02	1.4935E-02
3.0616E+02	1.4933E-02
3.1564E+02	1.4931E-02
3.2534E+02	1.4929E-02
3.3526E+02	1.4927E-02
3.4542E+02	1.4925E-02
3.5582E+02	1.4922E-02
3.6646E+02	1.4920E-02
3.7735E+02	1.4918E-02
3.8849E+02	1.4915E-02
3.9990E+02	1.4913E-02
4.1157E+02	1.4910E-02
4.2352E+02	1.4908E-02
4.3574E+02	1.4905E-02

4.4825E+02	1.4902E-02
4.6106E+02	1.4899E-02
4.7416E+02	1.4897E-02
4.8757E+02	1.4894E-02
5.0130E+02	1.4891E-02
5.1535E+02	1.4888E-02
5.2972E+02	1.4884E-02
5.4443E+02	1.4881E-02
5.5949E+02	1.4878E-02
5.7490E+02	1.4875E-02
5.9067E+02	1.4871E-02
6.0680E+02	1.4868E-02
6.2332E+02	1.4864E-02
6.4022E+02	1.4860E-02
6.5752E+02	1.4856E-02
6.7523E+02	1.4853E-02
6.9334E+02	1.4849E-02
7.1189E+02	1.4845E-02
7.3086E+02	1.4840E-02
7.5028E+02	1.4836E-02
7.7016E+02	1.4832E-02
7.9050E+02	1.4827E-02
8.1132E+02	1.4823E-02
8.3262E+02	1.4818E-02
8.5442E+02	1.4814E-02
8.7674E+02	1.4809E-02
8.9957E+02	1.4804E-02
9.2294E+02	1.4799E-02
9.4686E+02	1.4793E-02
9.7134E+02	1.4788E-02
9.9639E+02	1.4783E-02
1.0220E+03	1.4777E-02
1.0483E+03	1.4771E-02
1.0751E+03	1.4765E-02
1.1026E+03	1.4759E-02
1.1307E+03	1.4753E-02
1.1595E+03	1.4747E-02
1.1890E+03	1.4740E-02
1.2191E+03	1.4734E-02
1.2500E+03	1.4727E-02
1.2815E+03	1.4720E-02
1.3138E+03	1.4713E-02
1.3469E+03	1.4706E-02
1.3808E+03	1.4699E-02
1.4154E+03	1.4691E-02
1.4508E+03	1.4683E-02
1.4871E+03	1.4675E-02
1.5242E+03	1.4667E-02
1.5622E+03	1.4659E-02
1.6011E+03	1.4651E-02
1.6409E+03	1.4642E-02
1.6816E+03	1.4633E-02
1.7233E+03	1.4624E-02
1.7660E+03	1.4615E-02
1.8096E+03	1.4605E-02
1.8543E+03	1.4595E-02
1.9000E+03	1.4585E-02
1.9468E+03	1.4575E-02
1.9947E+03	1.4565E-02
2.0437E+03	1.4554E-02
2.0939E+03	1.4543E-02
2.1452E+03	1.4532E-02
2.1977E+03	1.4520E-02
2.2515E+03	1.4509E-02
2.3065E+03	1.4497E-02

2.3628E+03	1.4484E-02
2.4204E+03	1.4472E-02
2.4794E+03	1.4459E-02
2.5398E+03	1.4446E-02
2.6015E+03	1.4432E-02
2.6648E+03	1.4418E-02
2.7295E+03	1.4404E-02
2.7957E+03	1.4390E-02
2.8634E+03	1.4375E-02
2.9328E+03	1.4360E-02
3.0038E+03	1.4344E-02
3.0764E+03	1.4329E-02
3.1507E+03	1.4312E-02
3.2268E+03	1.4296E-02
3.3046E+03	1.4279E-02
3.3843E+03	1.4261E-02
3.4659E+03	1.4244E-02
3.5493E+03	1.4225E-02
3.6347E+03	1.4207E-02
3.7221E+03	1.4188E-02
3.8116E+03	1.4168E-02
3.9031E+03	1.4148E-02
3.9968E+03	1.4128E-02
4.0927E+03	1.4107E-02
4.1908E+03	1.4085E-02
4.2912E+03	1.4063E-02
4.3940E+03	1.4041E-02
4.4992E+03	1.4018E-02
4.6068E+03	1.3994E-02
4.7170E+03	1.3970E-02
4.8297E+03	1.3946E-02
4.9451E+03	1.3921E-02
5.0632E+03	1.3895E-02
5.1840E+03	1.3868E-02
5.3077E+03	1.3841E-02
5.4343E+03	1.3814E-02
5.5638E+03	1.3786E-02
5.6964E+03	1.3757E-02
5.8321E+03	1.3727E-02
5.9709E+03	1.3697E-02
6.1130E+03	1.3666E-02
6.2584E+03	1.3634E-02
6.4073E+03	1.3601E-02
6.5596E+03	1.3568E-02
6.7154E+03	1.3534E-02
6.8750E+03	1.3499E-02
7.0382E+03	1.3464E-02
7.2053E+03	1.3427E-02
7.3763E+03	1.3390E-02
7.5513E+03	1.3352E-02
7.7304E+03	1.3313E-02
7.9137E+03	1.3273E-02
8.1013E+03	1.3232E-02
8.2933E+03	1.3190E-02
8.4897E+03	1.3147E-02
8.6908E+03	1.3103E-02
8.8966E+03	1.3058E-02
9.1072E+03	1.3012E-02
9.3227E+03	1.2965E-02
9.5433E+03	1.2917E-02
9.7690E+03	1.2868E-02
1.0000E+04	1.2817E-02

****

Test 2a

In test case a, the value of DripShieldThickness[m] was modified from 0.015 to 0.002. With this thickness, the drip shield should fail at 9163 years after its emplacement by hand-calculation. The test case realization successfully executed in Test 2a under the test conditions. The following is a copy of the *dsfailt.dat* file for the test case. The failure status of the drip shield is highlighted.

```
******************************************************************************
GENERATING MODULE: dsfailt
 Uniform corrosion of drip shield
 Thickness of drip shield vs time
 1  Failure Flag (=1 if failed, 0 otherwise)
 9163  yrs :  Drip shield failure time
 198  Number of time steps in this file
  Time[yr]      Thickness[m]
  0.0000E+00    2.0000E-03
  2.3102E+00    1.9995E-03
  4.6744E+00    1.9990E-03
  7.0940E+00    1.9985E-03
  9.5702E+00    1.9979E-03
  1.2104E+01    1.9974E-03
  1.4698E+01    1.9968E-03
  1.7352E+01    1.9962E-03
  2.0069E+01    1.9956E-03
  2.2849E+01    1.9950E-03
  2.5694E+01    1.9944E-03
  2.8605E+01    1.9938E-03
  3.1585E+01    1.9931E-03
  3.4635E+01    1.9924E-03
  3.7756E+01    1.9918E-03
  4.0950E+01    1.9911E-03
  4.4219E+01    1.9903E-03
  4.7564E+01    1.9896E-03
  5.0988E+01    1.9889E-03
  5.4492E+01    1.9881E-03
  5.8078E+01    1.9873E-03
  6.1747E+01    1.9865E-03
  6.5503E+01    1.9857E-03
  6.9347E+01    1.9849E-03
  7.3281E+01    1.9840E-03
  7.7306E+01    1.9831E-03
  8.1426E+01    1.9822E-03
  8.5643E+01    1.9813E-03
  8.9958E+01    1.9804E-03
  9.4374E+01    1.9794E-03
  9.8894E+01    1.9784E-03
  1.0352E+02    1.9774E-03
  1.0825E+02    1.9764E-03
  1.1310E+02    1.9753E-03
  1.1806E+02    1.9742E-03
  1.2313E+02    1.9731E-03
  1.2832E+02    1.9720E-03
  1.3364E+02    1.9708E-03
  1.3908E+02    1.9696E-03
  1.4464E+02    1.9684E-03
  1.5034E+02    1.9672E-03
  1.5617E+02    1.9659E-03
  1.6213E+02    1.9646E-03
  1.6824E+02    1.9633E-03
  1.7449E+02    1.9619E-03
  1.8088E+02    1.9605E-03
  1.8743E+02    1.9591E-03
  1.9413E+02    1.9576E-03
  2.0098E+02    1.9561E-03
```

2.0800E+02	1.9546E-03
2.1518E+02	1.9530E-03
2.2252E+02	1.9514E-03
2.3004E+02	1.9498E-03
2.3774E+02	1.9481E-03
2.4562E+02	1.9464E-03
2.5368E+02	1.9446E-03
2.6193E+02	1.9428E-03
2.7037E+02	1.9410E-03
2.7901E+02	1.9391E-03
2.8785E+02	1.9372E-03
2.9690E+02	1.9352E-03
3.0616E+02	1.9332E-03
3.1564E+02	1.9311E-03
3.2534E+02	1.9290E-03
3.3526E+02	1.9268E-03
3.4542E+02	1.9246E-03
3.5582E+02	1.9223E-03
3.6646E+02	1.9200E-03
3.7735E+02	1.9176E-03
3.8849E+02	1.9152E-03
3.9990E+02	1.9127E-03
4.1157E+02	1.9102E-03
4.2352E+02	1.9076E-03
4.3574E+02	1.9049E-03
4.4825E+02	1.9022E-03
4.6106E+02	1.8994E-03
4.7416E+02	1.8965E-03
4.8757E+02	1.8936E-03
5.0130E+02	1.8906E-03
5.1535E+02	1.8875E-03
5.2972E+02	1.8844E-03
5.4443E+02	1.8812E-03
5.5949E+02	1.8779E-03
5.7490E+02	1.8745E-03
5.9067E+02	1.8711E-03
6.0680E+02	1.8676E-03
6.2332E+02	1.8639E-03
6.4022E+02	1.8603E-03
6.5752E+02	1.8565E-03
6.7523E+02	1.8526E-03
6.9334E+02	1.8487E-03
7.1189E+02	1.8446E-03
7.3086E+02	1.8405E-03
7.5028E+02	1.8362E-03
7.7016E+02	1.8319E-03
7.9050E+02	1.8275E-03
8.1132E+02	1.8229E-03
8.3262E+02	1.8183E-03
8.5442E+02	1.8135E-03
8.7674E+02	1.8086E-03
8.9957E+02	1.8037E-03
9.2294E+02	1.7985E-03
9.4686E+02	1.7933E-03
9.7134E+02	1.7880E-03
9.9639E+02	1.7825E-03
1.0220E+03	1.7769E-03
1.0483E+03	1.7712E-03
1.0751E+03	1.7653E-03
1.1026E+03	1.7593E-03
1.1307E+03	1.7532E-03
1.1595E+03	1.7469E-03
1.1890E+03	1.7405E-03
1.2191E+03	1.7339E-03
1.2500E+03	1.7272E-03

1.2815E+03	1.7203E-03
1.3138E+03	1.7132E-03
1.3469E+03	1.7060E-03
1.3808E+03	1.6986E-03
1.4154E+03	1.6911E-03
1.4508E+03	1.6833E-03
1.4871E+03	1.6754E-03
1.5242E+03	1.6673E-03
1.5622E+03	1.6590E-03
1.6011E+03	1.6505E-03
1.6409E+03	1.6418E-03
1.6816E+03	1.6329E-03
1.7233E+03	1.6239E-03
1.7660E+03	1.6145E-03
1.8096E+03	1.6050E-03
1.8543E+03	1.5953E-03
1.9000E+03	1.5853E-03
1.9468E+03	1.5751E-03
1.9947E+03	1.5646E-03
2.0437E+03	1.5539E-03
2.0939E+03	1.5430E-03
2.1452E+03	1.5318E-03
2.1977E+03	1.5203E-03
2.2515E+03	1.5086E-03
2.3065E+03	1.4966E-03
2.3628E+03	1.4843E-03
2.4204E+03	1.4717E-03
2.4794E+03	1.4588E-03
2.5398E+03	1.4456E-03
2.6015E+03	1.4322E-03
2.6648E+03	1.4184E-03
2.7295E+03	1.4042E-03
2.7957E+03	1.3898E-03
2.8634E+03	1.3750E-03
2.9328E+03	1.3599E-03
3.0038E+03	1.3444E-03
3.0764E+03	1.3285E-03
3.1507E+03	1.3123E-03
3.2268E+03	1.2957E-03
3.3046E+03	1.2787E-03
3.3843E+03	1.2613E-03
3.4659E+03	1.2435E-03
3.5493E+03	1.2253E-03
3.6347E+03	1.2067E-03
3.7221E+03	1.1876E-03
3.8116E+03	1.1680E-03
3.9031E+03	1.1481E-03
3.9968E+03	1.1276E-03
4.0927E+03	1.1067E-03
4.1908E+03	1.0853E-03
4.2912E+03	1.0634E-03
4.3940E+03	1.0409E-03
4.4992E+03	1.0180E-03
4.6068E+03	9.9447E-04
4.7170E+03	9.7042E-04
4.8297E+03	9.4581E-04
4.9451E+03	9.2063E-04
5.0632E+03	8.9486E-04
5.1840E+03	8.6848E-04
5.3077E+03	8.4148E-04
5.4343E+03	8.1386E-04
5.5638E+03	7.8558E-04
5.6964E+03	7.5665E-04
5.8321E+03	7.2704E-04
5.9709E+03	6.9673E-04

```
  6.1130E+03    6.6571E-04
  6.2584E+03    6.3397E-04
  6.4073E+03    6.0149E-04
  6.5596E+03    5.6824E-04
  6.7154E+03    5.3422E-04
  6.8750E+03    4.9940E-04
  7.0382E+03    4.6376E-04
  7.2053E+03    4.2729E-04
  7.3763E+03    3.8997E-04
  7.5513E+03    3.5177E-04
  7.7304E+03    3.1268E-04
  7.9137E+03    2.7267E-04
  8.1013E+03    2.3173E-04
  8.2933E+03    1.8983E-04
  8.4897E+03    1.4695E-04
  8.6908E+03    1.0306E-04
  8.8966E+03    5.8145E-05
  9.1072E+03    1.2179E-05
  9.3227E+03   -3.4863E-05
********************************************************************************
```

Test 2b

In test case b, the value of DripShieldCorrosionRate[m/yr] was changed to a constant value of 1.0e-5 m/yr. With this corrosion rate, the drip shield should fail at 1500 years after its emplacement by hand calculation. The test case realization successfully executed in Test 2b under the test conditions. The following is a copy of the *dsfailt.dat* file for the test case. The failure status of the drip shield is highlighted.

```
********************************************************************************
GENERATING MODULE: dsfailt
 Uniform corrosion of drip shield
 Thickness of drip shield vs time
 1  Failure Flag (=1 if failed, 0 otherwise)
 1500  yrs :  Drip shield failure time
 122  Number of time steps in this file
  Time[yr]      Thickness[m]
  0.0000E+00    1.5000E-02
  2.3102E+00    1.4977E-02
  4.6744E+00    1.4953E-02
  7.0940E+00    1.4929E-02
  9.5702E+00    1.4904E-02
  1.2104E+01    1.4879E-02
  1.4698E+01    1.4853E-02
  1.7352E+01    1.4826E-02
  2.0069E+01    1.4799E-02
  2.2849E+01    1.4772E-02
  2.5694E+01    1.4743E-02
  2.8605E+01    1.4714E-02
  3.1585E+01    1.4684E-02
  3.4635E+01    1.4654E-02
  3.7756E+01    1.4622E-02
  4.0950E+01    1.4591E-02
  4.4219E+01    1.4558E-02
  4.7564E+01    1.4524E-02
  5.0988E+01    1.4490E-02
  5.4492E+01    1.4455E-02
  5.8078E+01    1.4419E-02
  6.1747E+01    1.4383E-02
  6.5503E+01    1.4345E-02
  6.9347E+01    1.4307E-02
  7.3281E+01    1.4267E-02
  7.7306E+01    1.4227E-02
```

8.1426E+01	1.4186E-02
8.5643E+01	1.4144E-02
8.9958E+01	1.4100E-02
9.4374E+01	1.4056E-02
9.8894E+01	1.4011E-02
1.0352E+02	1.3965E-02
1.0825E+02	1.3917E-02
1.1310E+02	1.3869E-02
1.1806E+02	1.3819E-02
1.2313E+02	1.3769E-02
1.2832E+02	1.3717E-02
1.3364E+02	1.3664E-02
1.3908E+02	1.3609E-02
1.4464E+02	1.3554E-02
1.5034E+02	1.3497E-02
1.5617E+02	1.3438E-02
1.6213E+02	1.3379E-02
1.6824E+02	1.3318E-02
1.7449E+02	1.3255E-02
1.8088E+02	1.3191E-02
1.8743E+02	1.3126E-02
1.9413E+02	1.3059E-02
2.0098E+02	1.2990E-02
2.0800E+02	1.2920E-02
2.1518E+02	1.2848E-02
2.2252E+02	1.2775E-02
2.3004E+02	1.2700E-02
2.3774E+02	1.2623E-02
2.4562E+02	1.2544E-02
2.5368E+02	1.2463E-02
2.6193E+02	1.2381E-02
2.7037E+02	1.2296E-02
2.7901E+02	1.2210E-02
2.8785E+02	1.2122E-02
2.9690E+02	1.2031E-02
3.0616E+02	1.1938E-02
3.1564E+02	1.1844E-02
3.2534E+02	1.1747E-02
3.3526E+02	1.1647E-02
3.4542E+02	1.1546E-02
3.5582E+02	1.1442E-02
3.6646E+02	1.1335E-02
3.7735E+02	1.1226E-02
3.8849E+02	1.1115E-02
3.9990E+02	1.1001E-02
4.1157E+02	1.0884E-02
4.2352E+02	1.0765E-02
4.3574E+02	1.0643E-02
4.4825E+02	1.0517E-02
4.6106E+02	1.0389E-02
4.7416E+02	1.0258E-02
4.8757E+02	1.0124E-02
5.0130E+02	9.9870E-03
5.1535E+02	9.8465E-03
5.2972E+02	9.7028E-03
5.4443E+02	9.5557E-03
5.5949E+02	9.4051E-03
5.7490E+02	9.2510E-03
5.9067E+02	9.0933E-03
6.0680E+02	8.9320E-03
6.2332E+02	8.7668E-03
6.4022E+02	8.5978E-03
6.5752E+02	8.4248E-03
6.7523E+02	8.2477E-03
6.9334E+02	8.0666E-03

```
  7.1189E+02    7.8811E-03
  7.3086E+02    7.6914E-03
  7.5028E+02    7.4972E-03
  7.7016E+02    7.2984E-03
  7.9050E+02    7.0950E-03
  8.1132E+02    6.8868E-03
  8.3262E+02    6.6738E-03
  8.5442E+02    6.4558E-03
  8.7674E+02    6.2326E-03
  8.9957E+02    6.0043E-03
  9.2294E+02    5.7706E-03
  9.4686E+02    5.5314E-03
  9.7134E+02    5.2866E-03
  9.9639E+02    5.0361E-03
  1.0220E+03    4.7797E-03
  1.0483E+03    4.5174E-03
  1.0751E+03    4.2488E-03
  1.1026E+03    3.9740E-03
  1.1307E+03    3.6928E-03
  1.1595E+03    3.4050E-03
  1.1890E+03    3.1104E-03
  1.2191E+03    2.8090E-03
  1.2500E+03    2.5005E-03
  1.2815E+03    2.1847E-03
  1.3138E+03    1.8616E-03
  1.3469E+03    1.5309E-03
  1.3808E+03    1.1925E-03
  1.4154E+03    8.4614E-04
  1.4508E+03    4.9168E-04
  1.4871E+03    1.2891E-04
  1.5242E+03   -2.4234E-04
*****************************************************************************
```

Test Results (PASS/FAIL): The test case realization successfully executed in Tests 2a and 2b under the test conditions. Both cases demonstrate that the time of drip shield failure is correctly calculated by ds*failt.f* code. These results are submitted as evidence that objective 2 of SVR8 has been successfully tested. It meets the criterion specified in Test 2 in Attachment A, so the test result is **PASS.**

Test 3. Objective 3: Changes to specific failure depth thresholds (specified by parameter DSFractionThicknessPenetratedForFailureByCorrosion[] in tpa.inp) result in proportional changes to calculated corrosion failure time.

Environment variable:

Reference case: TPA_DATA=..\tpa51betaU
TPA_TEST=..\tpa51betaU

Test case: TPA_DATA=..\tpa51betaU
TPA_TEST=..\tpa51betaU

Path for archive of results

Reference case: Smurf: D\P8\P8-Reference_case
Test case : Smurf: D\P8\P8-Test3

Special input files or modifications to input files required : None

Special diagnostic code modifications required: None

Program modes to be used (append flags, scenario/model switches, etc.):

Reference case : append 21 (dsfail.ech and dsfail.rlt only)
Test case : append 21 (dsfail.ech and dsfail.rlt only)

Table 3 Original and Modified Values of Input Parameter for Test 3

Parameter	Original (reference case)	Modified (test case)
DripShieldCorrosionRate[m/yr]	logtriangular 2.0e-8, 2.98e-7, 6.4e-7	constant 1.0e-5
DSFractionThicknessPenetratedForFailureByCorrosion[]	1	0.75

Test Procedure, Pass/Fail criteria, and other relevant details are in **Attachment A**.

Analysis of results—Reference Case and Test Case:

Both the reference case and the test case realization successfully executed under the test conditions.

In the reference case, no failure of the drip shield in 10K years. A copy of the *dsfailt.dat* file for the reference case is included in Test 2.

In the test case, the values of DripShieldCorrosionRate[m/yr] and DSFractionThicknessPenetratedForFailureByCorrosion[] are modified as listed in Table 3 in the second column in the *tpa.inp*. With this corrosion rate and drip shield fraction thickness penetrated for failure by corrosion, the drip shield should fail at 1125 years after its emplacement by hand calculation, which is 3/4 of that calculated in Test 2b. The following is a copy of a section of the dsfail.rlt file and *the dsfailt.dat* file for the test case. The failure status of the drip shield is highlighted.

```
******************************************************************************
GENERATING MODULE: dsfailt
 Uniform corrosion of drip shield
 Thickness of drip shield vs time
 1  Failure Flag (=1 if failed, 0 otherwise)
 1125  yrs :  Drip shield failure time
 110  Number of time steps in this file
  Time[yr]      Thickness[m]
  0.0000E+00    1.1250E-02
  2.3102E+00    1.1227E-02
  4.6744E+00    1.1203E-02
  7.0940E+00    1.1179E-02
  9.5702E+00    1.1154E-02
  1.2104E+01    1.1129E-02
  1.4698E+01    1.1103E-02
  1.7352E+01    1.1076E-02
  2.0069E+01    1.1049E-02
  2.2849E+01    1.1022E-02
  2.5694E+01    1.0993E-02
  2.8605E+01    1.0964E-02
  3.1585E+01    1.0934E-02
```

3.4635E+01	1.0904E-02
3.7756E+01	1.0872E-02
4.0950E+01	1.0841E-02
4.4219E+01	1.0808E-02
4.7564E+01	1.0774E-02
5.0988E+01	1.0740E-02
5.4492E+01	1.0705E-02
5.8078E+01	1.0669E-02
6.1747E+01	1.0633E-02
6.5503E+01	1.0595E-02
6.9347E+01	1.0557E-02
7.3281E+01	1.0517E-02
7.7306E+01	1.0477E-02
8.1426E+01	1.0436E-02
8.5643E+01	1.0394E-02
8.9958E+01	1.0350E-02
9.4374E+01	1.0306E-02
9.8894E+01	1.0261E-02
1.0352E+02	1.0215E-02
1.0825E+02	1.0167E-02
1.1310E+02	1.0119E-02
1.1806E+02	1.0069E-02
1.2313E+02	1.0019E-02
1.2832E+02	9.9668E-03
1.3364E+02	9.9136E-03
1.3908E+02	9.8592E-03
1.4464E+02	9.8036E-03
1.5034E+02	9.7466E-03
1.5617E+02	9.6883E-03
1.6213E+02	9.6287E-03
1.6824E+02	9.5676E-03
1.7449E+02	9.5051E-03
1.8088E+02	9.4412E-03
1.8743E+02	9.3757E-03
1.9413E+02	9.3087E-03
2.0098E+02	9.2402E-03
2.0800E+02	9.1700E-03
2.1518E+02	9.0982E-03
2.2252E+02	9.0248E-03
2.3004E+02	8.9496E-03
2.3774E+02	8.8726E-03
2.4562E+02	8.7938E-03
2.5368E+02	8.7132E-03
2.6193E+02	8.6307E-03
2.7037E+02	8.5463E-03
2.7901E+02	8.4599E-03
2.8785E+02	8.3715E-03
2.9690E+02	8.2810E-03
3.0616E+02	8.1884E-03
3.1564E+02	8.0936E-03
3.2534E+02	7.9966E-03
3.3526E+02	7.8974E-03
3.4542E+02	7.7958E-03
3.5582E+02	7.6918E-03
3.6646E+02	7.5854E-03
3.7735E+02	7.4765E-03
3.8849E+02	7.3651E-03
3.9990E+02	7.2510E-03
4.1157E+02	7.1343E-03
4.2352E+02	7.0148E-03
4.3574E+02	6.8926E-03
4.4825E+02	6.7675E-03
4.6106E+02	6.6394E-03
4.7416E+02	6.5084E-03
4.8757E+02	6.3743E-03

```
  5.0130E+02    6.2370E-03
  5.1535E+02    6.0965E-03
  5.2972E+02    5.9528E-03
  5.4443E+02    5.8057E-03
  5.5949E+02    5.6551E-03
  5.7490E+02    5.5010E-03
  5.9067E+02    5.3433E-03
  6.0680E+02    5.1820E-03
  6.2332E+02    5.0168E-03
  6.4022E+02    4.8478E-03
  6.5752E+02    4.6748E-03
  6.7523E+02    4.4977E-03
  6.9334E+02    4.3166E-03
  7.1189E+02    4.1311E-03
  7.3086E+02    3.9414E-03
  7.5028E+02    3.7472E-03
  7.7016E+02    3.5484E-03
  7.9050E+02    3.3450E-03
  8.1132E+02    3.1368E-03
  8.3262E+02    2.9238E-03
  8.5442E+02    2.7058E-03
  8.7674E+02    2.4826E-03
  8.9957E+02    2.2543E-03
  9.2294E+02    2.0206E-03
  9.4686E+02    1.7814E-03
  9.7134E+02    1.5366E-03
  9.9639E+02    1.2861E-03
  1.0220E+03    1.0297E-03
  1.0483E+03    7.6736E-04
  1.0751E+03    4.9885E-04
  1.1026E+03    2.2405E-04
  1.1307E+03   -5.7188E-05
*************************************************
!! dsfail.rlt
!!
!!  Input file tpa.inp as supplied with TPA Version 5.1betaU Code.

!!  Validation nominal scenario reference case.

!! Created by: TPA 5.1betaU
!! Module: EXEC
!! Job started: Thu Mar 22 16:47:11 2007
!!
!! PURPOSE:
!!  DSFAIL Results


!!  with the output mode specified in "tpa.inp"


                       1 !! Realization
                       1 !! Subarea

!! SECTION: Drip shield failure status

            1.125000E+03  !! Drip shield failure time

            1.000000E-05  !! Drip shield corrosion rate (m/yr)

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

Test Results (PASS/FAIL): Both the reference case and the test case realization successfully executed under the test conditions. Both cases demonstrate that the changes to specific failure depth thresholds (specified by parameter DSFractionThicknessPenetratedForFailureByCorrosion[] in tpa.inp) resulted in proportional changes to calculated corrosion failure time. These results are submitted as evidence that objective 3 of SVR8 has been successfully tested. It meets the criterion specified in Test 3 in Attachment A, so the test result is **PASS.**

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 06002.01.354
Software Name: TPA	Version: TPA51betaT
Test ID: **P-9**	Test Series Name: Waste Package Corrosion

Test Method

- ☐ Code Inspection
- ■ Output Inspection
- ■ Hand Calculation
- ■ Spreadsheet
- ■ Graphical
- ☐ Comparison with External Code Results

Test Objective: See Attachment A

Test Environment Setup

Hardware (platform, peripherals): Desktop PC with Intel Pentium 4 processor.

Software (OS, compiler, libraries, auxiliary codes or scripts): Microsoft Windows XP

Input Data (files, data base, mode settings):

Assumptions, constraints, and/or scope of test:
See Attachment A

Test Procedure:
See Attachment A

Test Results

Location: See attached CD labeled "TPA Version 5.1 Validation Task P-9

Test Criterion and Analysis of Results: See Attachment A

Test Evaluation (Pass/Fail): Pass

Notes:

Tester: P. Shukla, H. Jung	Date: 01 May 2007

Attachment A

TPA Version 5.1 Validation Task P-9
Objectives, Assumptions, Test Descriptions

OBJECTIVES

The objective of Software Validation Report (SVR) P-9 is to verify process level calculations performed by the TPA module EBSFAIL (waste package failure). The specific issues to be addressed by SVR #9 are the following:

1. The ebsfail.f module provides correct input to the failt.f code.

2. Time varying corrosion potentials and passive current densities are correctly calculated.

3. Modification to the critical potential to account for the action of inhibiting anions is correctly calculated.

4. Times of failures by general corrosion and localized corrosion on welds and the waste package body are correctly reported by *failt.f*.

5. Changes to specified failure depth thresholds (i.e., fraction of total thickness at which waste package is assumed to have failed) result in proportional changes to calculated corrosion failure times.

6. Localized corrosion does not occur until the drift wall temperature falls below a threshold value for onset of seepage.

ASSUMPTIONS

For the purposes of this validation test, it is assumed:

- The input parameters and their distributions supplied by *tpa.inp* are consistent with the abstractions of the modeled processes.

- Previous validation testing of this module and testing of subsequent SCRs affecting this module have been properly performed, and may be cited as evidence of module performance.

TESTS

The following tests sequentially address the objectives of this SVR. During validation testing the validation teams may conduct additional testing, to be documented in the SVR, as necessary to understand and verify software performance related to the EBSFAIL module.

1. The tpameans.out file generated by reference case for TPA Version 5.1BetaT was used as the *tpa.inp* file. The input values of following five parameters were changed in accordance with the table below:

Parameter	Original Value	Input Value
InnerReferenceCurrReductionReactHighpH[C/(m2*yr)]	5.51e9	7.9e11
RefTemperaturePassiveCurrDens[K]	3.68e2	4.5e2
OuterDeltaEcritInh[mV]	800	900
TemperatureCoefficientOfErpInterceptWeld[mVSHE/C]	−10	−20
TempCoefOfOuterPackErpIntercept	−9.35026	−11.75

Then, the TPA code was executed for one reference case realization for subarea 3, and values of ire2hi, refTanod, deltaEcInh1, TerpInt, rptemo were examined in *ebsfail.inp*. These abbreviated parameter name sequentially correspond the parameters listed in the Table above.

PASS/FAIL CRITERIA

The parameter values of ire2hi, refTanod, deltaEcInh1, TerpInt, rptemo ebsfail.inp should appear as listed in the third column of the table.

RESULTS

Both the reference case and the test case realization successfully executed under the test conditions. The TPA code was executed according to the procedure outlined for this test case.

In the test case, the modified values of ire2hi, refTanod, deltaEcInh1, TerpInt and rptemo as listed in Table above were input in tpa.inp. The values of parameters, that were changed in *tpa.inp*, were noted. A copy of intermediate file *ebsfail.inp* is attached below, and the parameter values (that were changed) are highlighted.

```
****************************************************************************************! ! ebsfail.inp file, the input file for the failt.f standalone module
!
!  History: ebsfail.def is a legacy file with versions found in tpa32
!  03/18/06 previous version adding drip shield failure parameters
!  11/22/06 reformatted version
!
!  This file has 10 sections.  Each section has a description of its
!  respective contents
!
!  SECTION 1; CURRENT STATE
!
! Item 1 Current Realization
! Item 2 Current Subarea

                1 ! realization: current realization for run
                3 ! subarea: current subarea for run

!  SECTION 2 ; SIMULATION TIME
!
! Item 1 Simulation time

                10000.00 ! tend: simulation time length [yr]
```

```
!  SECTION 3 ; WASTE PACKAGE GEOMETRY
!
! Item 1 Waste Package Length [m]
! Item 2 Waste Package Diameter [m]
! Item 3 Waste Package Layer 1 Thickness [m]
! Item 4 Waste Package Layer 2 Thickness [m]
! Item 5 Weld Alloy Thickness [m]

        5.1650 ! wplen: wp length [m]
        1.6590 ! wpdia: wp diameter [m]
        0.2000E-01 ! cthick1: wp layers 1 thickness [m]
        0.5000E-01 ! cthick2: wp layers 2 thickness [m]
        2.0000E-02 ! thickness: weld alloy thickness [m]

!  SECTION 4 ; DRY OXIDATION OF WP OUTER OVERPACK
!
!  Item 1 Metal Grain Radius [micrometer]
!  Item 2 Terms In Infinite Series For WP Oxidation
!  Item 3 Boundary thickness [micrometer]
!  Item 4 Constant Relating Matrix And Grain Boundary Diff

        0.1375E+02 ! grainr: metal grain radius [micrometer]
        25 ! nseries: terms in infinite series for wp oxidation
        0.7000E-03 ! gbthick: bundary thickness [micrometer]
        0.1000E+21 ! constant1: constant relating matrix and grain boundary diff

!  SECTION 5 ; EVAPORATION-CONDENSATION
!
!  Item 1 Critical Relative Humidity 1
!  Item 2 Critical Relative Humidity 2
!  Item 3 Thickness Of Water Film [m]

        0.1500E+00 ! humdc1: crit. rel. hums
        0.2000E+00 ! humdc2: crit. rel. hums
        0.0000E+00 ! filmthk: thickness of water film [m]

!SECTION 6 ; WELD AREA PARAMETERS
!
!  Item 1 Erp Intercept [mVSHE]
!  Item 2 Temperature Coefficient Erp Intercept [mVSHE/C]
!  Item 3 Erp Slope [mVSHE], Slope of Efp vs log10(Cl)
!  Item 4 Temperature Coefficient of Erp Slope [mVSHE/C]
!  Item 5 Minimum Chloride Concentration For LC For Weld[mol/L]
!  Item 6 Critical Inhibitor To Chloride Ratio
!  Item 7 Increase In Critical Potential At [inh]/[Cl]=inhToClw  [mV]
!  Item 8 Weld Surface Fraction For Advective Transport

        1.0420E+03 ! ErpInt: Erp Intercept [mVSHE]
        -2.0000E+01 ! TErpInt: Temp Coef Erp Intercept [mVSHE/C]
        -5.8420E+02 ! ErpSlope: Erp Slope [mVSHE], Slope of Efp vs log10(Cl)
        3.7000E+00 ! TErpSlope: Temp Coeff of Erp Slope [mVSHE/C]
        0.1000E-02 ! clcritw: minimum chloride conc. for LC for weld[mol/L]
        0.3000E+00 ! inhToClw: critical inhibitor to chloride ratio
        0.8000E+03 ! deltaEcInhWeld: Increase in crit. pot. at [inh]/[Cl]=inhToClw  [mV]
        1.7219E-02 ! frac_weld_surf, weld surface fraction for advective transport
```

```
!  SECTION 7 ; CRITICAL POTENTIAL PARAMETERS
!  Ep: pitting potential [mVshe]
!  Erp: repassivation potential [mVshe]
!
!  Item 1:  Outer Overpack Ep Intercept[mV]
!  Item 2:  Temperature Coefficient Of Outer Overpack Ep Intercept[mV/degC]
!  Item 3:  Outer Overpack Ep Slope[mV]
!  Item 4:  Temperature Coefficient Of Outer Overpack Ep Slope[mV/degC]
!  Item 5:  Outer Overpack Erp Intercept[mV]
!  Item 6:  Temperature Coefficient Of Outer Overpack Erp Intercept[mV/degC]
!  Item 7:  Outer Overpack Erp Slope[mV]
!  Item 8:  Temperature Coefficient Of Outer Overpack Erp Slope[mV/degC]
!  Item 9:  Inner Overpack Ep Intercept[mV]
!  Item 10:  Temperature Coefficient Of Inner Overpack Ep Intercept[mV/degC]
!  Item 11:  Inner Overpack Ep Slope[mV]
!  Item 12:  Temperature Coefficient Of Inner Overpack Ep Slope[mV/degC]
!  Item 13:  Inner Overpack Erp Intercept[mV]
!  Item 14:  Temperature Coefficient Of Inner Overpack Erp Intercept[mV/degC]
!  Item 15:  Inner Overpack Erp Slope[mV]
!  Item 16:  Temperature Coefficient Of Inner Overpack Erp Slope[mV/degC]

        -0.5848E+03 ! xipto: outer overpack Ep intercept[mV]
        0.3920E+01 ! pttemo: temp. coef. of outer overpack Ep intercept[mV/degC]
        -0.2450E+02 ! slpto: outer overpack Ep slope[mV]
        -0.1100E+01 ! slpttemo: temp. coef. of outer overpack Ep slope[mV/degC]
        0.1255E+04 ! xirpo: outer overpack Erp intercept[mV]
        -0.1175E+02 ! rptemo: temp. coef. of outer overpack Erp intercept[mV/degC]
        -0.7520E+03 ! slrpo: outer overpack Erp slope[mV]
        0.5201E+01 ! slrptemo: temp. coef. of outer overpack Erp slope[mV/degC]
        -0.2000E+03 ! xipti: inner overpack Ep intercept[mV]
        0.0000E+00 ! pttemi: temp. coef. of inner overpack Ep intercept[mV/degC]
        -0.2400E+03 ! slpti: inner overpack Ep slope[mV]
        0.0000E+00 ! slpttemi: temp. coef. of inner overpack Ep slope[mV/degC]
        -0.1000E+05 ! xirpi: inner overpack Erp intercept[mV]
        0.0000E+00 ! rptemi: temp. coef. of inner overpack Erp intercept[mV/degC]
        0.0000E+00 ! slrpi: inner overpack Erp slope[mV]
        0.1000E+01 ! slrptemi: temp. coef. of inner overpack Erp slope[mV/degC]

!  Section 8; CORROSION POTENTIAL PARAMETERS
!       hi: high pH parameter
!       lo: low pH parameter
!
!  Item 1 pHtran:  transition pH between low pH and high pH behavior
!  Item 2 ire1hi, C/(m^2 yr), reference curr main red. react., outer overpack
!  Item 3 ire1lo, C/(m^2 yr), reference curr main red. react., outer overpack
!  Item 4 beta1hi, effective transf. coeff., high pH, outer overpack
!  Item 5 beta1lo, effective transf. coeff., low pH, outer overpack
!  Item 6 betahy1: transfer coefficient for water reduction, outer overpack
!
!  Item 7 ire2hi, C/(m^2 yr), reference curr main red. react., inner overpack
!  Item  8 ire2lo, C/(m^2 yr), reference curr main red. react., inner overpack
!  Item  9 beta2hi, effective transf. coeff., high pH, inner overpack
!  Item 10 beta2lo, effective transf. coeff., low pH, inner overpack
!  Item 11 betahy2:  transfer coefficient for water reduction, inner overpack
!
```

```
! Item 12 rkhy1 [Coul/(m^2 yr)], rate constant for water reduction outer overpack
! Item 13 g1hi, [J/mol], activation energies for main red. react., outer overpack
! Item 14 g1lo [J/mol], activation energies for main red. react., outer overpack
! Item 15 ghy1 [J/mol], activation energy water reduction, outer overpack
! Item 16 npH1hi, pH reaction order, outer overpack
! Item 17 npH1lo, pH reaction order, outer overpack
! Item 18 nO1hi, oxygen reaction order, outer overpack
! Item 19 nO1lo, oxygen reaction order, outer overpack
!
! Item 20 rkhy2 [Coul/(m^2 yr)], rate constant for water reduction, inner overpack
! Item 21 g2hi, [J/mol], activation energies for main red. react., outer overpack
! Item 22 g1lo [J/mol], activation energies for main red. react., outer overpack
! Item 23 ghy2 [J/mol], activation energy water reduction, outer overpack
! Item 24 npH2hi, pH reaction order, outer overpack
! Item 25 npH2lo, pH reaction order, outer overpack
! Item 26 nO2hi, oxygen reaction orders, outer overpack
! Item 27 nO2lo, oxygen reaction orders, outer overpack
!
! Item 28 aa(1,1) [C/m2/yr] Passive current density for WP outer overpack
! Item 29 aa(1,2)
! Item 30 aa(1,3)
! Item 31 aa(2,1) [C/m2/yr] Passive current density for WP inner overpack
! Item 32 aa(2,2)
! Item 33 aa(2,3)
! Item 34 g1anod [J/mol], act. energy general corrosion rate, outer overpack
! Item 35 g2anod [J/mol], act. energy general corrosion rate, inner overpack
! Item 36 refTanod [K], temperature at which passive curr. is specified
!
! Item 37 eexpt: measured galvanic couple potentia [VSHE]
! Item 38 rcoef: coef. for loc. corr. of outer overpack
! Item 39 rexpont: exponent for loc. corr. of outer overpack
! Item 40 rcoef2: coef. for loc. corr. of inner overpack
! Item 41 rexpont2: exponent for loc. corr. of outer overpack
! Item 42 cratehac: humd.air corr.rt
! Item 43 xcouple, efficiency of galvanic coupling
! Item 44 xread: factor for defining choice of crit. potential
! Item 45 clcrit1: min. chloride conc. for LC, outer overpack [mol/L]
! Item 46 clcrit2: min. chloride conc. for LC, inner overpack [mol/L]
! Item 47 inhToCl1: critical inhibitor to Cl ratio, outer overpack
! Item 48 inhToCl2: critical inhibitor to Cl ratio, inner overpack
! Item 49 deltaEcInh1: Incr in crit pot at [inh]/[Cl]=inhToCl1, [mV], outer
! Item 50 deltaEcInh2: Incr in crit pot at [inh]/[Cl]=inhToCl2, [mV], inner
! Item 51 xgas: oxygen partial pressure [atm]
! Item 52 scalthk: scale thickness
! Item 53 taus: tortuosity
! Item 54 spor:porosity

        0.6000E+01 ! pHtran: transition pH between low pH and high pH behavior
        0.5510E+10 ! ire1hi, C/(m^2 yr), reference curr main red. react., outer overpack
        0.7570E+10 ! ire1lo, C/(m^2 yr), reference curr main red. react., outer overpack
        0.2480E-01 ! beta1hi, effective transf. coeff., high pH, outer overpack
        0.1287E-01 ! beta1lo, effective transf. coeff., low pH, outer overpack
        0.0000E+00 ! betahy1: transfer coefficient for water reduction, outer overpack
        0.7900E+12 ! ire2hi, C/(m^2 yr), reference curr main red. react., inner overpack
        0.7570E+10 ! ire2lo, C/(m^2 yr), reference curr main red. react., inner overpack
```

0.2480E-01 ! beta2hi, effective transf. coeff., high pH, inner overpack
0.1287E-01 ! beta2lo, effective transf. coeff., low pH, inner overpack
0.5000E+00 ! betahy2: transfer coefficient for water reduction, inner overpack
0.0000E+00 ! rkhy1 [Coul/(m^2 yr)], rate constant for water reduction outer overpack
0.4000E+05 ! g1hi [J/mol], activation energies for main red. react., outer overpack
0.4000E+05 ! g1lo [J/mol], activation energies for main red. react., outer overpack
0.2500E+05 ! ghy1 [J/mol], activation energy water reduction, outer overpack
0.1897E-01 ! npH1hi, pH reaction order, outer overpack
0.2560E-01 ! npH1lo, pH reaction order, outer overpack
0.0248 ! nO1hi, oxygen reaction order, outer overpack
0.01287 ! nO1lo, oxygen reaction order, outer overpack
0.0000E+00 ! rkhy2 [Coul/(m^2 yr)], rate constant for water reduction, inner overpack
0.4000E+05 ! g2hi, [J/mol], activation energies for main red. react., outer overpack
0.4000E+05 ! g2lo, [J/mol], activation energies for main red. react., outer overpack
0.2500E+05 ! ghy2 [J/mol], activation energy water reduction, outer overpack
0.1897E-01 ! npH2hi, pH reaction order, outer overpack
0.2560E-01 ! npH2lo, pH reaction order, outer overpack
0.0248 ! nO2hi, oxygen reaction orders, outer overpack
0.01287 ! nO2lo, oxygen reaction orders, outer overpack
0.2084E+04 ! aa(1,1) [C/m2/yr]
0.0E+00 ! aa(1,2)
0.0E+00 ! aa(1,3)
0.1000E+05 ! aa(2,1) [C/m2/yr]
0.0E+00 ! aa(2,2)
0.0E+00 ! aa(2,3)
0.4470E+05 ! g1anod [J/mol], act. energy general corrosion rate, outer overpack
0.4470E+05 ! g2anod [J/mol], act. energy general corrosion rate, inner overpack
0.4500E+03 ! refTanod [K], temperature at which passive curr. is
0.0000E+00 ! eexpt: measured galvanic couple potentia [VSHE]
0.2500E-03 ! rcoef: coef. for loc. corr. of outer overpack
0.1000E+01 ! rexpont: exponent for loc. corr. of outer overpack
0.1000E+01 ! rcoef2: coef. for loc. corr. of inner overpack
0.1000E+01 ! rexpont2: exponent for loc. corr. of outer overpack
0.2500E-07 ! cratehac: humd.air corr.rt
0.0000E+00 ! xcouple, efficiency of galvanic coupling
0.0000E+00 ! xread: factor for defining choice of crit. potential
0.1000E-02 ! clcrit1: min. chloride conc. for LC, outer overpack [mol/L]
0.1000E-09 ! clcrit2: min. chloride conc. for LC, inner overpack [mol/L]
0.1000E+00 ! inhToCl1: critical inhibitor to Cl ratio, outer overpack
0.1000E+11 ! inhToCl2: critical inhibitor to Cl ratio, inner overpack
0.9000E+03 ! deltaEcInh1: Incr in crit pot at [inh]/[Cl]=inhToCl1, [mV], outer
0.0000E+00 ! deltaEcInh2: Incr in crit pot at [inh]/[Cl]=inhToCl2, [mV], inner
0.2100E+00 ! xgas: oxygen partial pressure [atm]
0.0E+00 ! scalthk: scale thick
0.1E+01 ! taus: tortuosity
0.1E+01 ! spor:porosity

! Section 9 ; Radiolysis parameters
!
! Item 55 deltaEo : Delta Potential Due To Radiolysis. [V]
! Item 56 lamb : Radiolysis decaying constant. [1/yr]
! Item 57 dense1 : Density of Outer Overpack. [kg/m3]
! Item 58 dense2 : Density of Inner Overpack. [kg/m3]
! Item 59 wtmol1 : Equivalent Weight of Outer Overpack. [kg/mol]
! Item 60 wtmol2 : Equivalent Weight of Inner Overpack. [kg/mol

```
          0.0000E+00 ! deltaEo: Delta Potential Due To Radiolysis. [V]
          0.7000E-04 ! lamb: Radiolysis decaying constant. [1/yr]
          0.869000E+04 ! dense1 [kg/m3]
          0.798000E+04 ! dense2 [kg/m3]
          0.259700E-01 ! wtmol1 [kg/mol]
          0.249400E-01 ! wtmol2 [kg/mol]

!  Section 10 ; Mechanical failure data
!
!  Item 61 yieldstr: yield strength [MPa]
!  Item 62 sfactor: safety factor
!  Item 63 dkic: fracture toughness [MPa-m**0.5]

          0.3103E+03 ! yieldstr: yield strength [MPa]
          0.1000E+01 ! sfactor: safety factor
          0.3040E+03 ! dkic: fracture toughness [MPa-m**0.5]

! Section 11 ; Runge-kutta control parameters
!
! Item 64 dtini
! Item 65 dtmax
! Item 66 errrel (same as eps)
! Item 67 errabs (same as tiny)

          0.1000E-02 ! dtini
          0.1000E+01 ! dtmax
          0.1000E-01 ! errrel (same as eps)
          0.1000E-29 ! errabs (same as tiny)

!end
*************************************************************************************
```

The test case demonstrates that correct inputs are passed from the *ebsfail.f* to the *failt.f* code via *ebsfail.inp*. These results are submitted as evidence that objective 1 of SVR9 has been successfully tested.

Test Results (PASS/FAIL): **PASS**

2a. The following equation for corrosion potential was independently programmed in MATLAB® Version 7.4.0.287.

$$E_{corr} = \frac{E_a^a - E_a^{ef}}{Z_r \beta_r^{ef} F} - \frac{E_a^a T}{Z_r \beta_r^{ef} F T_{ref}^a} + \frac{RT}{Z_r \beta_r^{ef} F} \ln\left[\left(\frac{[H^+]}{1mol/L}\right)^{n_o}\left(\frac{pO_2}{1\ atm}\right)^{n_H} \frac{i_r^{ref}}{i_a^o} \frac{C_{O_2}^{bulk}(T)}{C_{O_2}^{bulk}(T_{ref})}\right]$$

where

E_{corr} — Corrosion potential (Volts, vs. Standard Hydrogen Electrode)

E_a^a — Activation energy for the anodic current density [J/mol], as specified by the input parameter OuterActivationEnergyPassiveCurrDens [J/mol]

E_a^{ef}	—	effective activation energy, J/mol, as specified by the input parameter OuterActivationEnergyReductionReactLowpH [J/mol] for pH < 6, and OuterActivationEnergyReductionReactHighpH[J/mole] for pH > 6
Z_r	—	number of electrons in the cathodic reaction, 4
T_{ref}	—	reference temperature [K]
i_a^o	—	anodic current density at reference temperature[Coul/(m^2yr)], as specified by the input parameter AA_1_1[C/m2/yr]
i_r^{ref}	—	reference current density [Coul/(m^2yr)], as specified by the input parameter OuterReferenceCurrReductionReactLowpH[C/(m2*yr)] for pH <6, and OuterReferenceCurrReductionReactHighpH[C/(m2*yr)] for pH >6
F	—	Faraday's constant = 96486.7 [C/mol]
$C_{O_2}^{bulk}(T)$	—	dissolved oxygen concentration in solution as a function of temperature [mol/kg]
$C_{O_2}^{bulk}(T_{ref})$	—	dissolved oxygen concentration in solution at the reference temperature [mol/kg]
β_r^{ef}	—	dimensionless effective charge transfer coefficient, as specified by the input parameter OuterChargeTransferCoefReductionReactLowpH for pH < 6, and OuterChargeTransferCoefReductionReactHighpH for pH > 6
T_{ref}^a	—	reference temperature for anodic current density [K], as specified by the input parameter RefTemperaturePassiveCurrDens[K]
T	—	temperature of the system[K]
n_H	—	dimensionless constant, as peicified by the input parameter OuterEffectiveReactionOrderHLowpH for pH < 6, and OuterEffectiveReactionOrderHHighpH for pH > 6
n_o	—	dimensionless constant, as speicified by the input parameter OuterChargeTransferCoefReductionReactLowpH for pH < 6, and OuterChargeTransferCoefReductionReactHighpH for pH > 6
	—	partial pressure of oxygen in atmosphere, 0.21 atmosphere [3.09 psi]
R	—	Universal gas constant, 8.31447215 J K^{-1} ·mol^{-1}
$[H^+]$	—	Hydrogen ion concentration [M], 10^{-pH}

First, the *tpameans.out* file generated by reference case for TPA Version 5.1BetaT was used as the *tpa.inp* file, and the following parameters specified in *tpa.inp* according to the following table.

Values of Parameters to Calculate Corrosion Potential		
Parameter	**Value at pH < 6 [parameter name in tpa.inp]**	**Value at pH > 6 [parameter name in tpa.inp]**
E_a^a (kJ/mol)	44.7	44.7
E_a^{ef} (kJ/mol)	40	40
i_a^o [Coul/(m^{2}yr)]	3427	3427
T_{ref}^a (K)	368.15	368.15
T_{ref} (K)	298.15	298.15
β_r^{ref}	0.01287	0.0248
n_H	0.0256	0.01897
i_r^{ref} [Coul/(m^{2}yr)]	7.57×10^9	5.51×10^9
n_o	0.01287	0.0248

TheTPA code was executed for one reference case realization for subarea 3. The information needed to implement the corrosion potential model in MATLAB®, such as waste package surface temperature and pH as a function of repository emplacement time was imported in the MATLAB® program by reading the data in file *ebstrh.dat*.

The MATLAB® code was executed. The calculate value of corrosion potential by TPA code, which is stored in gencorrfail.out was compared to the ones estimated by the MATLAB® .

Pass/Fail criteria

The relative difference between two calculated values at each time step should be less than 5 percent.

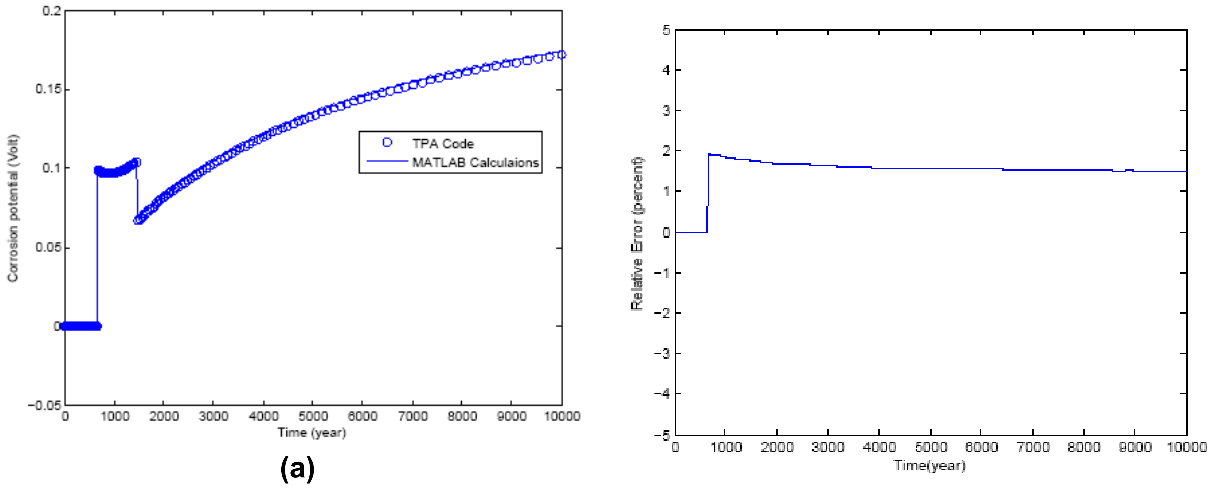
Results

The TPA and MATLAB® code were executed as described. The results of calculations are presented in Figure 1(a) and 1(b).

The corrosion potential calculated by the TPA code and by the MATLAB® are presented in Figure 1a, and residual error in corrosion potential at each time step is presented in Figure 1b. The maximum residual error between two calculated values of corrosion potential is less that 2 percent.

Test Results (PASS/FAIL): **PASS**

2b. In TPA code, the passive current density is used to compute the general corrosion rate. The passive current density at a given temperature is computed by the following expression



(a)

(b)

Figure 1. Simulation Results for Test Case 2a: (A) Comparison of Corrosion Potential Obtained Using the TPA and the MATLAB® Codes, (B) Relative Residual Error (In Percent) Between Corrosion Potential Values Obtained Using the TPA and the MATLAB® Code.

$$i_a(T) = i_a^0 exp\left[-\frac{E_a^a}{R}\left(\frac{1}{T} - \frac{1}{T_{ref}^a}\right)\right]$$

where

$i_a(T)$	—	passive current density at temperature T
i_a^0	—	passive current density at T_{ref}^a [C/(m^2 yr)], as defined by parameter AA_1_1[C/m2/yr]
E_a^a	—	effective activation energy for the anodic current density [J/mol], as specified by the input parameter OuterActivationEnergyPassiveCurrDens[J/mol]
R	—	Universal gas constant, 8.314 [J/mol-K]
T_{ref}^a	—	reference temperature for passive current density [K], as specified by the input parameter RefTemperaturePassiveCurrDens[K]

Using the passive current density, the corrosion rate is computed by the expression

$$CR = \frac{i^a(T)E_w}{F\rho}$$

where

CR	—	general corrosion rate [m/year]
$i^a(T)$	—	passive current density [C/(m^2 yr)] at temperature T
E_w	—	equivalent molecular weight [kg/mol],as specified by the input parameter EquivalentWeightOuterOverpack[kg/mol]
F	—	Faraday's constant, 96486.7 C/mol

ρ — Material density [kg/m^3], as specified by the input parameter DensityOuterOverpack[kg/m^3]

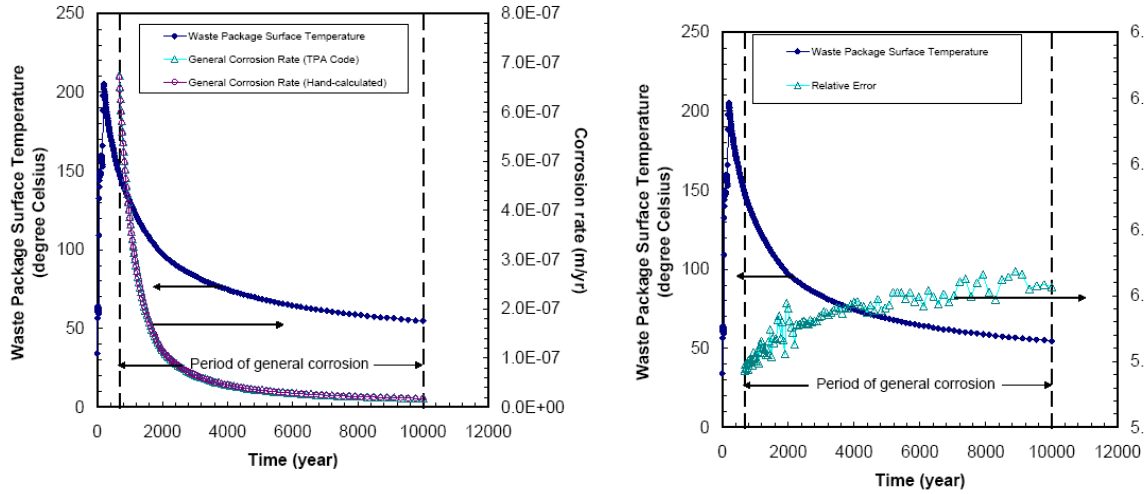
First, the *tpameans.out* file generated by reference case for TPA Version 5.1BetaT was used as the *tpa.inp* file, and the following parameters values listed in the table were specified in *tpa.inp*.

Values of Parameters to Passive Current Density and Corrosion Rate	
Parameter	**Value**
E_a^a (kJ/mol)	44.7
i_a^o [Coul/(m^{2}yr)]	3427
E_w	0.02597
T_{ref}^a (K)	368.15
ρ (kg/m^3)	8690

The TPA code was executed for one reference case realization for subarea 3. The general corrosion rate at each time step is stored in file *gencorrfail.out*. The waste package surface temperature for each time step was imported into a Microsoft excel file. The corrosion rate was independently calculated and compared to the values estimated by the TPA code for each time step.

Pass/Fail criteria
The relative difference between two calculated values at each time step should be less than 5%.

Results: The TPA code was executed as outlined above. The results of simulations are presented in Figure 2a and 2b. The general corrosion rate calculated by TPA code and hand-calculated (H-C) values at each time step are plotted in Figure 2a. The corresponding relative error between two values are plotted in Figure 2b. The relative residual errors between two values for each timestep are less than 0.6 percent which indicate that pasive current density is accurately estimated in the TPA code.



(a) (b)

Figure 2: Simulation results for test case 2b: (a) The TPA and hand-calculated values of general corrosion rate versus simulation time, (b) The relative error between two corrosion rates versus simulation time.

Test Results (PASS/FAIL): **PASS**

---

3. The repassivation potential for welded and mill-annealed Alloy 22 is separately calculated in TPA code. The following empirical relationship is implemented in the TPA code to estimate the repassivation potential.

$$E_{crit}(T) = A_1 + A_2 T + (B_1 + B_2 T)\log_{10}\left(\frac{[Cl^-]}{c_0}\right) + \Delta E_{crit}$$

where

E_{crit}(T) — repassivation potential for localized corrosion initiation (mV_{SHE}) at temperature T

A_1 — intercept constant [mV_{SHE}], as specified by the input parameter OuterOverpackErpIntercept or ErpInterceptWeld

A_2 — intercept slope constant (mV/^{o}C), as specified by the input parameter TempCoefOfOuterPackErpIntercept or TemperatureCoefficientOfErpInterceptWeld

B_1 — chloride concentration intercept constant, (mV_{SHE}), as specified by the input parameter OuterOverpackErpSlope or ErpSlopeWeld

B_2 — chloride concentration intercept slope constant,(mV/^{o}C), as specified by the input parameter TempCoefOfOuterPackErpSlope or TemperatureCoefficientOfErpSlopeWeld TempCoefOfOuterPackErpSlope or TemperatureCoefficientOfErpSl opeWeld , TempCoefOfOuterPackErpSlope or TemperatureCoefficientOfErpSl opeWeld

$\left[Cl^{-}\right]$ — chloride ion concentration of in-drift water (M)

c_o — constant, 1M

ΔE_{crit} — correction term in critical potential, (mV_{SHE})

The term ΔE_{crit} accounts for the inhibiting effect of oxyanions such as nitrate, sulfate, or bicarbonate on localized corrosion. The experimental results have shown that in the presence of oxyanaions, E_{crit} increases sharply. The term ΔE_{crit} is computed by the following expression

$$\Delta E_{crit} = \Delta E^{0}_{crit} \frac{min(r,r_n)}{r_n}$$

where

ΔE_{crit}^{0} — critical potential constant, (mV_{SHE}), as specified by OuterDeltaEcritInh or WeldDeltaEcritInh

The term r in the expression for ΔE_{crit} is a linear combination of oxyanion to chloride concentration ratios defined as

$$r = \frac{[NO_3^{-}]}{[Cl^{-}]} + \frac{r_n}{r_s}\frac{[SO_4^{2-}]}{[Cl^{-}]} + \frac{r_n}{r_c}\frac{[CO_3^{2-}] + [HCO_3^{-}]}{[Cl^{-}]}$$

where

r_n — nitrate inhibitor constant, as specified by the input parameter OuterInhibitingNitrateToCl or WeldInhibitingNitrateToCl

r_c — carbonate inhibitor constant, as specified by the input parameter OuterInhibitingCarbonateToCl or WeldInhibitingCarbonateToCl

r_s — sulphate inhibitor constant, as specified by the input parameter OuterInhibitingSulfateToCl or WeldInhibitingSulfateToCl

The *tpameans.out* file generated by reference case for TPA Version 5.1BetaT was used as the *tpa.inp file*. The values of A_1, A_2, B_1, B_2, ΔE_{crit}^{0} , r_n, r_s, and r_c were specified in *tpa.inp* according to the following table.

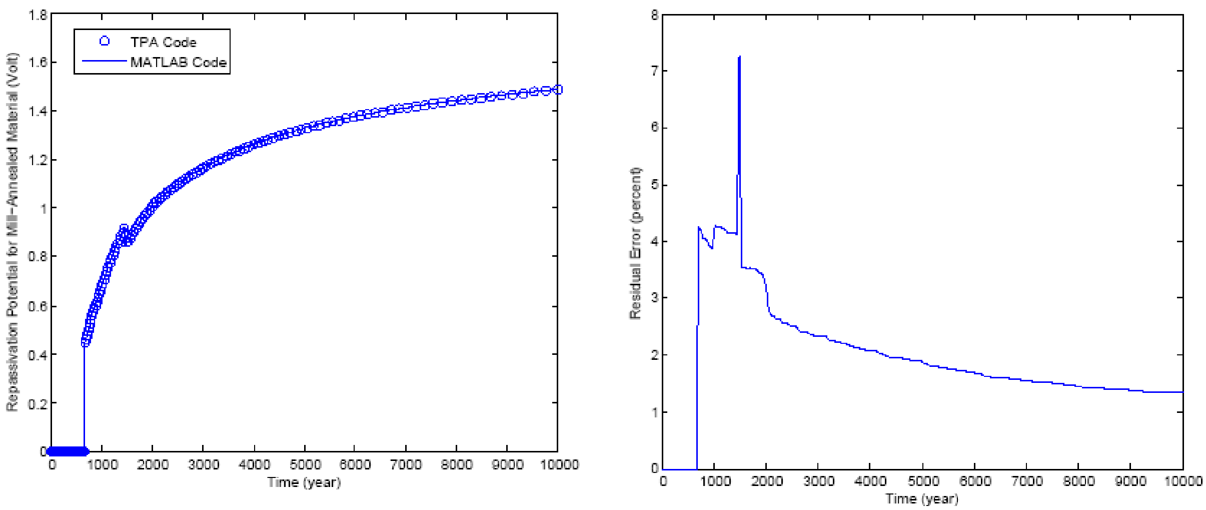
Parameters Values Used to Estimate the Repassivation Potential E_{crit}.								
Metallurgical Condition	A_1	A_2	B_1	B_2	ΔE_{crit}^{0} (mV)	r_n	r_s	r_c
Mill-Annealed	1591.2	−13.1	−362.7	2.3	800	0.1	0.5	0.2
Thermally Aged (Welded Alloy 22)	1041.2	−10.0	−584.2	3.7	800	0.3	0.5	0.2

The TPA code was again executed again for one realization and subarea 3. The repassivation potential for mill-annealed Alloy 22 is stored in *failt.out,* and for welded material in *weldfail.out*.

The equations for repassivation potential with the aforementioned parameter values was independently programmed in MATLAB® . The temperature of the waste package surface and corresponding simulation time step was imported from files *ebstrhc.inp* and *corrode.out*. The chloride concentration of in-drift water at each time step and was imported from file *chlrdmf.dat*. The value of r, which is pre-computed by the near field environment module at each time step for welded and mill-annealed Alloy 22 and stored in file *ebstrhc.inp*, was also imported in MATLAB® code. The MATLAB® code was executed and values of repassivation potential for mill-annealed and welded materials were compared to the ones generated by TPA code at time step.

Pass/Fail criteria
The relative difference between two calculated values at each time step should be less than 10 percent.

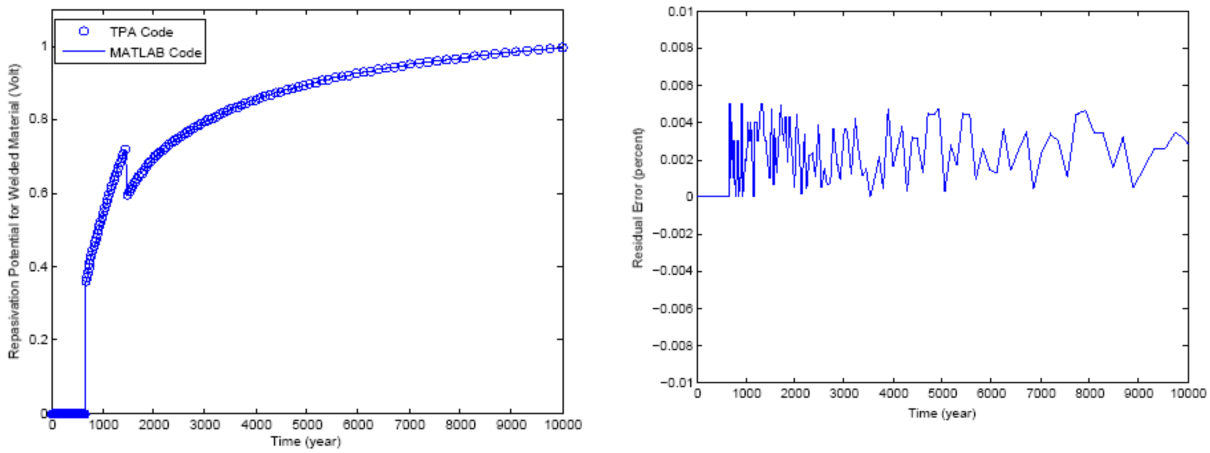
Results:
Both TPA and MATLAB® codes were executed according to the procedure outlined above. The results of the simulation for mill-annealed Alloy 22 are presented in Figure 3. The calculated values of repassivation potential at each time step for mill-annealed Alloy 22 using the TPA and the MATLAB code are presented in Figure 3a. The corresponding relative residual error between two values are presented in Figure 3b. The maximum relative residual error is less than 10 percent for each timestep.



(a) (b)

Figure 3: Simulation results for test case 3a: (a) The repassivation potential as a function of simulation time for mill-annealed Alloy 22 as calculated by TPA and MATLAB® code, (b) The relative error between the two repassivation potential versus simulation time.

Similarly, the results of the simulation for welded Alloy 22 are presented in Figure 4. The calculated values of repassivation potential at each time step for welded Alloy 22 using the TPA and the MATLAB code are presented in Figure 4a. The corresponding relative residual errors between two values for each timestep are presented in Figure 4b. The maximum relative residual error is less than 10 percent.



(a) (b)

Figure 4: Simulation results for test case 3b: (a) The repassivation potential as a function of simulation time for wleded Alloy 22 as calculated by the TPA and MATLAB® code, (b) The relative residual errors between the two repassivation potentials as a function of simulation time.

Test Results (PASS/FAIL): **PASS**

4a. First, the time of waste package failure due to general corrosion was tested. The *tpameans.out* file generated by reference case for TPA Version 5.1BetaT was used as the *tpa.inp* file. The input values of the following six parameters were changes in accordance with the table below:

Parameter	Value
CriticalRelativeHumidityHumidAirCorrosion	0.2
CriticalRelativeHumidityAqueousCorrosion	0.2
OuterActivationEnergyPassiveCurrDens[J/mol]	0
AA_1_1[C/m2/yr]	3.2E5
OuterOverpackErpIntercept	100000
ErpInterceptWeld	100000

By assigning the same values of CriticalRelativeHumidityHumidAirCorrosion and CriticalRelativeHumidityAqueousCorrosion, the humid air corrosion is deactivated. Similarly, by assigning a large values of OuterOverpackErpIntercept and ErpInterceptWeld, it is ensured that localized corrosion will not activate. In the test, the temperature independent general corrosion rate is implemented by assigning OuterActivationEnergyPassiveCurrDens[J/mol] to zero. In addition, the general corrosion rate is increased by four orders of magnitude to ensure that waste package outer container thickness reduces to zero before 10,000 years. The waste package thickness should change linearly with time due to temperature-independent general corrosion rate. The TPA code was executed for one reference case realization for subarea 3.

The general corrosion rate at each time step and time of failure for mill-annealed and welded Alloy 22 is stored in file *corrode.out* and *weldfail.out*, respectively. The time of failures were hand-calculated (H-C) for both materials and compared to the values provided by the TPA code.

Pass/Fail criteria
The relative difference between two computed values of times of failures should be less than 5 percent.

Results:
The TPA code was simulated using the procedure outlined above. The results are summarized in the following Table.

Summary of Results for Test Case 4a

	Hand-Calculation		TPA Code	
	WP Body	Welds	WP Body	Welds
Initiation Time for general corrosion (years)	657.5191	666.3513	657.5191	666.3513
Time of Failure (yrs)	2675.3989	2684.2311	2675.3615	2684.2493
Net General Corrosion Time (yrs)	2017.8798	2017.8798	2017.8484	2017.8980
	Ave. 2017.8798		Ave. 2017.8732	
	Ratio (H-C/TPA) = 1.000003			

The times of failures for the waste package body (WP Body) and the welds (Welds) provided by TPA code are consistent with the values obtained by hand-calculation.

The computed results demonstrate that the failure times due to general corrosion for the WP Body and the Welds are correctly reported by EBSFAIL. The relative difference between the hand-calculated values and TPA code values for failure time is much less than 5 percent for both mill-annealed and welded materials. These results are presented as evidence that test objective has been successfully met.

Test Results (PASS/FAIL): **PASS**

4b. The time of waste package failure due to localized corrosion was tested. The *tpameans.out* file generated by reference case for TPA Version 5.1BetaT was used as the *tpa.inp* file. The input values of following two parameters were changes in accordance with the table below:

Parameter	Value
OuterOverpackErpIntercept	-100000
ErpInterceptWeld	-100000

The large negative values of OuterOverpackErpIntercept and ErpInterceptWeld ensures that the corrosion potential is much larger than the repassivation potential for mill-annealed and welded Alloy 22. The TPA code was executed for one reference case realization for subarea 3. The time of failure due to localized corrosion for mill-annealed and welded Alloy 22 is stored in file *failt.cum* and *weldfail.out*. The time of failure was hand-calculated and compared to the values provided by the TPA code.

Pass/Fail criteria
The relative difference between two computed values of time of failure should be less than 5 percent.

Results
The TPA code was simulated using the procedure outlined above. The results are summarized in the following Table.

Summary of Results for Test Case 4b

	Hand-Calculation		TPA Code	
	WP Body	Welds	WP Body	Welds
Start Time (Initiation Time) (yrs)	657.6148	666.3780	657.6148	666.3780
Finish Time (Time of Failure) (yrs)	737.6148	746.3780	737.6150	746.8600
Net Localized Corrosion Time (yrs)	80.0000	80.0000	80.0002	80.0020
	Ave. 80.0000		Ave. 80.0011	
	Ratio (H-C/TPA) = 9.9999E-01			

The times of failures for the waste package body (WP Body) and the welds (Welds) provided by TPA code are consistent with the values obtained by hand-calculation.

These results demonstrate that the waste package failure times due to localized corrosion for the WP Body and the Welds are correctly reported by EBSFAIL. The relative difference between the hand-calculated values and TPA code values for failure time is much less than 5 percent for both mill-annealed and welded materials.

These results are presented as evidence that test objective has been successfully met.

Test Results (PASS/FAIL): **PASS**

5a. The test procedure outlined in 4a was repeated with additional change in values of the two parameters according to the following table

Parameter	**Value**
WPFractionThicknessPenetratedForFailureByCorrosion[]	0.75
WPWeldFractionThicknessPenetratedForFailureByCorrosion[]	0.75

The time of waste package failure should reduce by 25 percent by changing values of the two parameters from 1 to 0.75. The output values of time of waste package failure by TPA code were compared to the hand-calculated values. The relative difference between two computed values was less than 5 percent.

Pass/Fail criteria
The relative difference between two computed values of time of failure should be less than 5 percent.

Results:
The TPA code was simulated using the procedure outlined for test case 5a. The results are summarized in the following Table.

Summary of Results for Test 5a

	Hand-Calculation		TPA Code	
	WP Body	Welds	WP Body	Welds
Start Time (Initiation Time) (yrs)	657.5191	666.3513	657.5191	666.3513
Finish Time (Time of Failure) (yrs)	2170.9260	2179.7612	2170.9067	2179.7582
Net General Corrosion Time (yrs)	1513.4099	1513.4099	1513.3876	1513.4069
	Ave. 1513.4099		Ave. 1513.3972	
	Ratio (H-C/TPA) = 1.000008			

The times of failures for the waste package body (WP Body) and the welds (Welds) provided by TPA code are consistent with the values obtained by hand-calculation.

The computed results demonstrate that the EBSFAIL failure times for the WP Body and the Welds by general corrosion are correctly reported by EBSFAIL. The relative difference between the hand-calculated values and TPA code values for failure time is much less than the 5 percent for both mill-annealed and welded materials.

The following table summarizes the net times at two different values of fraction (i.e., 1 and 0.75) in the case of general corrosion. As shown in this table, the net times are reduced approximately 25 percent by reducing values of failure criteria from 1 to 0.75.

Changes of Net Times at Different Specified Failure Depth Threshold in the Case of General Corrosion Mode.

Specified Failure Depth Thresholds (fraction)	Ave. Net Time by Hand-Calculation (yrs)	Ave. Net Time by TPA Code (yrs)
1 0.75	2017.8789 1513.4099	2017.8732 1513.3972
Fraction of Changes of Net Time		
-0.25	-0.2499	-0.2500
	Ave. -0.2499	

These results are presented as evidence that test objective has been successfully met.

Test Results (PASS/FAIL): **PASS**

5b. The test procedure outlined in 4b was repeated with additional changes in values of the two parameters according to the following table

Parameter	Value
WPFractionThicknessPenetratedForFailureByCorrosion[]	0.75
WPWeldFractionThicknessPenetratedForFailureByCorrosion[]	0.75

The time of failure should reduce by 25 percent because of the change in values of the above two parameters. The output values of time of failure by TPA code were compared to the hand-calculated values.

Pass/Fail criteria
The relative difference between two computed values of time of failure should be less than 5 percent.

Results:
The TPA code was simulated using the procedure outlined for test case 5b. The results are summarized in the following Table.

Summary of Results for Test Case 5b

	Hand-Calculation		TPA Code	
	WP Body	Welds	WP Body	Welds
Start Time (Initiation Time) (yrs)	657.6148	666.3780	657.6148	666.3780
Finish Time (Time of Failure) (yrs)	717.6148	726.3780	718.6390	726.3776
Localized Corrosion Failure Time (yrs)	60.0000	60.0000	61.0242	59.9996
	Ave. 60.0000		Ave. 60.5119	
	Ratio (H-C/TPA) = 9.9145E-01			

The times of failures for the waste package body (WP Body) and the welds (Welds) provided by TPA code are consistent with the values obtained by hand-calculation.

The computed results demonstrate that the failure times by localized corrosion for the WP Body and the Welds are correctly reported by EBSFAIL. This is also supported by the very low value of ratio (8.46E-1), which is much less than 5 percent as a criterion.

The following Table summarizes the net times at two different values of fraction (i.e., 1 and 0.75) in the case of localized corrosion. As shown in this table, the net times are reduced approximately 25 percent by reducing values of fractions from 1 to 0.75.

Changes of Net Time at Different Specified Failure Depth Threshold in the Case of Localized Corrosion Mode.		
Specified Failure Depth Thresholds (fraction)	Ave. Net Time by Hand-Calculation (yrs)	Ave. Net Time by TPA Code (yrs)
1 0.75	80.0000 60.0000	80.0011 60.5119
Fraction of Changes of Net Time		
-0.25	-0.2500	-0.2436
	Ave. -0.2468	

These results are presented as evidence that this objective has been successfully tested.
Test Results (PASS/FAIL): **PASS**

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6. This procedure tested the onset of localized when drift wall temperature falls below a threshold value. The *tpameans.out* file generated by reference case for TPA Version 5.1BetaT was used as the *tpa.inp* file. The corrosion potential model for Alloy 22 in the TPA code predicts higher values in low pH environment than in high pH. The repassivation potential model predicts a low value for high chloride and low nitrate concentration solutions. Using these two facts, the following parameters values were in *tpa.inp* changed according to the following table.

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DriftDegradationScenarioFlag(yes=1,no=0)	0
DSFractionThicknessPenetratedForFailureByCorrosion[]	0
EnvironmentII_Cl_Subarea_3[mol/L]	50.0 mol/L
EnvironmentII_pH_Subarea_3[]	3
EnvironmentII_NO3_Subarea_3[mol/L]	0.01 mol/L
SeepageThresholdT[C]	90 °C

These parameter values ensure that the repassivation potential for localized corrosion initiation is much lower than the corrosion potential at each time step in Environment II. The TPA code was executed for one reference case realization for subarea 3. The time for localized corrosion initiation for mill-annealed and welded material is recorded in files *failt.out* and *weldfail.out*. The drift wall temperature as a function of simulation time is recorded in *nfenv.rlt* for each time step. The simulation time was obtained from the file when drift wall temperature reaches the value of SeepageThresholdT[C] as specified in *tpa.inp*. The corresponding localized corrosion initiation time was obtained from output files *fail.out* and *weldfail.out*. The localized initiation time and the time when drift wall temperature reaches the value of SeepageThresholdT[C] were found to be same.

Pass/Fail criteria
The localized corrosion initiation temperature is at or below the value specified by input parameter SeepageThresholdT[C].

Results:

The tpa code was executed as mentioned above. The drift wall temperature reached to 89.84 °C at time 1601.11 years. The localized corrosion of mill-annealed Alloy 22 started at time 1601.11 years. Similarly, localized corrosion welded material also started 1601.11 years. The results of this test are presented in Figure 5 as shown below. The blue diamond symbols represent the drift wall temperature versus simulation time, the pink and green symbols represent the waste package (mill-annealed Alloy 22) and welded material thickness.

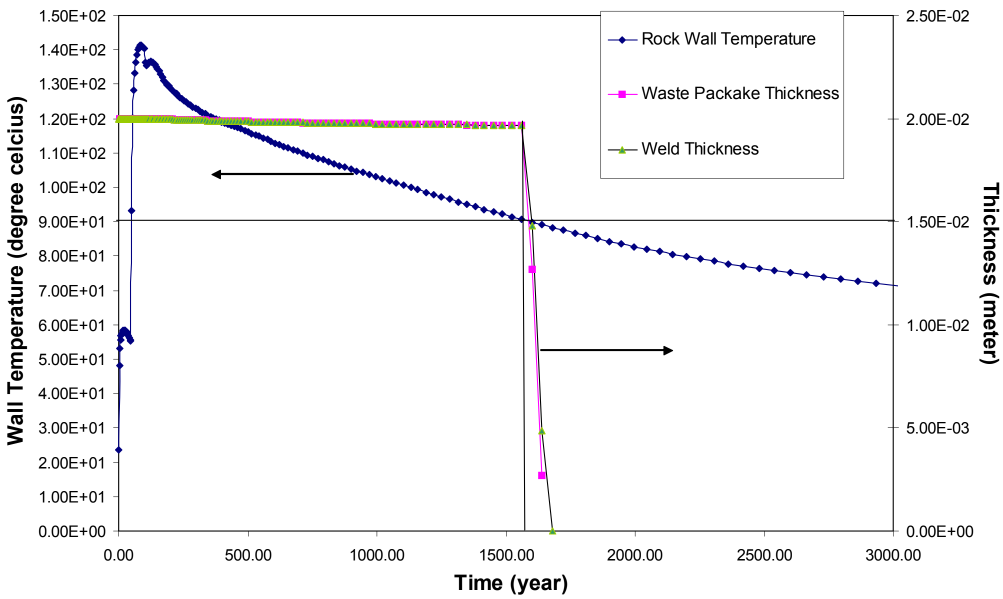


Figure 5: Simulation results for test case 6.

Test Results (PASS/FAIL): **PASS**

SOFTWARE VALIDATION REPORT (SVR)

SVTR#:	Project#: 20.06002.01.354
Software Name: TPA	Version: 5.1betaT, 5.1betaU
Test ID: **P-10**	Test Series Name: **Releases from the Engineered Barrier System**

Test Method

code inspection	x spreadsheet
x output inspection	x graphical
hand calculation	comparison with external code results

Test Objective: Verify the functionalities implemented in RELEASET.

Test Environment Setup

Hardware (platform, peripherals): Various desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): Windows XP

Input Data (files, data base, mode settings): See the Attachments A through I for descriptions of input data for tests 1 through 9

Assumptions, constraints, and/or scope of test: (none)

Test Procedure:
A total of nine tests were developed for this TPA Version 5.1 validation task.
See the Attachments A through I for descriptions of test procedures for tests 1 through 9.

Test Results

Location: See attached CDs labeled “TPA Version 5.1 Validation Task P10"

Test Criteria or Expected Results:.
See the Attachments A through I for descriptions of test criteria for tests 1 through 9.

Test Evaluation (Pass/Fail): **Pass**

Notes: Summaries of Analyses for Tests 1–9 can be found in Attachments A–I.

Tester: Hakan Basagaoglu Robert Rice	Date: April 27, 2007

Attachment A
TPA Version 5.1 Validation Task P-10
Test 1 Description

Test Method	
code inspection	x spreadsheet
x output inspection	x graphical
hand calculation	comparison with external code results
Test Objective: Verify the functionalities implemented in RELEASET.	
Test Environment Setup	
Hardware (platform, peripherals): Desktop computers Software (OS, compiler, libraries, auxiliary codes or scripts): Windows XP Input Data (files, data base, mode settings): See the Attachments A through I for descriptions of input data for tests 1 through 9.	
Assumptions, constraints, and/or scope of test: (none)	
Test Procedure: Execute the TPA code for 10,000 yr, 100,000 yr, and 1,000,000 yr using the mean value data file for Subarea 3. Plot the release rates from *ebsnef2.dat* for I-129, Tc-99, Pu-239, Pu-240, Np237, JP239, and JP 240, and verify the results are consistent for overlapping times (e.g., over 10,000 yrs, for 10,000 yr, 100,000 yr, and 1,000,000 yr simulations; over 100,000 yrs, for 100,000 yr and 1,000,000 yr simulations).	
Test Results	
Location: P10\TPA_Validation\Test1 Test Criterion or Expected Results: The release rates are expected to be independent of the simulation length chosen and the results should be consistent for overlapping times. Test Evaluation (Pass/Fail): **Pass**	
Notes: See following pages of this attachment for analysis of results.	
Tester: Hakan Basagaoglu Robert Rice	Date: April 27, 2007

Results:

TPA was run first using the **mean value data file** for 10,000 years (10Ky hereafter); however, the model results did not show any releases from the EBS and UZ during this time period. Part of the screen output is given below:

```
    exec: time of drip shield mechanical failure =      388.5  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Corrosion Breach on WP Welded Areas
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  2904  ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
     ebsrel: running glass waste form
                    There is no EBS release
exec: calling uzft
                    There is no UZ release
exec: calling szft
                    There is no SZ release
exec: calling dcagw
                    There is no GW release
                    There is no release
exec: end realizations
exec: Peak Mean Dose is 0.00000E+00 rem/yr at      0.0 yr, based on     1 realizations.
```

Therefore, TPA was executed using a single realization by setting *StartAtRealization* =1 and *StopAtRealization* = 1 was in *tpa.inp*. Hence, “realization #1" was used for Test 1.

TPA was run for Subarea 3 using the reference case for the realization #1 for the simulation period of 10Ky, 100Ky, and 1000Ky. Waste packages failed by localized corrosion within the first 10 Ky. Waste packages failed by mechanical events at t>30 Ky. Screen summary of each simulation (with a different simulation length) is shown below.

10Ky simulation

```
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      501.3  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =     1660.0  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    149 at TPA time =   1640.9 yr
 *** failed WPs:  149   out of  2904  ***
```

100Ky simulation

```
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      435.7  yr
    exec: time of drip shield failure by general corrosion =   68722.0  yr
    exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =     1167.8  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
```

*** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from MECHANICAL event = 378 at TPA time = 31600.0 yr
*** failed WPs: 378 out of 526 ***

1000Ky simulation
exec: calling mechdriver (drip shield)
exec: time of drip shield mechanical failure = **435.7** yr
exec: time of drip shield failure by general corrosion = 68722.0 yr
exec: calling nfenv
exec: calling ebsfail
ebsfail: time of corrosion breach on welded areas = 1167.8 yr
*** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
*** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from MECHANICAL event = 378 at TPA time = 39700.0 yr
*** failed WPs: 378 out of 526 ***

The release rates of I129, Tc129, Pu239, Pu240, Np237, JP239, and JP 240 from EBS in the first 10Ky from TPA runs for 10Ky, 100Ky, and 1000Ky simulation lengths are shown in Fig. 1a - Fig. 1g The source of data was ebsnef2.dat.

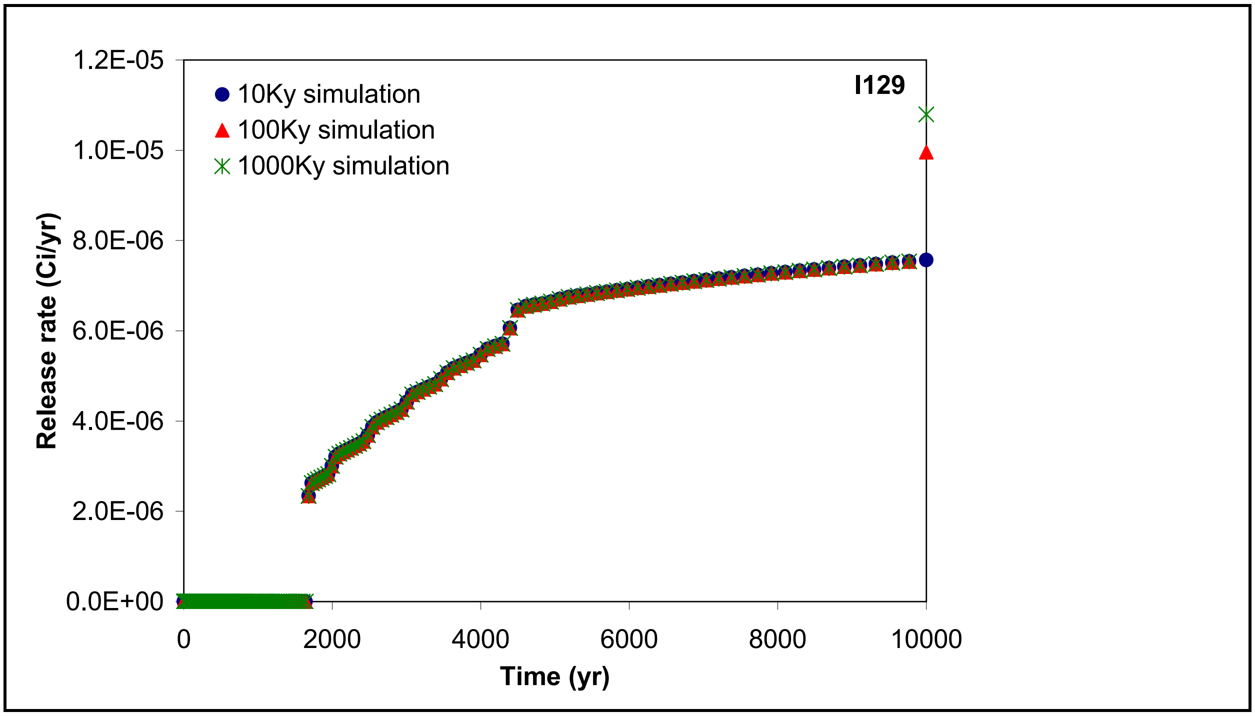


Fig. 1a. Release rates of I129 from the EBS (Engineered Barrier Systems) in the first 10Ky resulting from TPA runs for 10Ky, 100Ky, and 1000Ky long simulations.

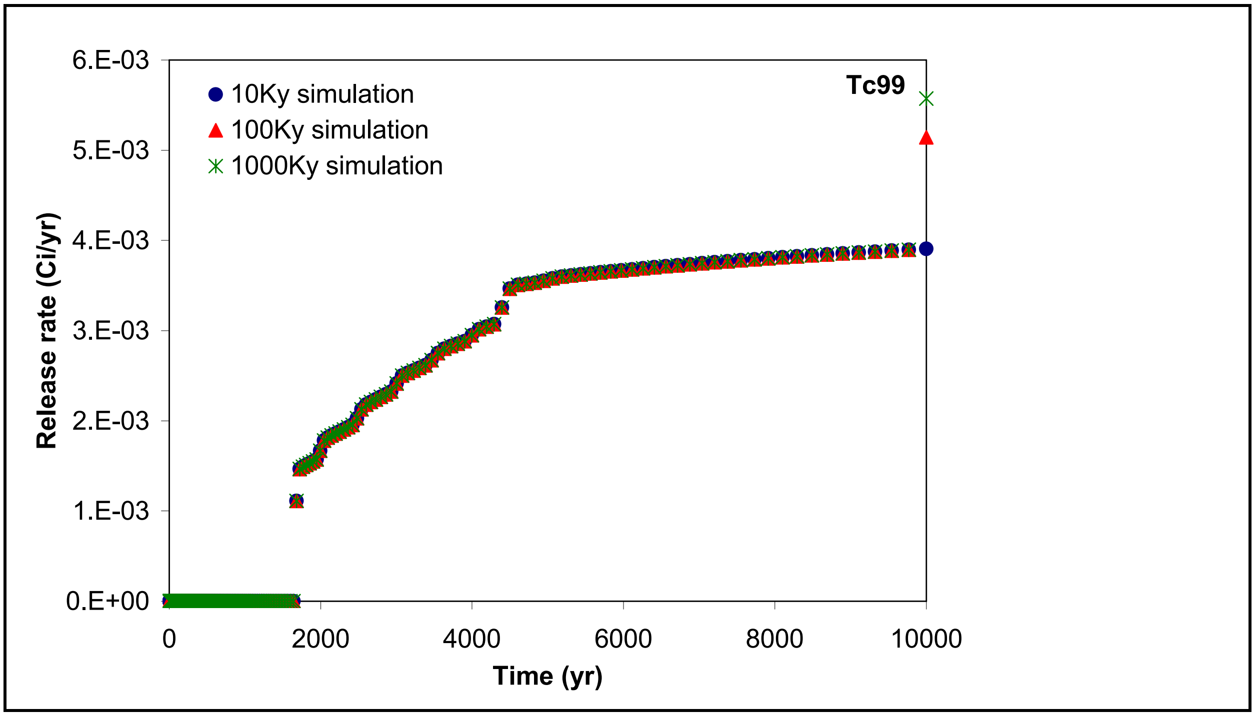


Fig. 1b. Release rates of Tc99 from the EBS in the first 10Ky resulting from TPA runs for 10Ky, 100Ky, and 1000Ky long simulations.

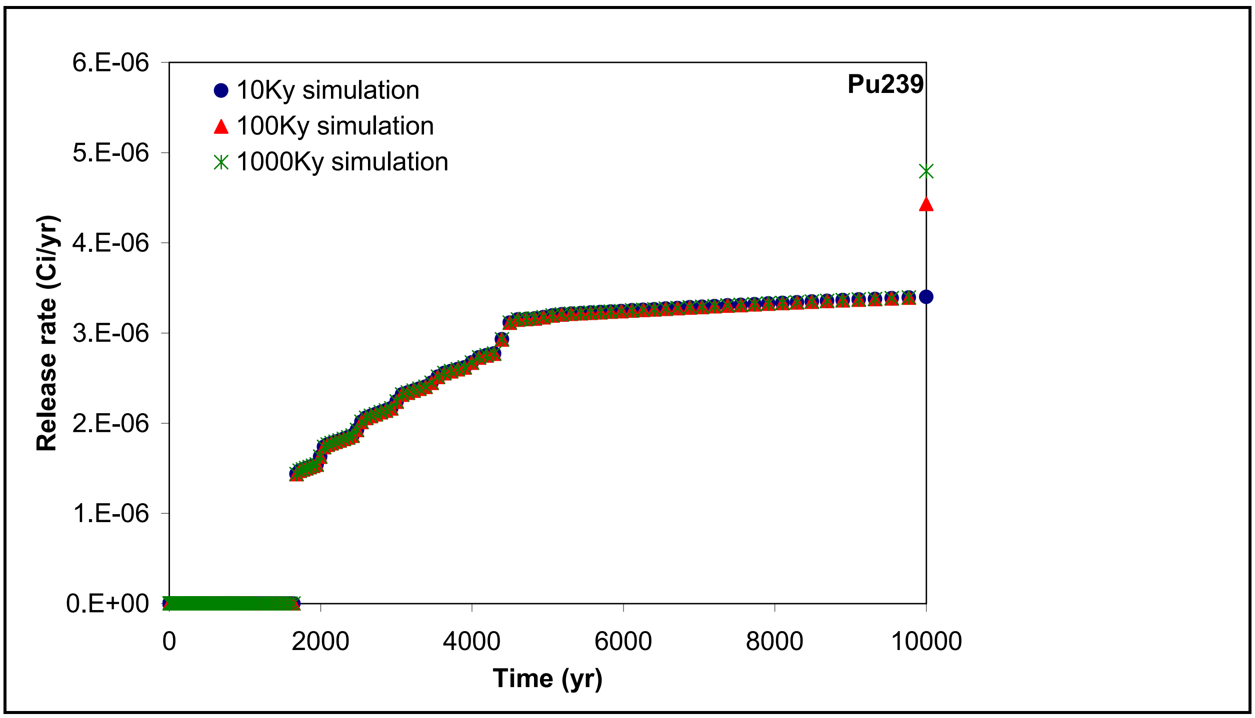


Fig. 1c. Release rates of Pu239 from the EBS in the first 10Ky resulting from TPA runs for 10Ky, 100Ky, and 1000Ky long simulations.

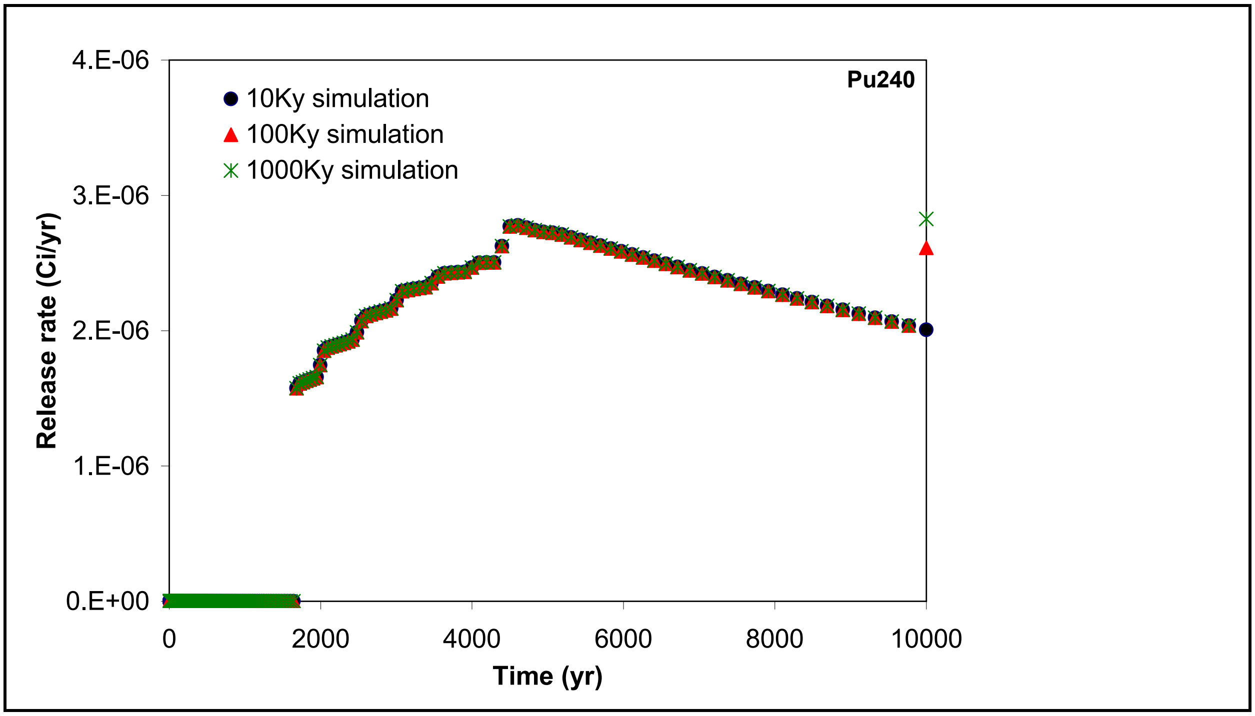


Fig. 1d. Release rates of Pu240 from the EBS in the first 10Ky resulting from TPA runs for 10Ky, 100Ky, and 1000Ky long simulations.

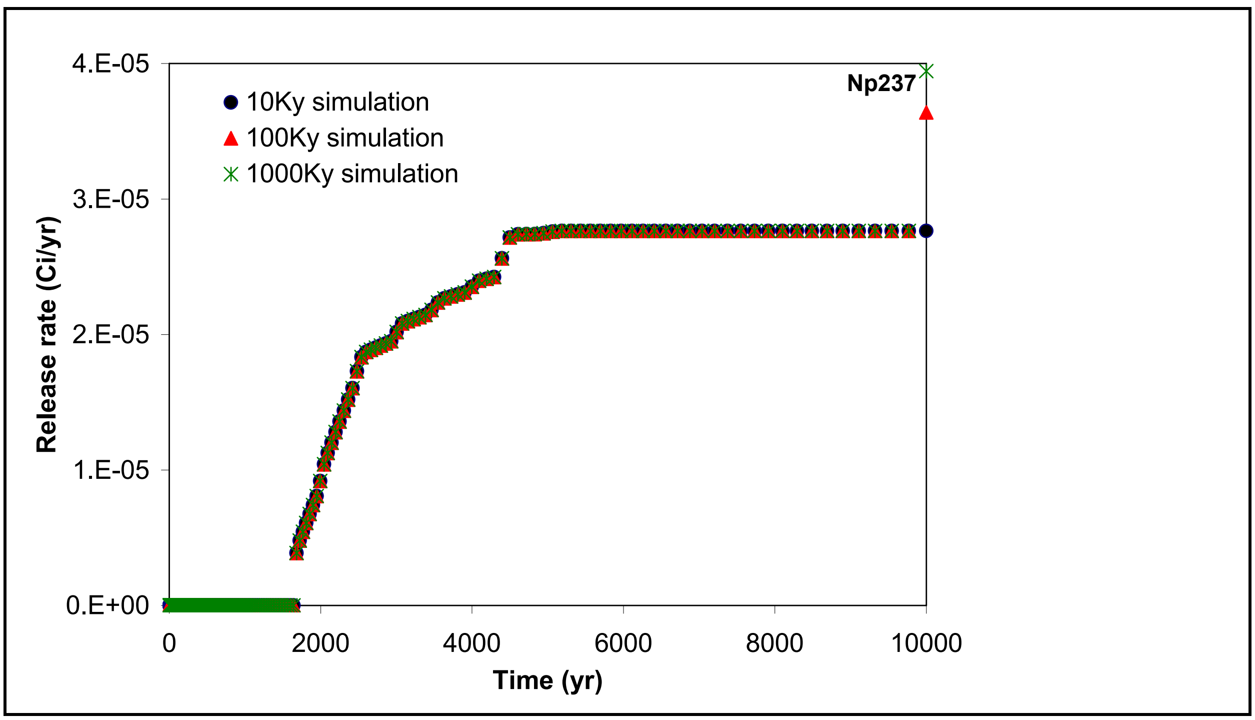


Fig. 1e. Release rates of Np237 from the EBS in the first 10Ky resulting from TPA runs for 10Ky, 100Ky, and 1000Ky long simulations.

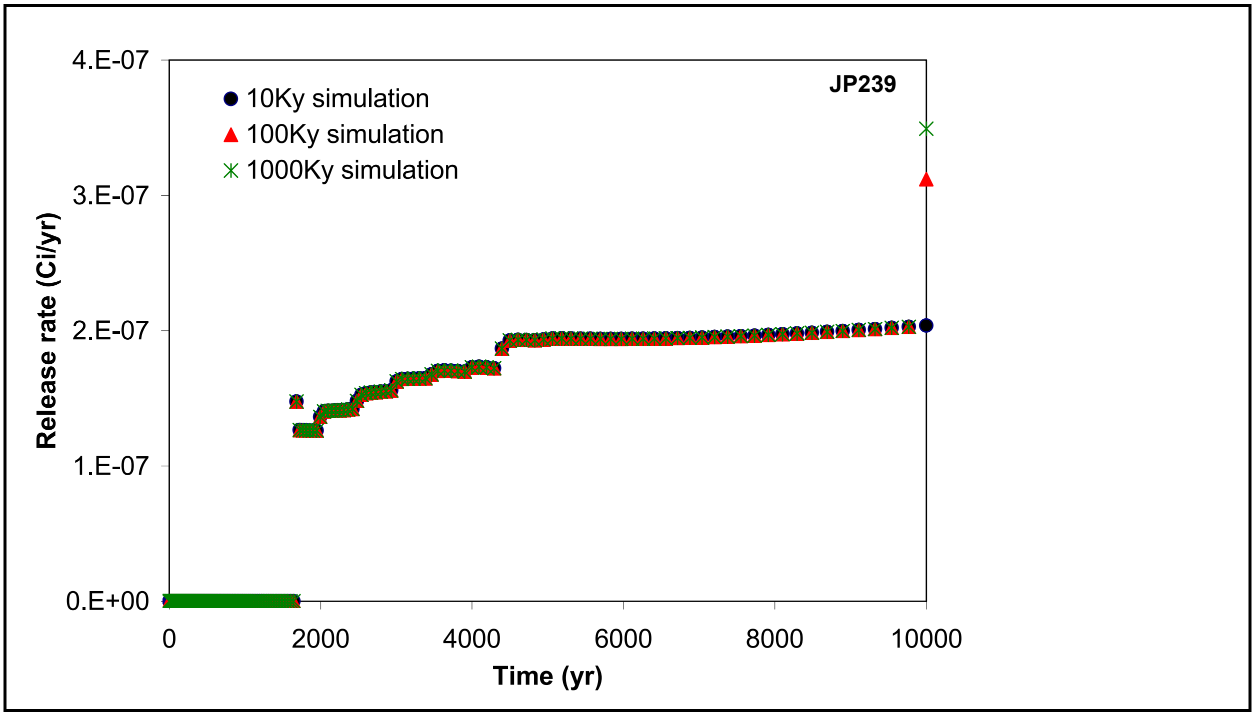


Fig. 1f. Release rates of JP239 from the EBS in the first 10Ky resulting from TPA runs for 10Ky, 100Ky, and 1000Ky long simulations.

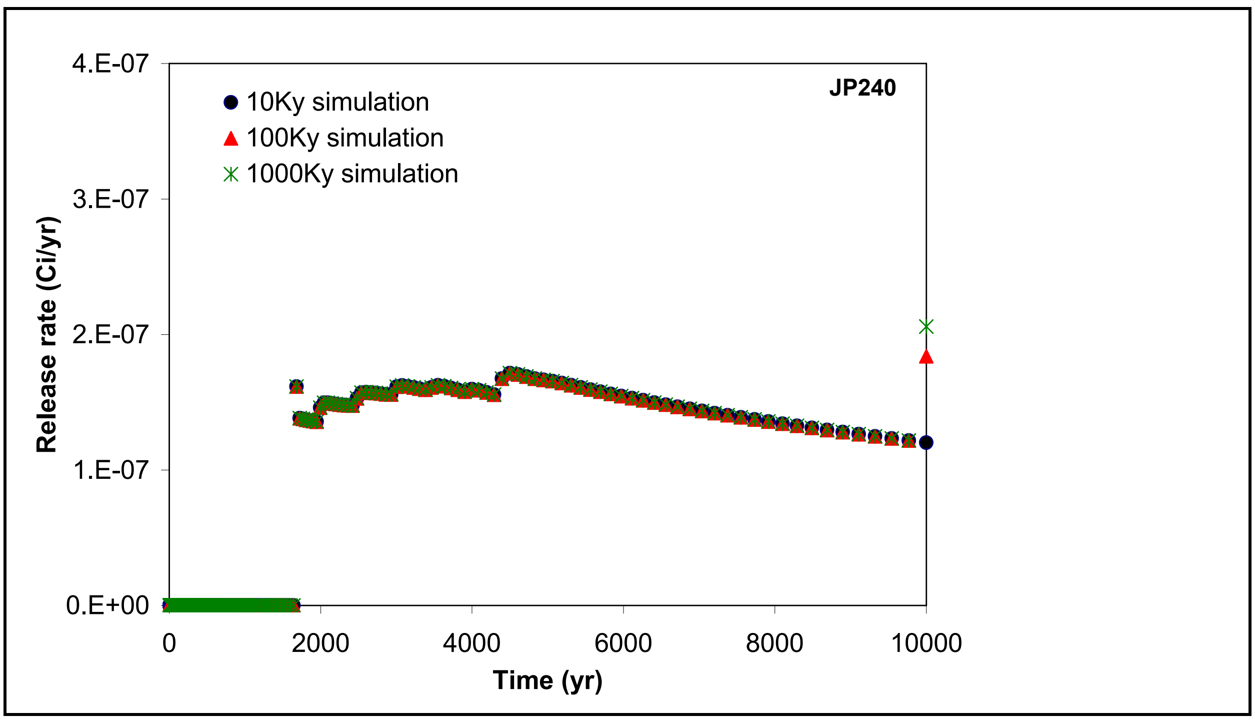


Fig. 1g. Release rates of JP240 from the EBS in the first 10Ky resulting from TPA runs for 10Ky, 100Ky, and 1000Ky long simulations.

Figs. 1a -g revealed that the release rates of I-129, Tc-99, Pu-239, Pu-240, Np237, JP239, and JP240 from the EBS are identical over the overlapped simulation length of <10Ky, resulting from TPA runs for 10Ky, 100Ky, and 1000Ky. However, the release rates at t=10Ky resulting from TPA runs for 10Ky, 100Ky, and 1000Ky differed due to interpolation of release rates calculated at different time steps for t≥10Ky in TPA runs for 100Ky and 1000Ky long simulations (in these simulations, the number of time steps during the compliance period was 201, and after the compliance period it was 100). This issue was elaborated further in the subsequent section.

Next, the release rates of I-129, Tc-99, Pu-239, Pu-240, Np237, JP239, and JP240 from EBS for the overlapping period of 100Ky from TPA runs for 100Ky and 1000Ky were plotted and the results are shown in Fig. 2a through 2g:

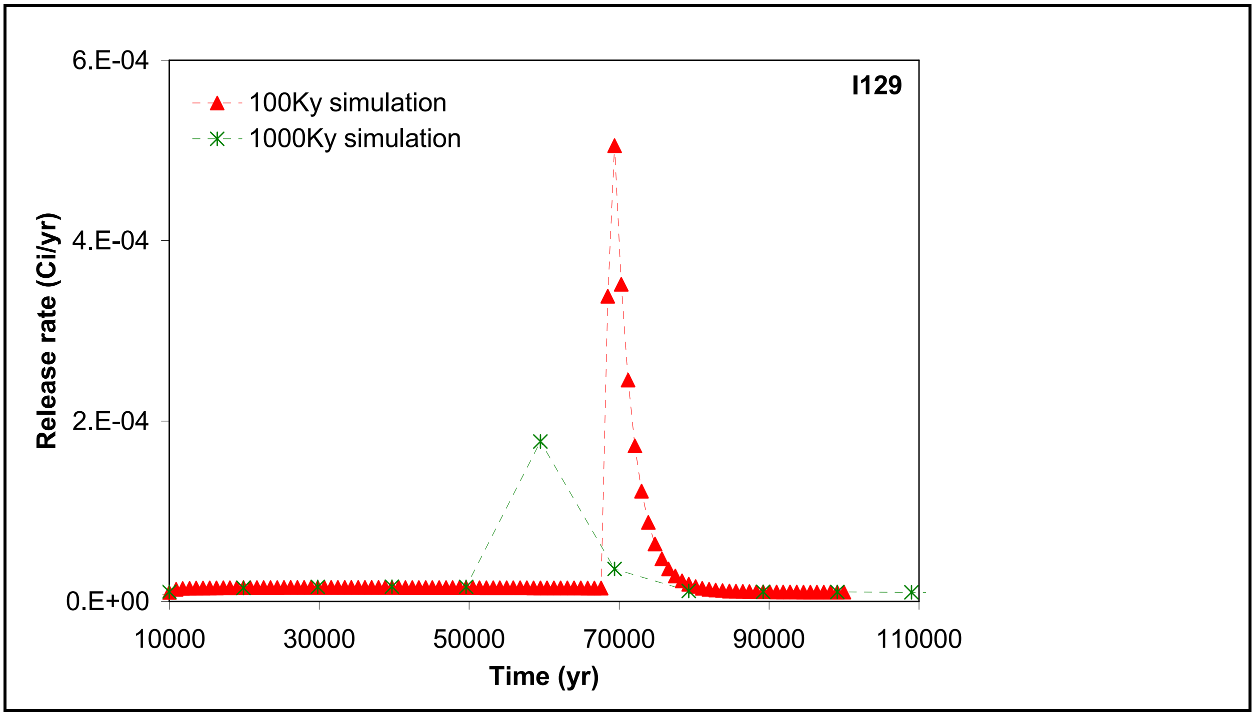


Fig. 2a. Release rates of I129 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations.

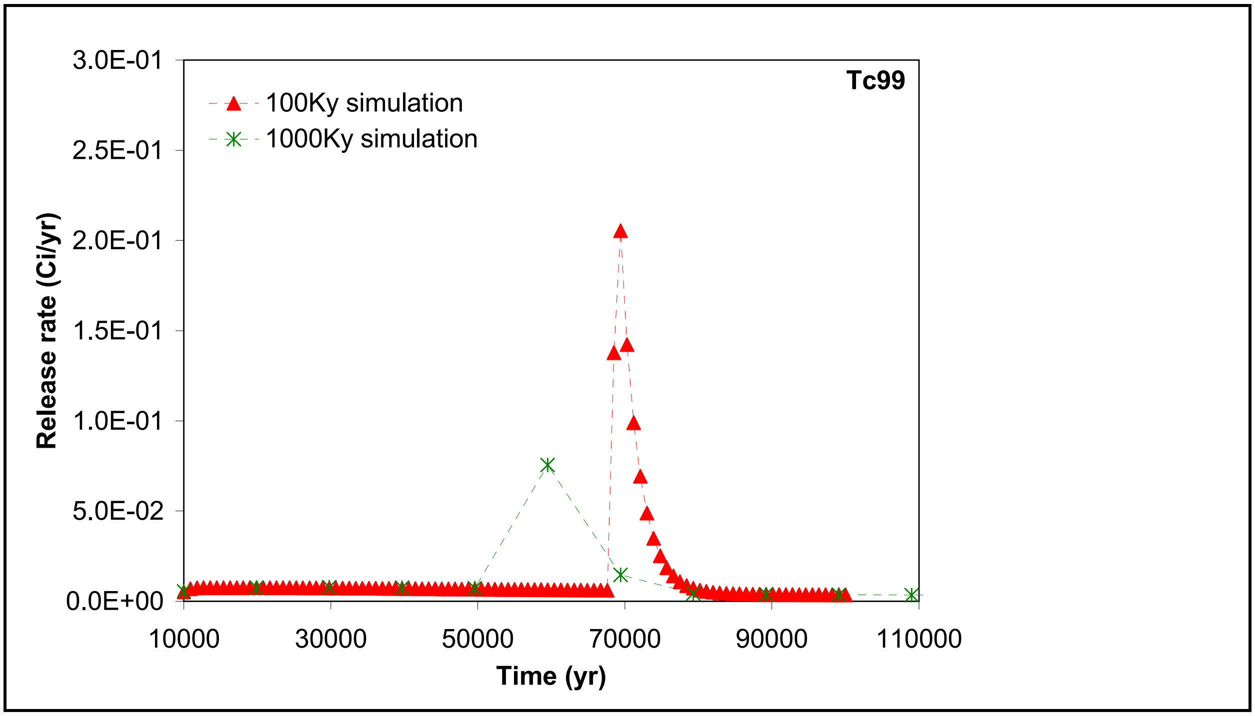


Fig. 2b. Release rates of Tc99 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations.

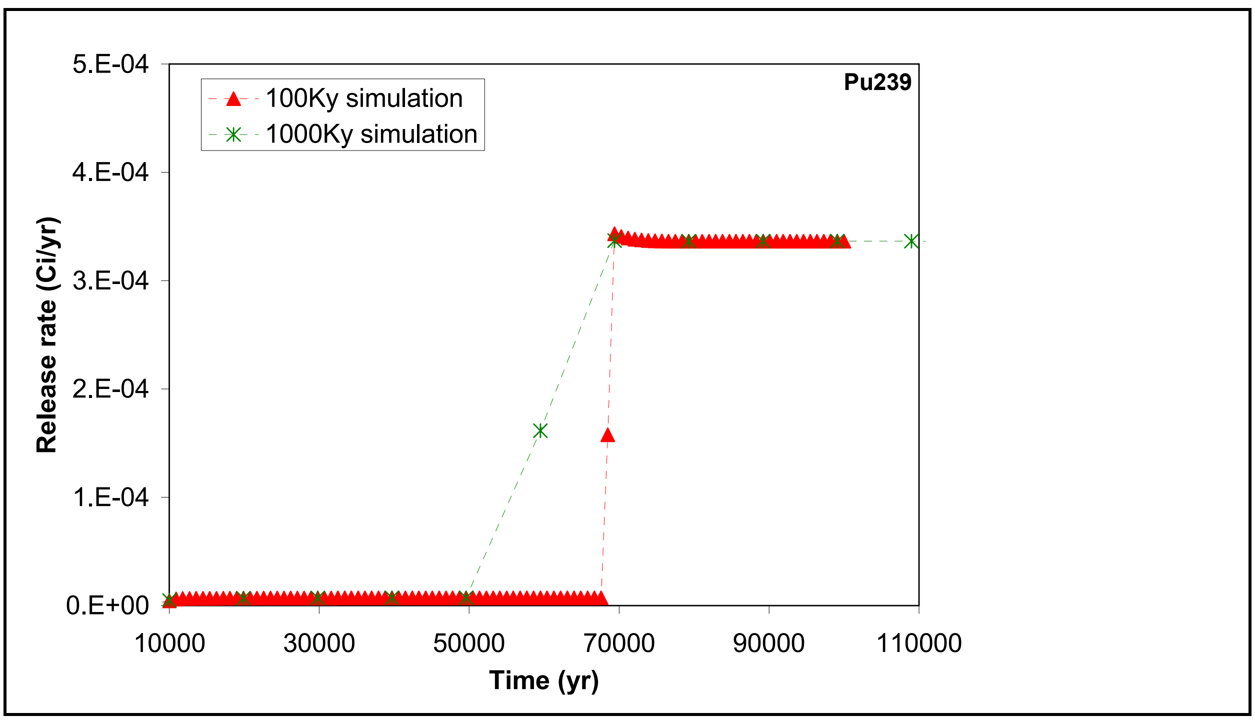


Fig. 2c. Release rates of Pu239 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations.

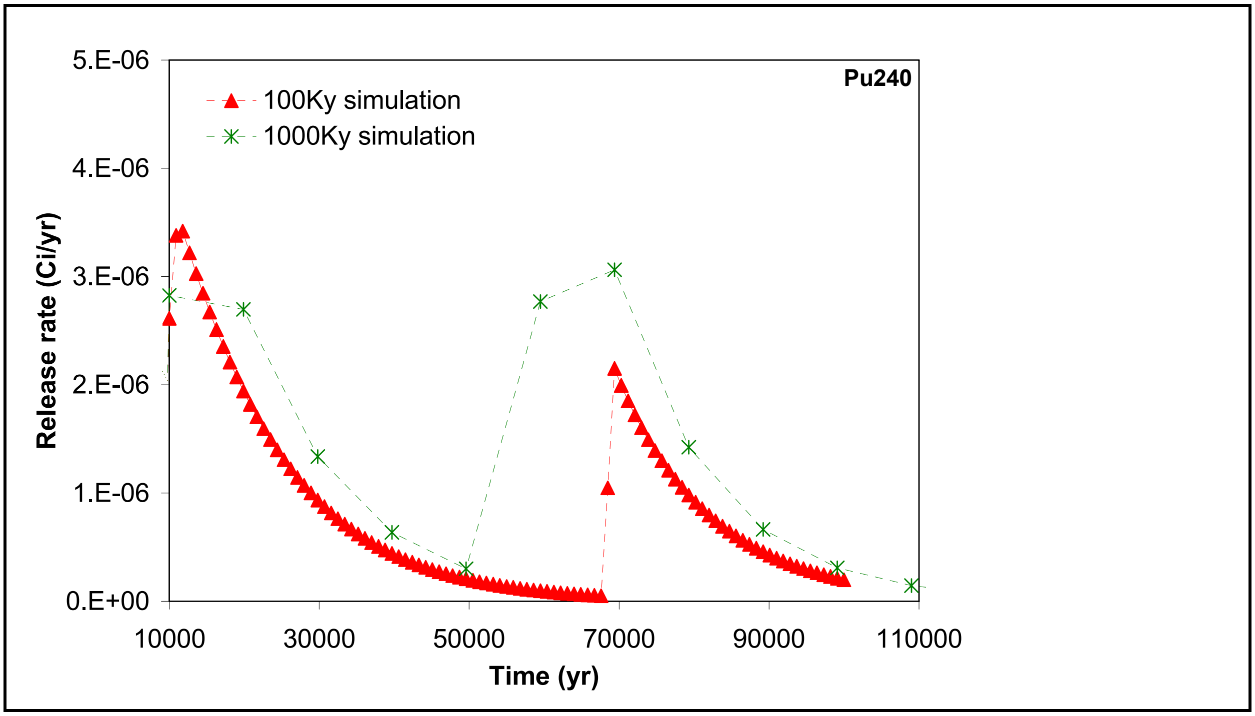


Fig. 2d. Release rates of Pu240 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations.

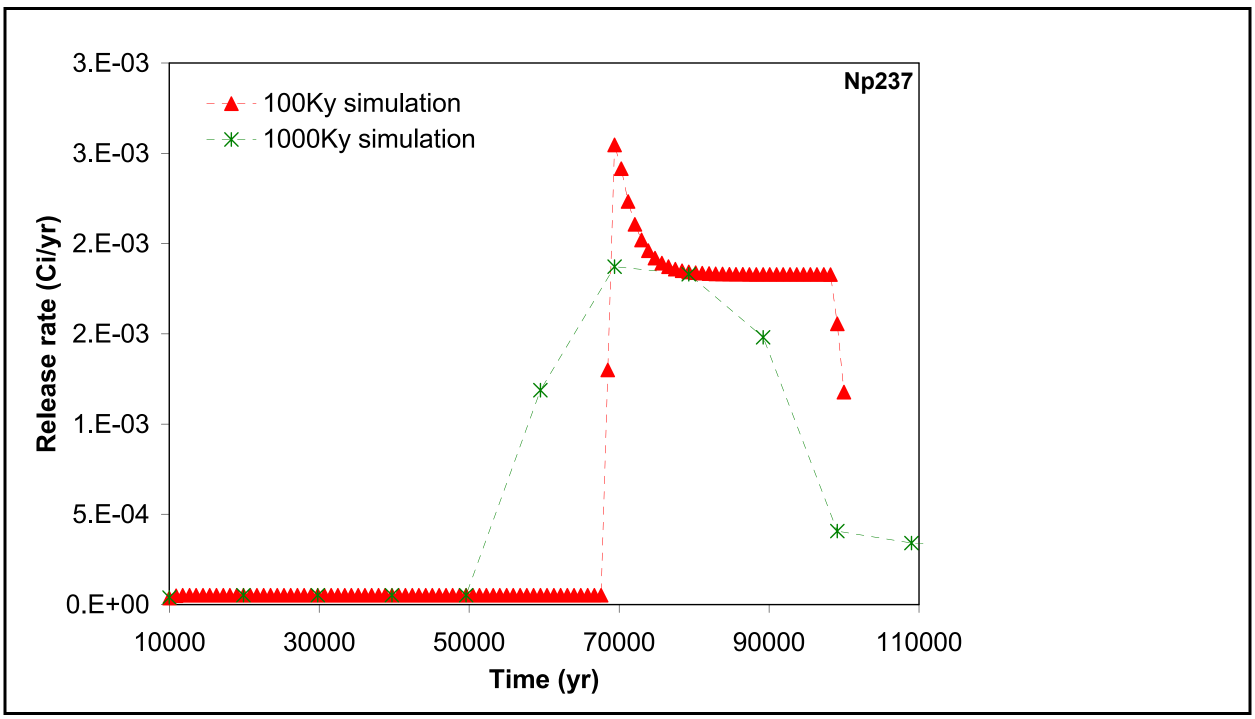


Fig. 2e. Release rates of Np237 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations.

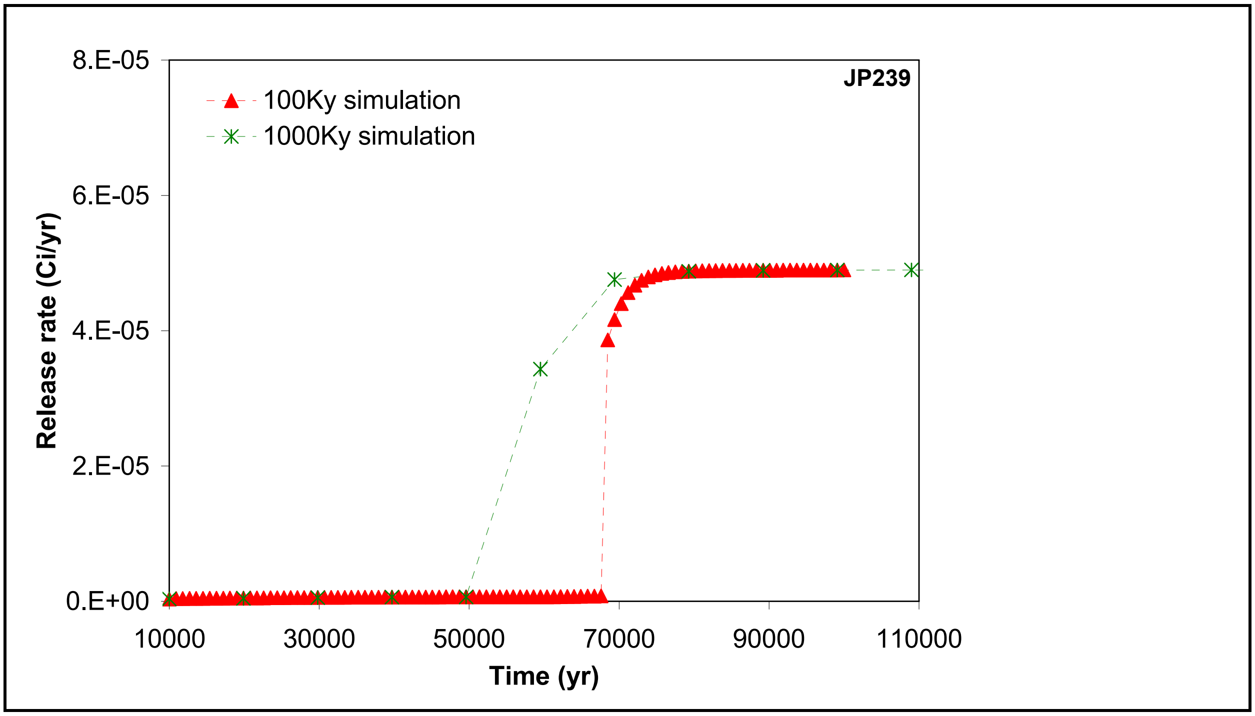


Fig. 2f. Release rates of JP239 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations.

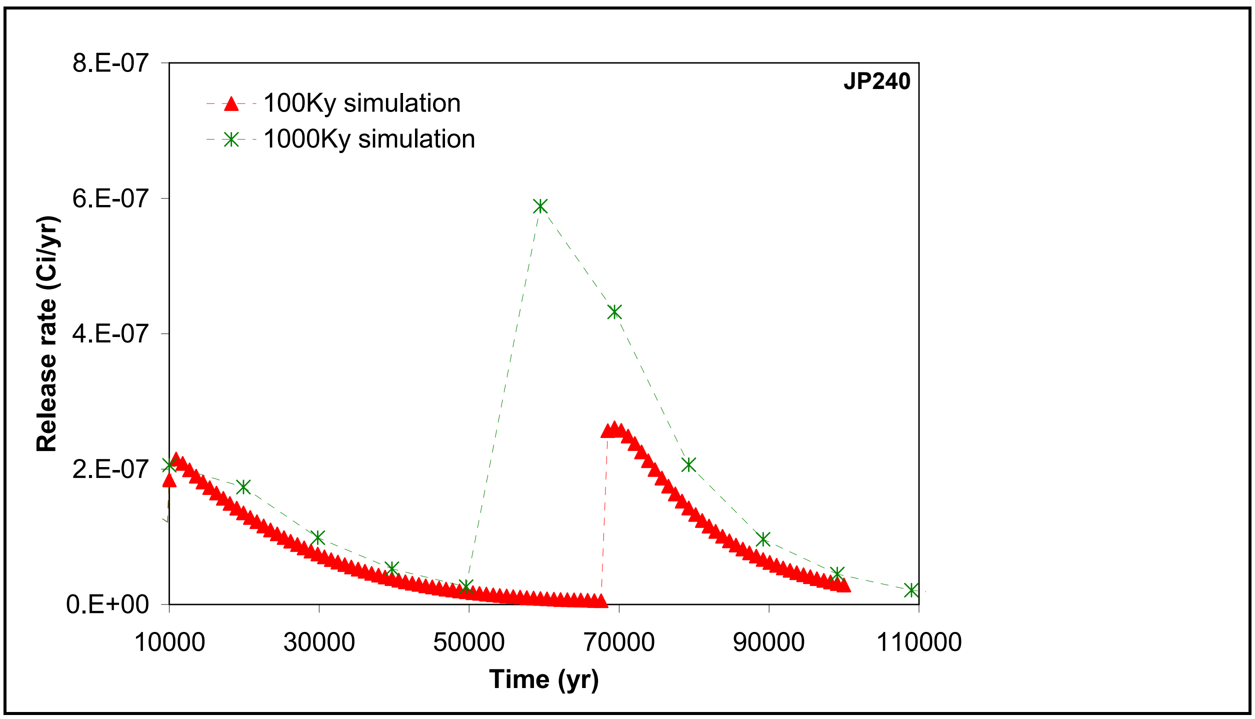


Fig. 2g. Release rates of JP240 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations.

Unlike the release rates for the overlapping 10Ky, the release rates computed for the overlapping period of 100Ky from TPA runs for 100Ky and 1000Ky did not match. It seems that the disparity was due to the number of the time steps taken after the compliance period for the 100Ky and 1000Ky long simulations. To verify this, the number of time steps after the compliance period was set to 100 for the 100Ky long simulation, and to 1000 for the 1000Ky simulation. The results are shown in Figs. 3a-g. The results for 1000Ky simulations with a total number of time steps (TS in the plots) equal to 100 were also included in the plots for comparison (the source of data for these plots were ebsnef2.dat):

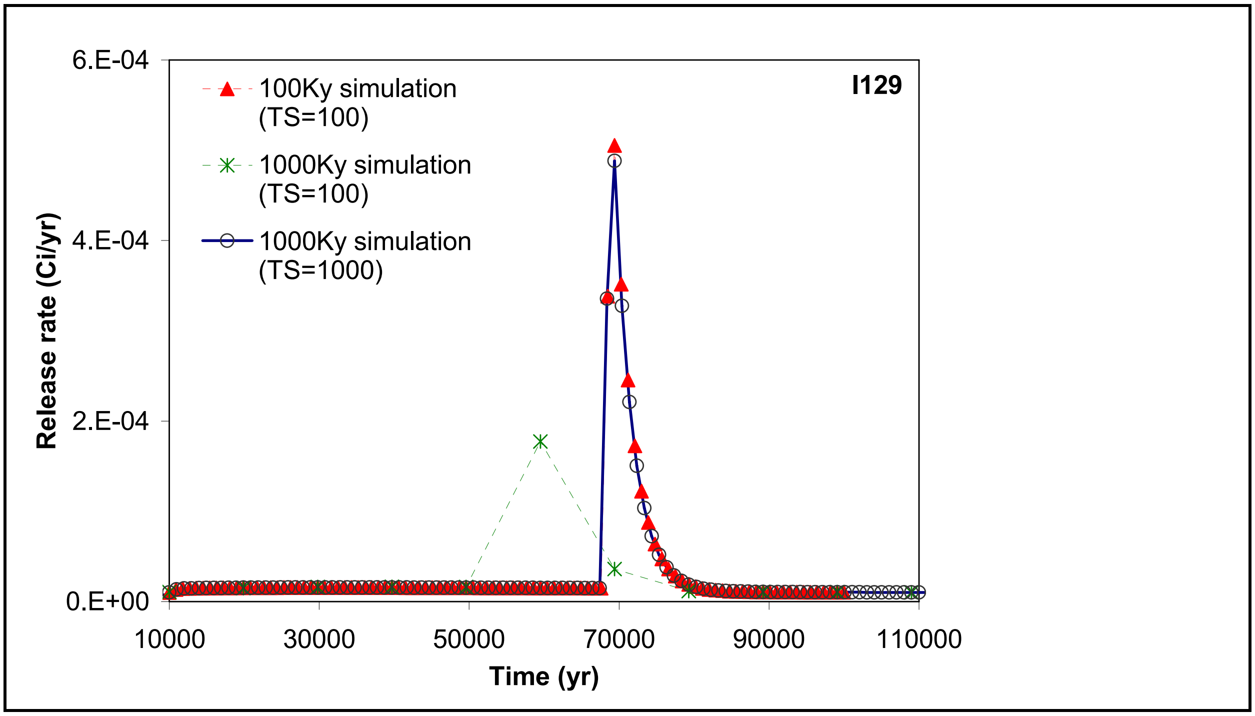


Fig. 3a. Release rates of I129 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations. The number of time steps (TS) was set to 100 for 100Ky and 1000 for 1000Ky simulations.

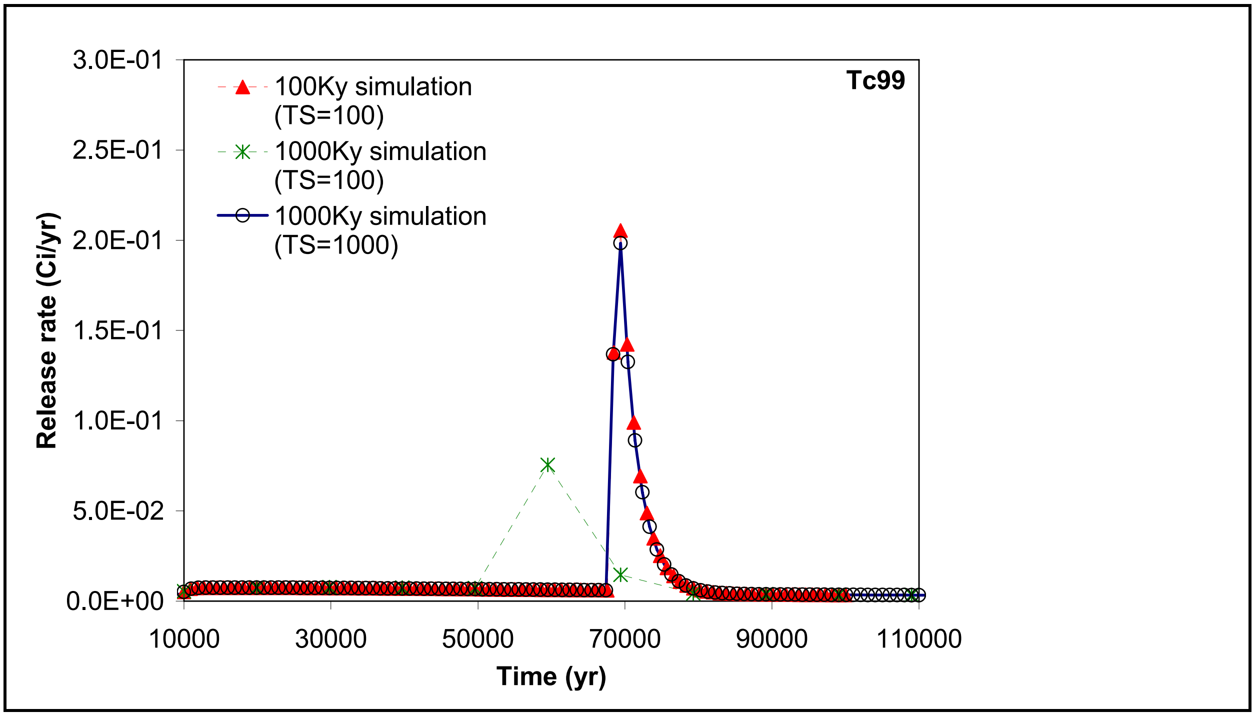


Fig. 3b. Release rates of Tc99 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations. The number of time steps (TS) was set to 100 for 100Ky and 1000 for 1000Ky simulations.

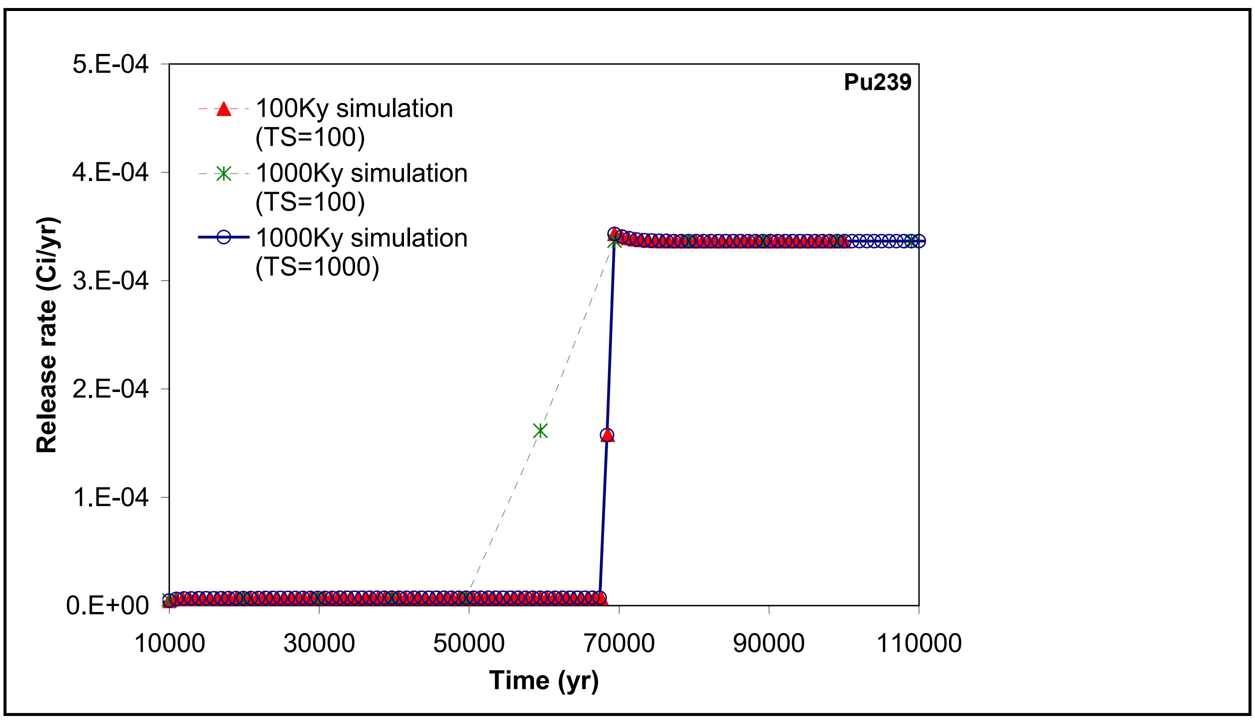


Fig. 3c. Release rates of Pu239 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations. The number of time steps (TS) was set to 100 for 100Ky and 1000 for 1000Ky simulations.

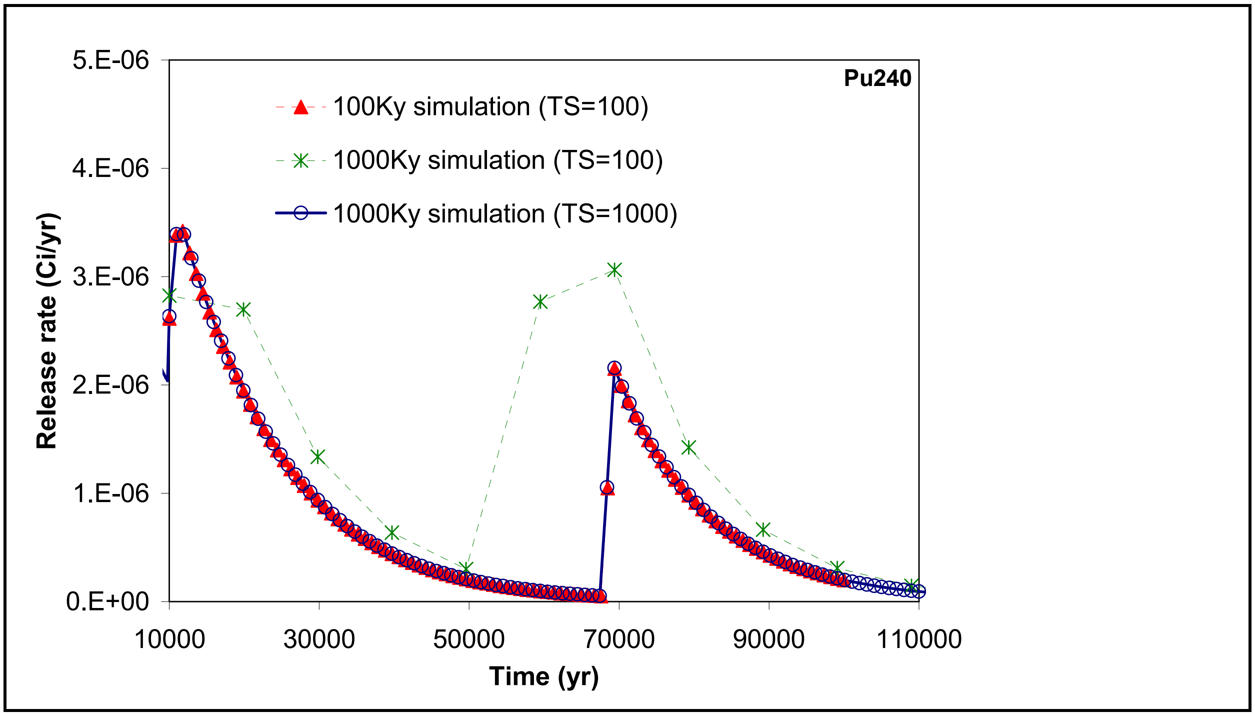


Fig. 3d. Release rates of Pu240 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations. The number of time steps (TS) was set to 100 for 100Ky and 1000 for 1000Ky simulations.

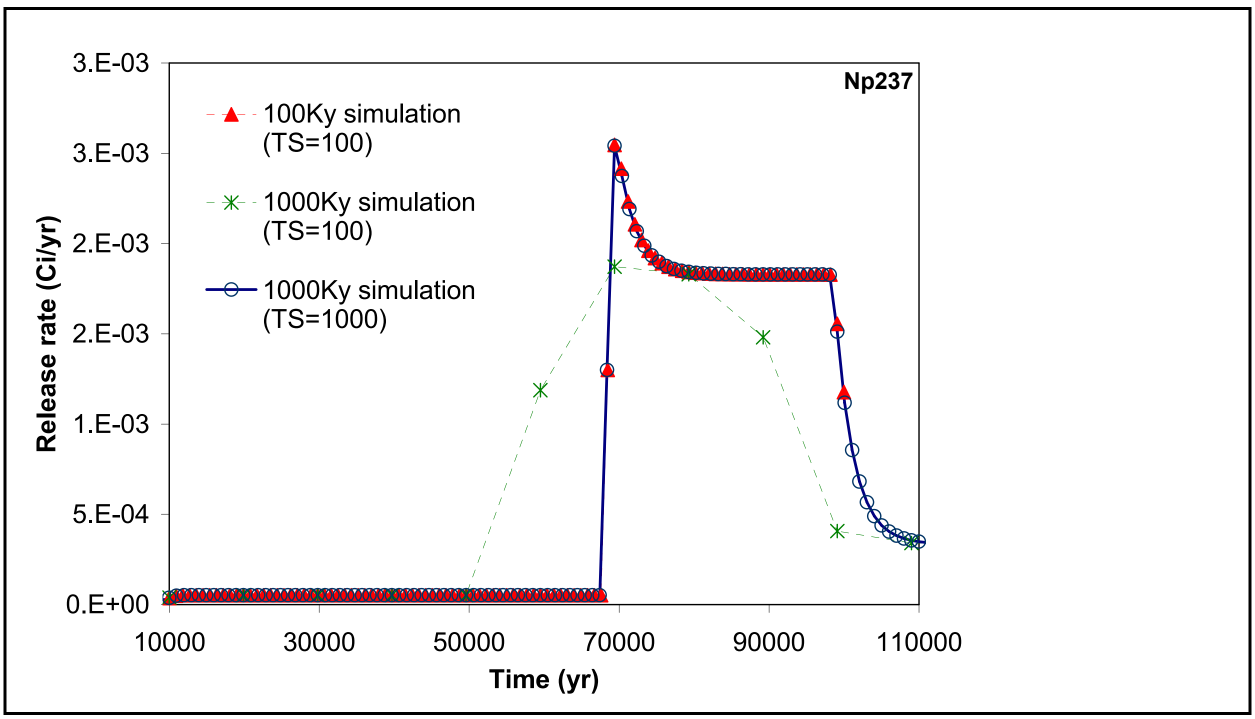


Fig. 3e. Release rates of Np237 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations. The number of time steps (TS) was set to 100 for 100Ky and 1000 for 1000Ky simulations.

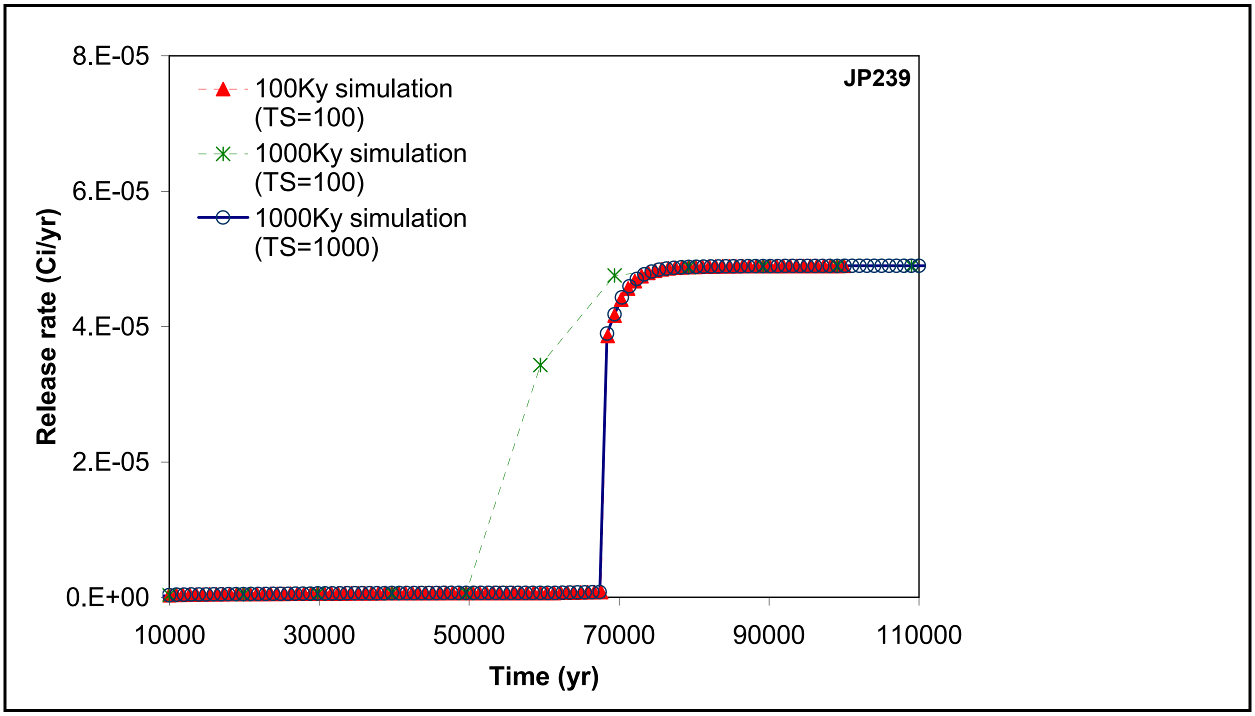


Fig. 3f. Release rates of JP239 from the EBS in the first 100Ky resulting from TPA runs for 100Ky, and 1000Ky long simulations. The number of time steps (TS) was set to 100 for 100Ky and 1000 for 1000Ky simulations.

Hence, an agreement for the 100Ky and 1000Ky simulations for the release rates over the overlapping 100Ky period was achieved by increasing the number of time steps after the compliance period tenfold for the 1000Ky long simulations, so that the length of each time step was identical for the two runs.

In summary,

1. The release rates for I-129, Tc-99, Pu-239, Pu-240, Np237, JP239 and JP240 were identical for the overlapping period of the first 10Ky,
2. The release rates for I-129, Tc-99, Pu-239, Pu-240, Np237, JP239 and JP240 were identical for the overlapping period of the first 100Ky when the number of time steps after the compliance period was increased by ten times for the 1000Ky simulations than for the 100Ky long simulations.

Hence, the release rates were independent of the total simulation length if a proper number of time steps (after the compliance period) was chosen for TPA runs with different simulation lengths. For a properly chosen number of time steps for TPA runs with different total simulation lengths, the release rates were identical over the overlapping time periods.

Test1 Evaluation Pass/Fail: **PASS**

Attachment B
TPA Version 5.1 Validation Task P-10
Test 2 Description

<table>
<tr><td colspan="2">Test Method
x code inspection
x output inspection
hand calculation</td></tr>
<tr><td colspan="2">spreadsheet
graphical
comparison with external code results</td></tr>
<tr><td colspan="2">Test Objective: Verify the functionalities implemented in RELEASET.</td></tr>
<tr><td colspan="2">Test Environment Setup
Hardware (platform, peripherals): Desktop computers
Software (OS, compiler, libraries, auxiliary codes or scripts): XP
Input Data (files, data base, mode settings): See the attachment.</td></tr>
<tr><td colspan="2">Assumptions, constraints, and/or scope of test: (none)</td></tr>
<tr><td colspan="2">Test Procedure:
Execute the TPA code mean value data file for 10,000 yr and for Subarea 3. Examine data files, source code, and output files to verify the C-14 parameters are removed from tpa.inp.</td></tr>
<tr><td colspan="2">Test Results
Location: P10\TPA_Validation\Test2
Test Criterion or Expected Results: C-14 parameters would be removed from data files, source code and output files.
Test Evaluation (Pass/Fail): Pass</td></tr>
<tr><td colspan="2">Notes: See following pages of this attachment for analysis of results.</td></tr>
<tr><td>Tester: Hakan Basagaoglu
Robert Rice</td><td>Date: April 27, 2007</td></tr>
</table>

Results:

TPA was run first using the **mean value data file** for 10Ky; however, the model results did not show any releases from the EBS and UZ during this time period. Therefore, tpa.inp (realization #1) was used for Test 2.

Input File: the following statements were commented out in the input file (tpa.inp):

<u>C14</u>

<u>** rwr 4-10-06; SCR626; remove C14 variables</u>
<u>** 22</u>
<u>** 13</u>

<u>** rwr 4-10-06; SCR626; remove C14 variables</u>
<u>** **   chain 10</u>
<u>** 1</u>
<u>** C14</u>
<u>**   chain 11</u>

and C14 was not specified anywhere else in the input file.

Source Code:
There is no entry and statement associated with C14 in ebsrel.f90

Output files: No entry was found for C14 in ebsrel.rlt, ebsnef.dat, ebsnef2.dat

Test 2 Evaluation (Pass/Fail): PASS

Attachment C
TPA Version 5.1 Validation Task P-10
Test 3 Description

<table>
<tr><td colspan="2">Test Method
code inspection
x output inspection
hand calculation
x spreadsheet
x graphical
comparison with external code results</td></tr>
<tr><td colspan="2">Test Objective: Verify the functionalities implemented in RELEASET.</td></tr>
<tr><td colspan="2">Test Environment Setup
Hardware (platform, peripherals): Desktop computers
Software (OS, compiler, libraries, auxiliary codes or scripts): XP
Input Data (files, data base, mode settings): See the attachment.</td></tr>
<tr><td colspan="2">Assumptions, constraints, and/or scope of test: (none)</td></tr>
<tr><td colspan="2">Test Procedure:

Execute the TPA code mean value data file for 10,000 yr and for Subarea 3. If there is no weld failure, force weld failure by decreasing the weld thickness and make sure weld failure is the earliest occurring failure mode. Verify that the data in ebsflo.dat and the release rates in ebsnef2.dat include the weld failure time.</td></tr>
<tr><td colspan="2">Test Results
Location: D:\TPA_Validation\Test3
Test Criterion or Expected Results: Data in ebsflo.dat and the release rates in ebsnef2.dat should include the weld failure time and the releases should occur after the failure time.

Test Evaluation (Pass/Fail): Pass</td></tr>
<tr><td colspan="2">Notes: See following pages of this attachment for analysis of results.</td></tr>
<tr><td>Tester: Hakan Basagaoglu</td><td>Date: April 27, 2007</td></tr>
</table>

Results:

TPA was run first using the **mean value data file** for 10Ky; however, the model results did not show any releases from the EBS and UZ during this time period. Therefore, tpa.inp (realization #1) was used for Test 3 in the subsequent sections.

First, the weld thickness was kept at its default value of 0.02 m (reference case). Part of the screen output is shown below:

```
constant
WPWeldThickness[m]
2.0e-2
```

```
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      501.3  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =     1660.0  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    149 at TPA time =   1640.9 yr
 *** failed WPs:  149   out of  2904  ***
```

In this simulation, the corrosion breach occurred on welded areas at t=1660 yr, which resulted in waste packages (WP) failure. The reported times for the corrosion breach on welded areas (t=1660 yr) and failed WPs from localized corrosion (t=1640.9 yr) differed by ~20 yr in the screen output file, although they indicate the same process. The times were different, because the WP failure time reported by exec.f was in TPA times.

Next, the weld thickness was reduced to 0.0002 m (i.e., 100 times smaller than the weld thickness in the reference case) to promote early localized corrosion welded areas and early WPs failure . Part of the screen output is shown below:

```
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      501.3  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =      988.4  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    149 at TPA time =    971.3 yr
 *** failed WPs:  149   out of  2904  ***
```

In this case, corrosion breach on welded areas occurred earlier than in the reference case with a relatively thicker weld. Although corrosion breach on welded areas took place at t~988 yr, the percolating water did not reach failed WPs until t~1600 yr (in ebsflo.dat) (Fig. 4). Therefore, the releases from EBS should not occur for t<1600 yr.

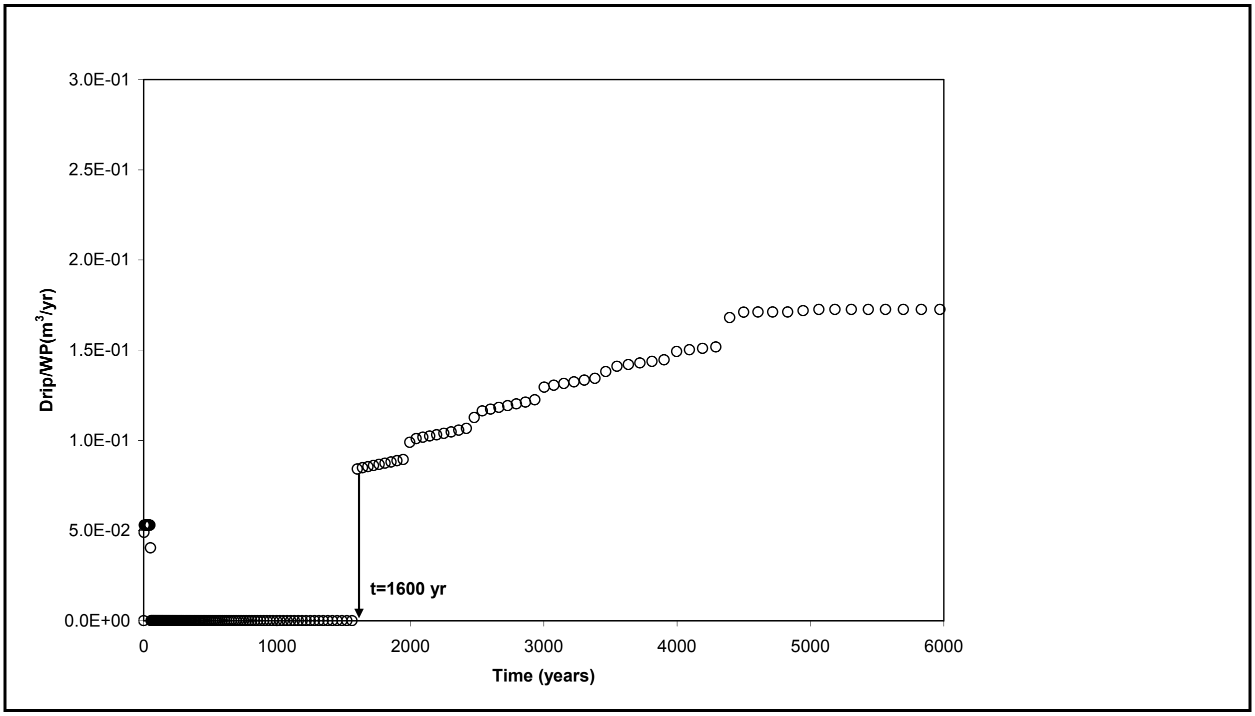


Fig. 4. Deep percolation rate (water flux rate) from the EBS.

The release rates reported in ebsnef2.dat indicate that all releases occurred at t≥1600 yr, which is consistent with the flow data reported in ebsflo.dat. A part of ebsflo.dat is shown below. The release rates of Cm 245, Cm246, and U238 are shown in Fig. 5 as an example:

Cm 245		Cm 246		U238	
Time	Releases	Time	Releases	Time	Releases
1380.80	0.00E+00	1380.80	0.00E+00	1380.80	0.00E+00
1415.40	0.00E+00	1415.40	0.00E+00	1415.40	0.00E+00
1450.80	0.00E+00	1450.80	0.00E+00	1450.80	0.00E+00
1487.10	0.00E+00	1487.10	0.00E+00	1487.10	0.00E+00
1524.20	0.00E+00	1524.20	0.00E+00	1524.20	0.00E+00
1562.20	0.00E+00	1562.20	0.00E+00	1562.20	0.00E+00
1601.10	0.00E+00	1601.10	0.00E+00	1601.10	0.00E+00
1640.90	0.00E+00	1640.90	6.12E-09	1640.90	2.65E-23
1681.60	7.85E-09	1681.60	6.22E-09	1681.60	2.56E-08
1723.30	1.65E-08	1723.30	6.27E-09	1723.30	5.38E-08
1766.00	2.56E-08	1766.00	6.32E-09	1766.00	8.38E-08
1809.60	3.59E-08	1809.60	6.36E-09	1809.60	1.18E-07
1854.30	4.74E-08	1854.30	6.41E-09	1854.30	1.56E-07
1900.00	5.99E-08	1900.00	6.46E-09	1900.00	1.98E-07
1946.80	7.34E-08	1946.80	6.51E-09	1946.80	2.43E-07
1994.70	7.28E-08	1994.70	6.88E-09	1994.70	2.42E-07
2043.70	1.10E-07	2043.70	7.31E-09	2043.70	3.68E-07
2093.90	1.32E-07	2093.90	7.41E-09	2093.90	4.42E-07

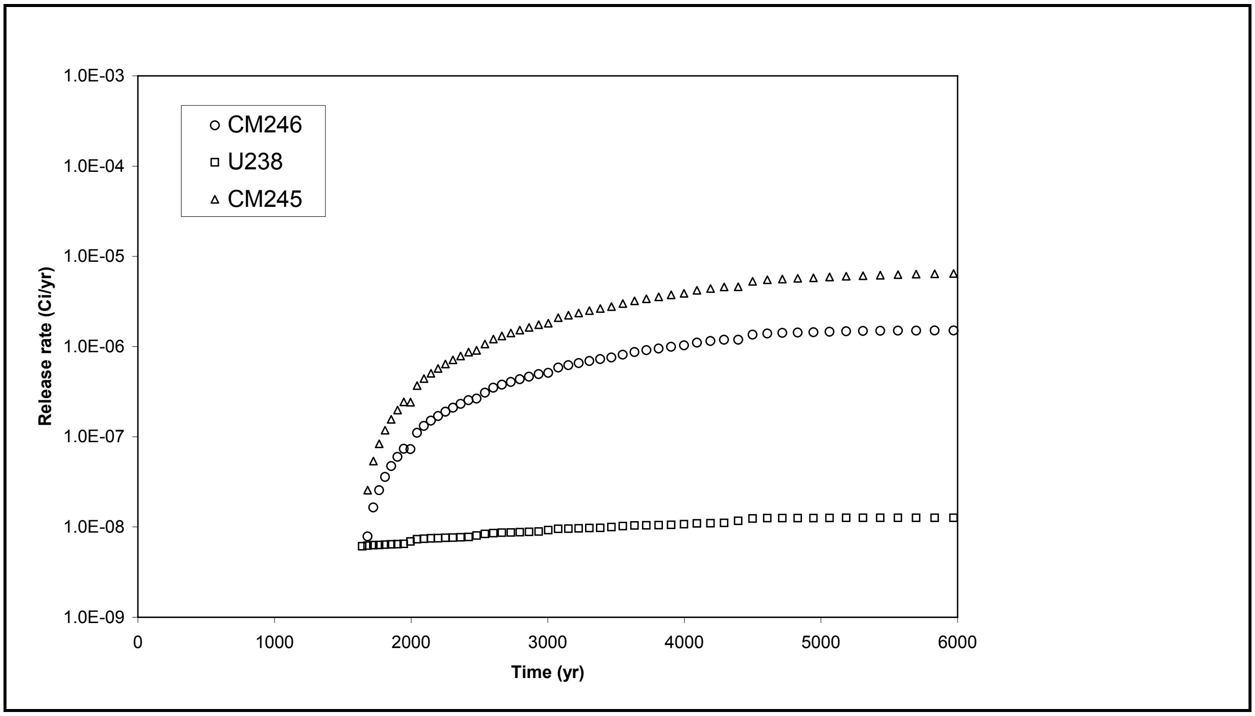


Fig. 5. The release rates of CM245, CM246, and U238 from the EBS.

In the current version of TPA, the percolating water cannot contact the failed WPs if the drift wall temperature is higher than the seepage threshold temperature. Hence, in order to force the early arrival of percolating water to EBS, the seepage threshold temperature was increased (arbitrarily) ten-fold in the following simulation. Part of the screen output file was given below.

```
exec: calling uzflow
      Mean Annual Infiltration at Start(AAI0):    6.9049E+00
exec: calling driftdriver
exec: calling nfenvFI
exec: calling dsfail
dataFile= dsfailt.dat
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      501.3  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =      694.9  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    149 at TPA time =    693.3 yr
 *** failed WPs:  149   out of  2904  ***
exec: calling ebsrel
```

Fig. 6 shows that the early arrival of water to the waste packages and hence early releases of radionuclides from failed waste packages (Fig. 7) when the effect of the seepage threshold temperature is suppressed.

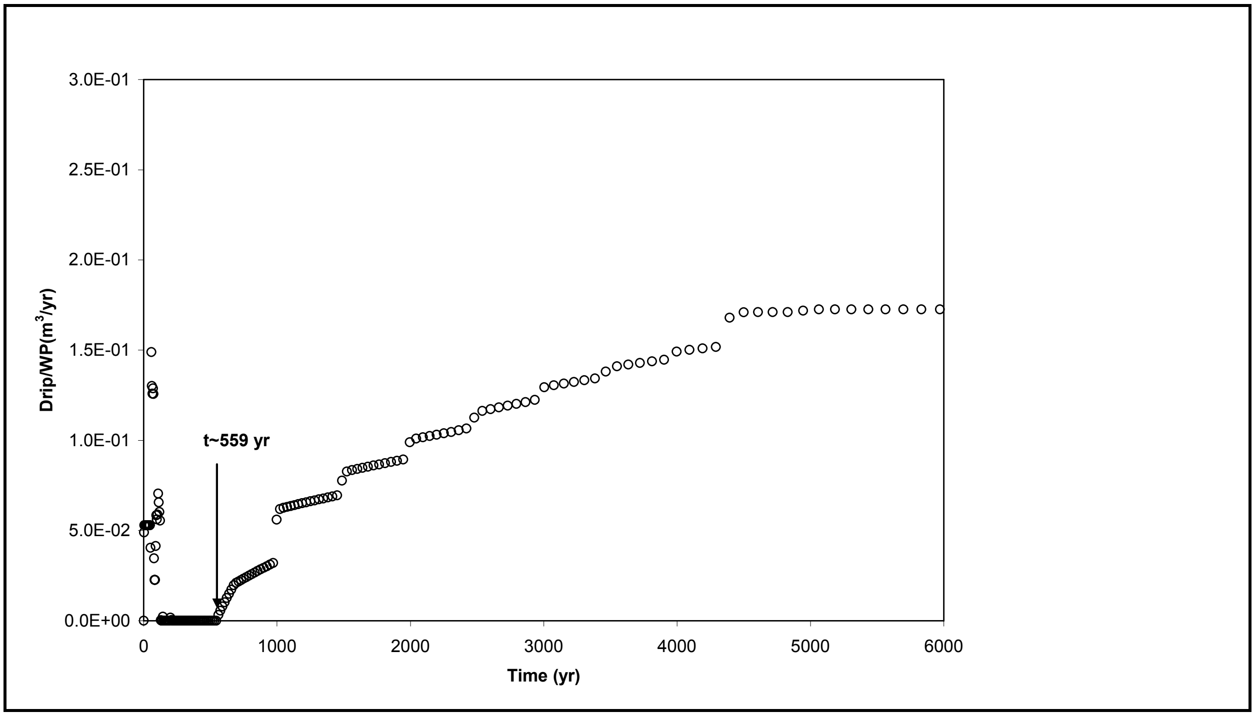


Fig. 6. Deep percolation rate (water flux rate) from the EBS (the source of data was ebsflo.dat).

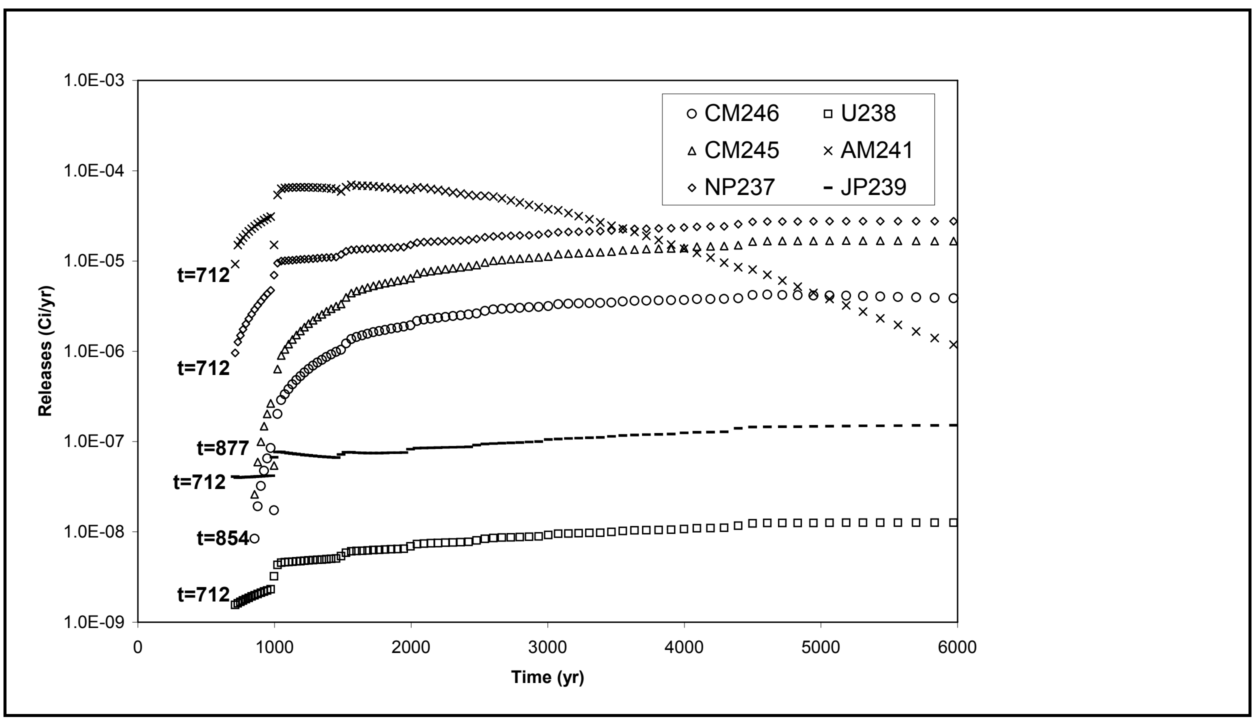


Fig. 7. The release rates of CM245, CM246, U238, AM241, NP237, and JP239 from the EBS (the source of data was ebsnef2.dat).

The WP failure occurred due to corrosion breaches on welded areas. The releases from the EBS (t~712 year) started shortly after WP failure (t~694 yr) by localized corrosion (Fig. 7). Because no other failure mechanisms were activated in this simulation and the effect of the seepage threshold temperature was suppressed, the release from the EBS is solely controlled by localized corrosion breaches on welded areas, and the release time of radionuclides complied well with the time of corrosion on welded areas. Hence, the weld failure time correctly passed to ebsflo.dat (including flow factors) and ebsnef2.dat (including the release rates).

Test 3 Evaluation (Pass/Fail): PASS.

Attachment D
TPA Version 5.1 Validation Task P-10
Test 4 Description

Test Method

code inspection	spreadsheet
x output inspection	graphical
hand calculation	comparison with external code results

Test Objective: Verify the functionalities implemented in RELEASET.

Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): XP

Input Data (files, data base, mode settings): See the attachment.

Assumptions, constraints, and/or scope of test: (none)

Test Procedure:

Execute the TPA code mean value data file for 10,000 yr and all subareas and activate the APPEND file. Verify that *relcum.out* is written for SF and glass in the *relcumsf.out* and *relcumglass.out* files. Also, verify that *relcum.out* is written to *ebsrel.rlt* for SF and glass for all subareas.

Test Results

Location: P10\TPA_Validation\Test4

Test Criterion or Expected Results: *relcum.out* would be written for SF and glass in the *relcumsf.out* and *relcumglass.out* files. *relcum.out* would be written to *ebsrel.rlt* for SF and glass for all subareas.

Test Evaluation (Pass/Fail): **Pass**

Notes: See following pages of this attachment for analysis of results.

Tester: Hakan Basagaoglu Robert Rice	Date: April 27, 2007

Results:

TPA was run first using the **mean value data file** for 10Ky; however, the model results did not show any releases from the EBS and UZ during this time period. Therefore, tpa.inp (realization #1) was used for Test 4 in the subsequent sections. The model run was conducted for 10 Subareas from Subarea 1 to Subarea 10. The number of failed waste packages in each subarea is listed below:

```
    subarea   1 of  10
 *** failed WPs:  27   out of  526  ***
    subarea   2 of  10
 *** failed WPs:  0   out of  1062  ***
   subarea   3 of  10
 *** failed WPs:  149   out of  2904  ***
   subarea   4 of  10
 *** failed WPs:  0   out of  1793  ***
   subarea   5 of  10
 *** failed WPs:  74   out of  1452  ***
   subarea   6 of  10
 *** failed WPs:  0   out of  343  ***
  subarea   7 of  10
 *** failed WPs:  0   out of  696  ***
   subarea   8 of  10
 *** failed WPs:  0   out of  931  ***
  subarea   9 of  10
 *** failed WPs:  0   out of  723  ***
   subarea  10 of  10
*** failed WPs:  0   out of  1747  ***
```

In this simulation, waste packages failed only in Subareas 1, 3, 5.

The results from ebsrel.rlt are summarized below:

```
          1 !! Realization
          1 !! Subarea
379     Waste packages subject to immediate flow through
147     Waste packages subject to immediate flow through
          2 !! Subarea
0       Waste packages subject to immediate flow through
0       Waste packages subject to immediate flow through
         3 !! Subarea
2090    Waste packages subject to immediate flow through
814     Waste packages subject to immediate flow through
          4 !! Subarea
0       Waste packages subject to immediate flow through
0    Waste packages subject to immediate flow through
          5 !! Subarea
1045    Waste packages subject to immediate flow through
407     Waste packages subject to immediate flow through
          6 !! Subarea
0       Waste packages subject to immediate flow through
0       Waste packages subject to immediate flow through
          7 !! Subarea
0       Waste packages subject to immediate flow through
0       Waste packages subject to immediate flow through
          8 !! Subarea
0       Waste packages subject to immediate flow through
```

0 Waste packages subject to immediate flow through
9 !! Subarea
0 Waste packages subject to immediate flow through
0 Waste packages subject to immediate flow through
10 !! Subarea
0 Waste packages subject to immediate flow through
0 Waste packages subject to immediate flow through

ebsrel.rlt has 20 sets of data (for 10 subareas), one for spent fuel (sf) and one for glass.

relcum.out

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00
8	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00

0 Waste packages subject to immediate flow through

***relcumsf.out* (for SF)**

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00
8	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00

0 Waste packages subject to immediate flow through

relcumglass.out

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00
8	0	1.0000E+04	0.0000E+00	0.0000E+00	0.0000E+00

0 Waste packages subject to immediate flow through

In summary:

1. The results from the “last subarea” were saved in relcumsf.out for spent fuel (sf) and in relcumglass.out for glass.
2. ebsrel.rlt has 20 sets of data (for 10 subareas), one for sf and one for glass. The results for Subarea 10 in ebsrel.rlt are consistent with the results in relcumsf.out and relcumoutglass.out

However, because there was no waste package failure (and no immediate flow through waste packages) in Subarea 10 and both relcumsf.out and relcumoutglass.out reports the results for the last Subarea, the results do not seem to be conclusive. Therefore, we <u>repeated</u> the same simulation for <u>Subarea 5</u> only to strengthen the validation of the Test 4. A summary of screen output file is shown below:

```
------------------------------------------------------------------
   subarea   5 of  10          realization    1 of  500
------------------------------------------------------------------
exec: calling uzflow
      Mean Annual Infiltration at Start(AAI0):    6.9049E+00
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
dataFile= dsfailt.dat
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      399.9  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =     1511.6  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     74 at TPA time =   1487.1 yr
 *** failed WPs:  74   out of  1452  ***
------------------------------------------------------------------
```

<u>relcumsf.out</u> **<u>(for SF)</u>**

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	53	1.4871E+03	0.0000E+00	1.5242E+03	1.5242E+03
8	992	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

1045 Waste packages subject to immediate flow through

<u>relcumglass.out</u>

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00

6	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	21	1.4871E+03	0.0000E+00	1.5242E+03	1.5242E+03
8	386	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

407 Waste packages subject to immediate flow through

relcum.out

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.4508E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	21	1.4871E+03	0.0000E+00	1.5242E+03	1.5242E+03
8	386	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

407 Waste packages subject to immediate flow through

In brief,

1) The number of waste packages for spent fuel (sf) and glass subject immediate flow through reported in ebsrel.rlt (on page p10 D2) in Subarea 5 is consistent with the data reported in relcumsf.out and relcumglass.out. The first set of results for each Subarea in ebsrel.rlt corresponds to sf and the second set of results corresponds to glass. When the simulation was conducted for all subareas, ebsrel.rlt reported results for sf and glass separately for each Subarea. Therefore, for 10 Subareas, there were a total of 20 data sets (see page p10 D2)
2) The last data set used in the analyses was saved in relcum.out. The analyses was completed for sf first, and then for glass. Once the calculations for glass were completed, the results for sf was overwritten by the results for glass in relcum.out.

Test 4 Evaluation (Pass/Fail): PASS

Attachment E
TPA Version 5.1 Validation Task P-10
Test 5 Description

Test Method	
code inspection	x spreadsheet
x output inspection	x graphical
hand calculation	comparison with external code results

Test Objective: Verify the functionalities implemented in RELEASET.

Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): XP

Input Data (files, data base, mode settings): See the following pages of this attachment.

Assumptions, constraints, and/or scope of test: (none)

Test Procedure:
Execute the TPA code mean value data file for 10,000 yr and for Subarea 3. If there is no drift degradation, and no initial failures, drip shield mechanical failure, WP corrosion failure (localized and general), or weld failure, force these events to occur. Then, examine, using *tpa.inp* values, the factors Fr, Fd, Fwc, Fwm1, Fwm2, and Fid in *ebsflo.dat* file and verify those factors are correctly calculated **(Bullet 3)**. Verify water does not enter the WP if the temperature is above boiling or a threshold value by examining information in the files *ebsflo.dat* and *ebssf.dat* **(Bullet 2)**. Verify Fmult is correctly calculated using *tpa.inp* values. Verify $q_{in}()$ and $q_{out}()$ are correctly calculated by failure mode (try all seven of the active RELEASET failure modes) and that $q_{in}()$ and $q_{out}()$ are equal for the flowthrough model (and after the bathtub is fillled) by running RELEASET in standalone mode and examining flow rates in *ebsnef.dat*. Verify the general and localized failure times and the weld failure times are correctly transferred from EBSFAIL to the EBSREL/RELEASET input files. Verify the number of WPs failed by failure mode is correctly computed using Pallowance and Pcontact **(Bullet 1)** and tracked in *wpsfail.res* and *wpsfail2.res* (the former contains the WP failures as calculated in previous versions of the TPA code and the latter contains the WP failures in the current code that are passed from EBSREL to RELEASET in the *ebsrel.inp* file). Verify the last two columns in the *infilper.res* file contains WP-weighted average flow rates (i.e., weighted by the number of WPs in RELEASET calculations).

Test Results

Location: P10\TPA_Validation\Test5

Test Criterion or Expected Results: Calculated values of flow factors would be consistent with conditions imposed in their definitions. Delays in outflows with the bathtub model whereas no delays with the flowthrough model. Mass-balance equation for water would be met at all times when flowthrough model is used, or after bathtub is filled up when the bathtub model is used. The failure times would be correctly passed between EBSFAIL to the RBSREL/RELEASET input files. The number of failed WPs would be correctly calculated based on Pallowance and Pcontact. The weighted-average flow rates would be in the last two-columns of *infilper.res*.

Test Evaluation (Pass/Fail): **Pass**

Notes: See following pages of this attachment for analysis of results.

Tester: Hakan Basagaoglu Robert Rice	Date: April 26, 2007

Results:

All the aforementioned failure modes described under **Bullet 3** in the test procedure above was forced by setting:

DefectiveFractionOfWPs/cell=0.1048808848170152
WPFractionThicknessPenetratedForFailureByCorrosion[]=0.01
WPWeldThickness[m]=2.0e-6

---

exec: calling mechdriver (drip shield)
    exec: time of **drip shield mechanical failure** = 388.5 yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling nfenv
exec: calling ebsfail
    ebsfail: time of **corrosion breach on welded areas** = 582.9 yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    ebsfail: time of WP breach by general corrosion = 1077.0 yr
exec: calling mechdriver (waste package)
exec: failed **WPs from INITIAL event** = 15 at TPA time = 0.0 yr
exec: failed **WPs from LOC CORR** event = 131 at TPA time = 574.9 yr
exec: failed **WPs from GEN CORR** event = 2758 at TPA time = 1075.1 yr
*** failed WPs: all WPs failed (2904) ***
exec: calling ebsrel

The source code for all flow factors was ebsflo.dat. Time series of calculated F_r and F_d are shown in Fig. 8.

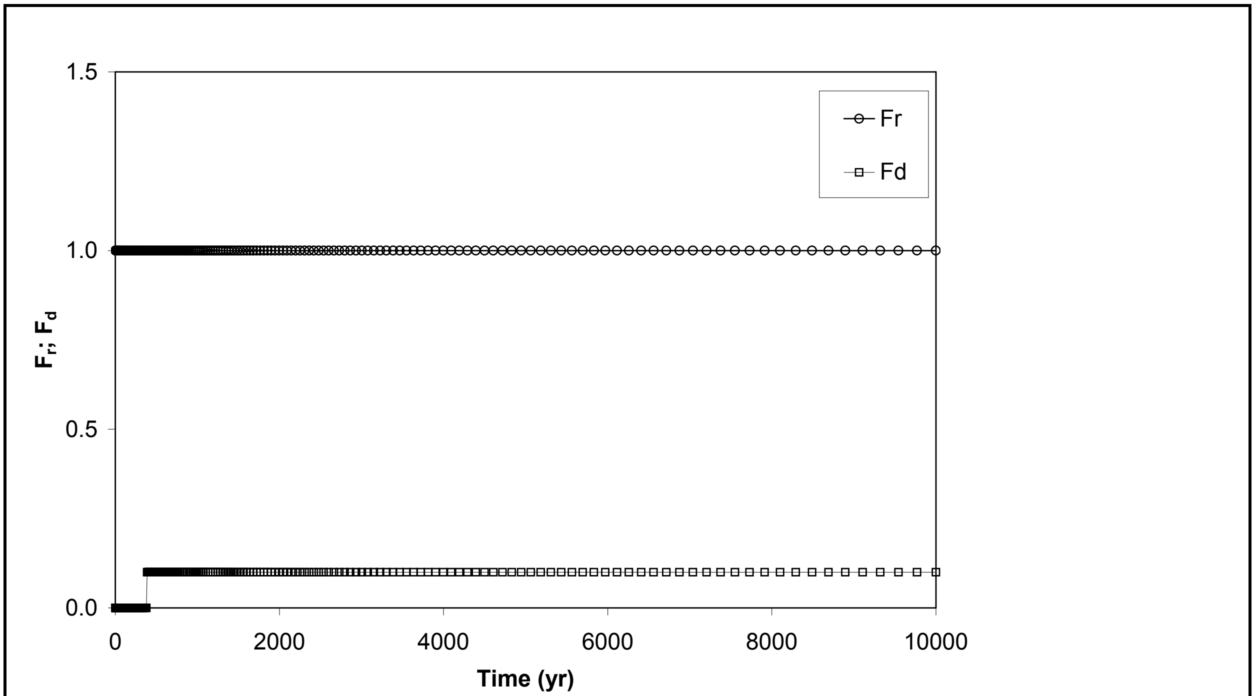


Fig. 8. Time series of F_r and F_d resulting from a TPA simulation for 10Ky.

The ‘SeepageRubbleFactor’, F_r =1.0 in tpa.inp and no condition was specified in TPA for the change of its value. After the model run, F_r =1 over the entire simulation period. Hence, F_r has been **correctly** calculated in the plot above.

The drip shield seepage factor, F_d , takes a value of zero until the earliest breaching time of the drip-shield. It takes a value of 1 if the drip-shield undergoes general corrosion. If the drip-shield does not undergo general corrosion, its value is determined by the sampled parameter InitialSeepageReductionFractionByMechFailedDS, once the drip shield is breached by mechanical failure. InitialSeepageReductionFractionByMechFailedDS is sampled from a log-uniform distribution in the range of 0.01- 1.0. In this validation test, drip-shield failure due to mechanical failure occurred at t~388 year, and hence Fd=0 until t~388. The drip-shield did not undergo general corrosion; therefore, F_d is determined by InitialSeepageReductionFractionByMechFailedDS for the rest of the simulation and its value was 0.1, which lies in the range of 0.01-1.0 as specified in tpa.inp. Hence, F_d has been **correctly** calculated.

InitialSeepageReductionFractionWeldLC, is the seepage reduction factor that accounts for waste package failure by localized corrosion of welded areas. It is a sampled parameter and was sampled from a loguniform distribution in the range of 0.001-0.1. In the absence of disruptive events, InitialSeepageRedeuctionFractionWeldedLC represents the increase in flow factor F_{wc} when weld localized corrosion occurs. F_{wc}=0 prior to localized corrosion (t<575), and took a value of 0.01 up to t=1100 yr. 0.01 is in the range of values specified for InitialSeepageReductionFractionWeldLC in tpa.inp. At t~1100, all waste packages failed by general corrosion; therefore, F_{wc}=1 for t>1100 year (Fig. 9). Hence, F_{wc} has been **correctly** calculated.

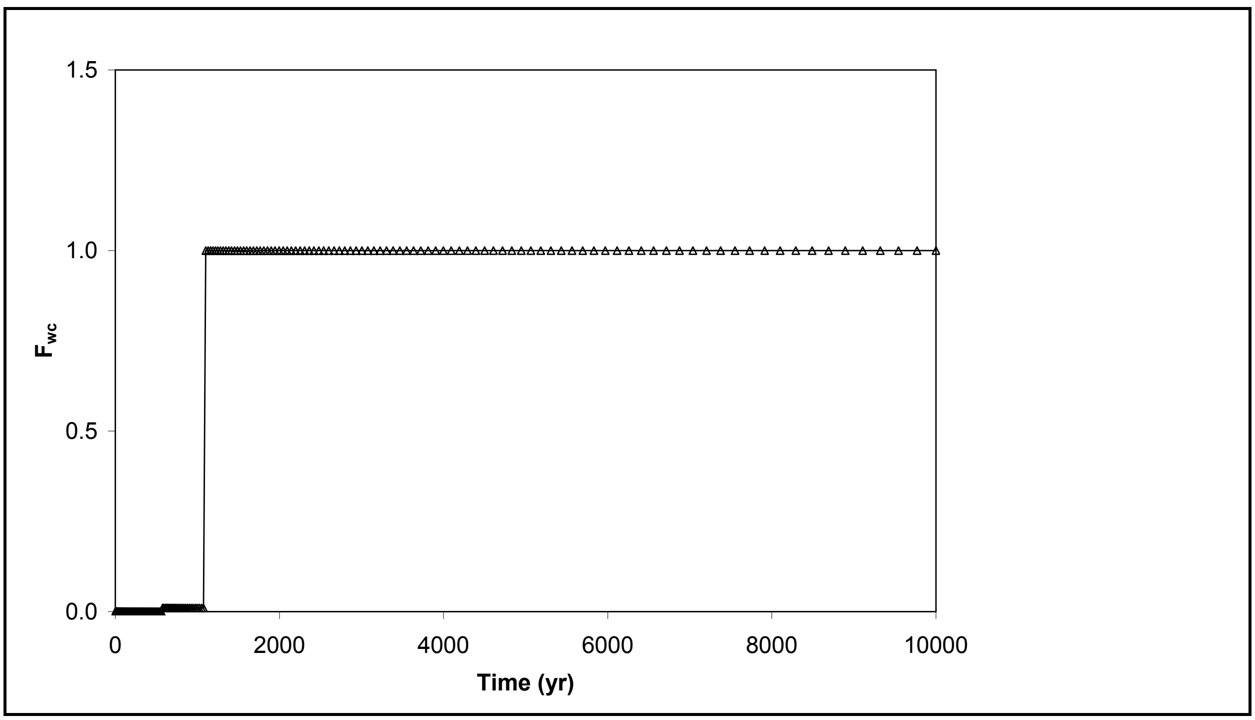


Fig. 9. Time series of F_{wc} resulting from a TPA simulation for 10Ky.

InitialSeepageReductionFractionByMechFailedWP, is the seepage reduction factor associated with the mechanical failure of WPs. It is a sampled parameter and was sampled from a uniform distribution in the range of 0.01-1.0. In this test run, it was zero until WP failure by localized corrosion (t=575 yr). It took a value of 0.01 over the period starting from WP failure by localized corrosion (t=575 yr) to WP failure by general corrosion (t=1100 yr). 0.01 lies in the range of 0.01-1.0 as specified in tpa.inp (Fig. 10). The results are reasonable, but not conclusive on the accuracy of F_{wm} calculations.

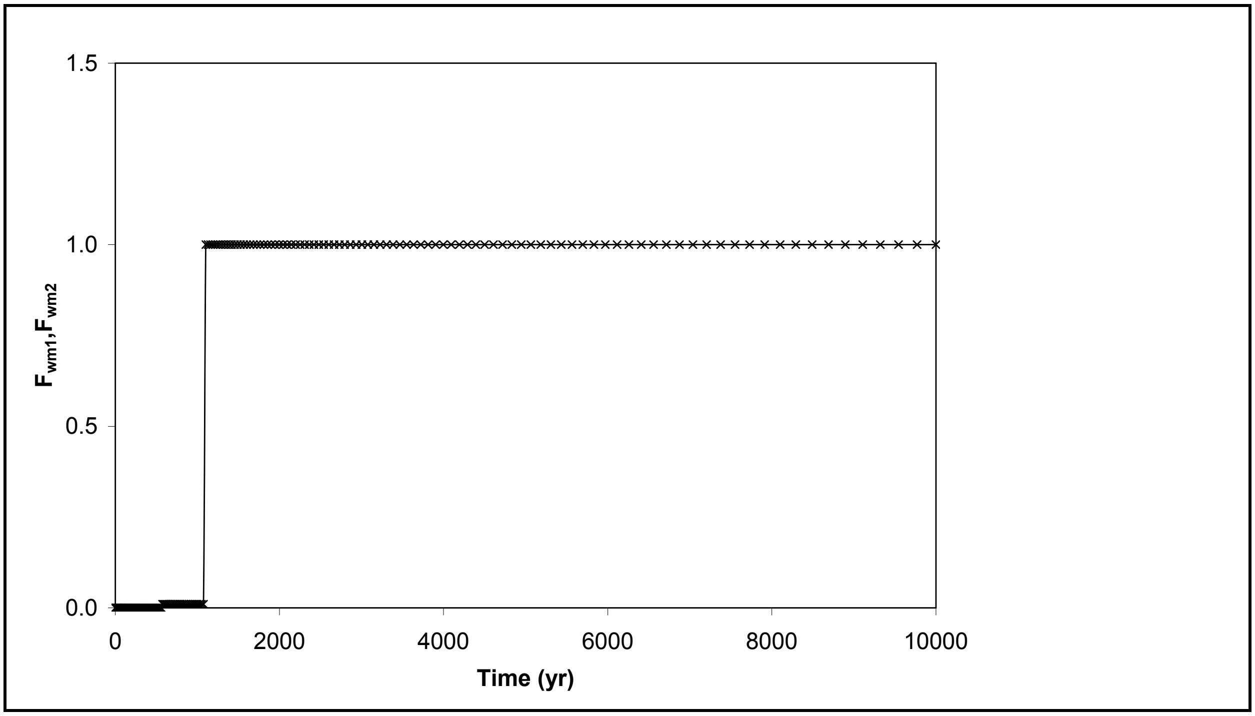


Fig. 10. Time series of F_{wm} resulting from a TPA simulation for 10Ky.

In order to have a more conclusive test results for InitialSeepageReductionFractionByMech FailedWP, we forced mechanical failure by setting DripShieldBulkHeadTributaryArea to 230 m^2 (the default value was 2.3 m^2 in tpa.inp). A summary of screen output is given below:

---

exec: calling nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas = **582.9** yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    ebsfail: time of WP breach by general corrosion = 1077.0 yr
exec: calling mechdriver (waste package)
exec: failed WPs from INITIAL event = 15 at TPA time = 0.0 yr
exec: failed WPs from **MECHANICAL event** = 1312 at TPA time = **388.5** yr
exec: failed WPs from GEN CORR event = 1577 at TPA time = **1075.1** yr
 *** failed WPs: all WPs failed (2904) ***
exec: calling ebsrel

An increment in F_{wm} due to the mechanical event at t~388 yr and corrosion on welded areas at t~583 yr were captured well in Fig. 11. F_{wm}=1 when general corrosion occurred at t~1077 yr. InitialSeepageReductionFractionbyMechFailedWP is a sampled parameter and is sampled from a uniform distribution in the range of 0.01-1.0. InitialSeepageReductionFractionbyMechFailed WP=0.505, which lies in the range of 0.01-1.0. InitialSeepageReductionFractionWeldL=0.01, which lies in the range of 0.001-0.1, as specified in tpa.inp. F_{wm}=1 for t>1102 yr as the general corrosion took place. Hence, F_{wm} has been correctly calculated.

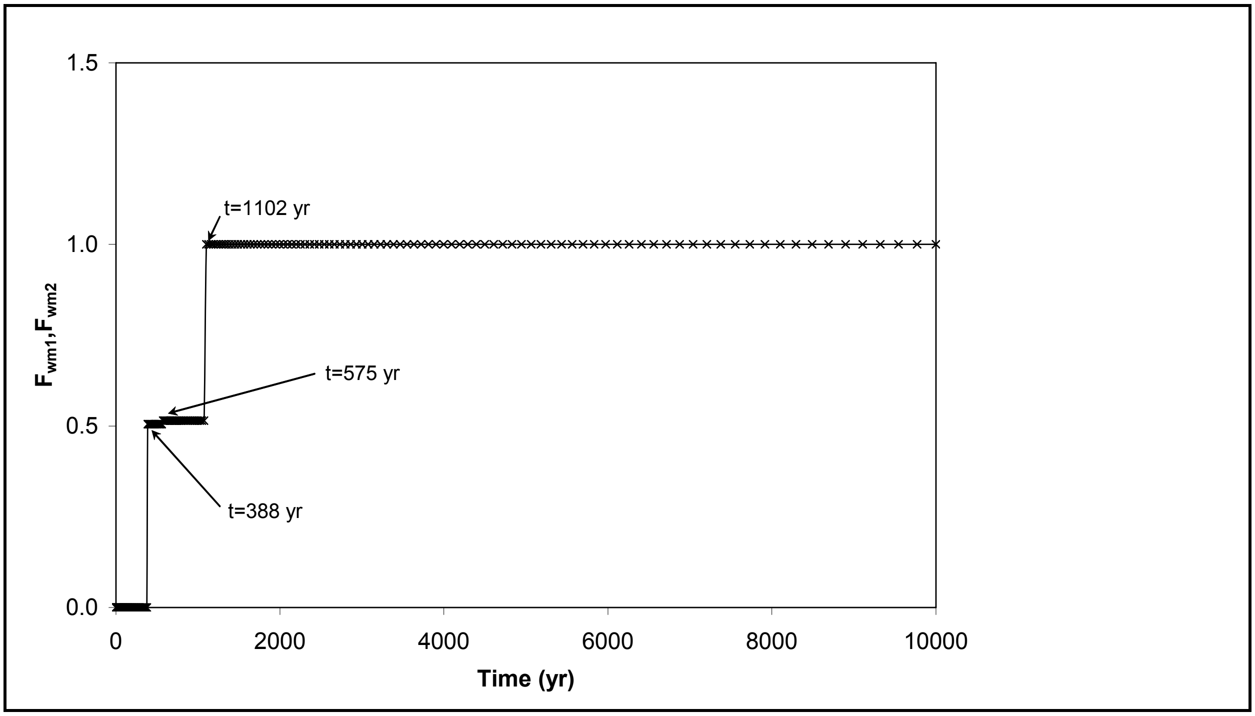


Fig. 11. Time series of F_{wm1}, F_{wm2} resulting from a TPA simulation for 10Ky.

InitialSeepageReductionFractionInitiallyDefWP accounts for the seepage reduction due to initial failure of WPs and is the value of F_{id} when initial failure occurs. It is a sampled parameter, and was sampled from a loguniform distribution in the range of 0.001, 0.1. F_{id} took a value of 0.01 at t=0 when initial failures occurred. Its value is in the range of prescribed bounds in TPA. At t~575 yr, F_{id} =0.02 when weld localized corrosion occurred. The change from 0.01 to 0.02 was due to the sampled value of 0.01 for InitialSeepageReductionFractionWeldL, which lies in the range of 0.001-0.1, as specified in TPA. F_{id} =1 for t>1102 yr as the general corrosion took place. Hence, F_{id} has been **correctly** calculated (Fig. 12).

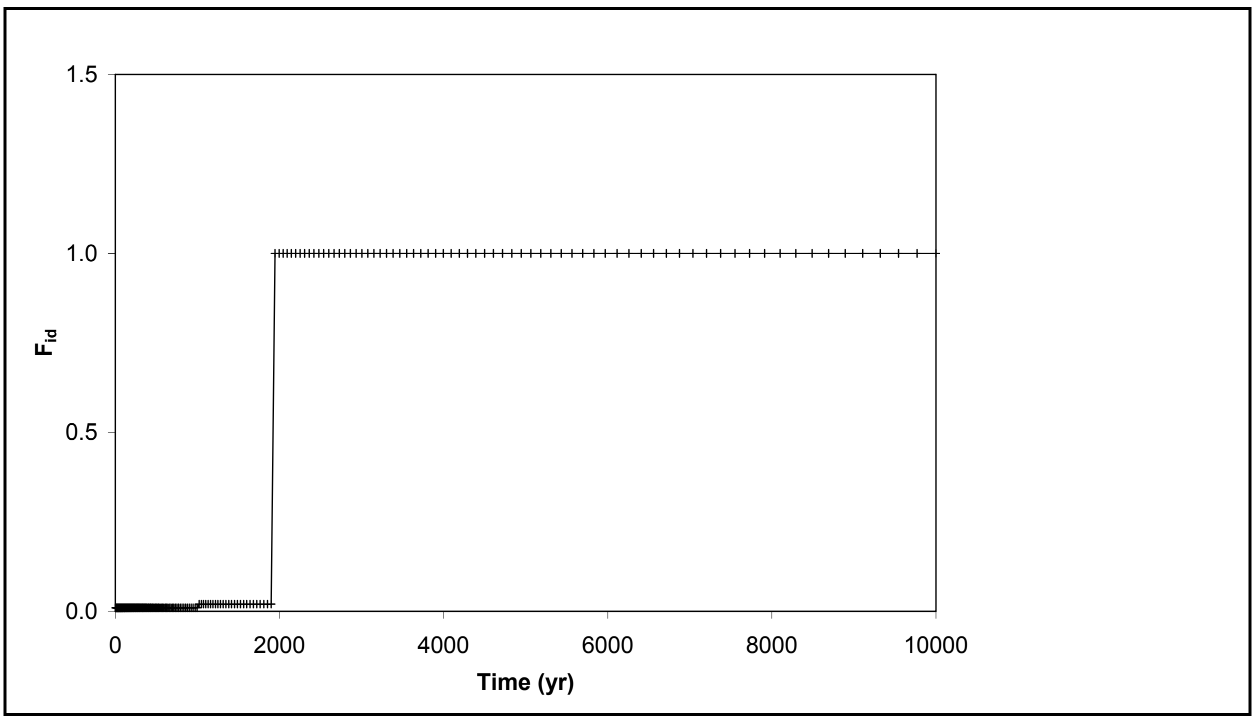


Fig. 12. Time series of F_{id} resulting from a TPA simulation for 10Ky.

Bullet 2, (effect of the seepage threshold temperature on flows and releases)**:**

Seepage threshold temperature (SeepageThresholdT[C] in tpa.inp) is a sampled parameter and is sampled from a triangular distribution (100°C, 105°C, 125°C). The mean value was 110 °C. FlagSeepageThreshold was 1 (indicating that the seepage threshold is activated in calculations). The drip shield temperature (under tempdsoA in thermal.dbg) and the mean value of Seepage ThresholdT[C] are shown in the figure below.

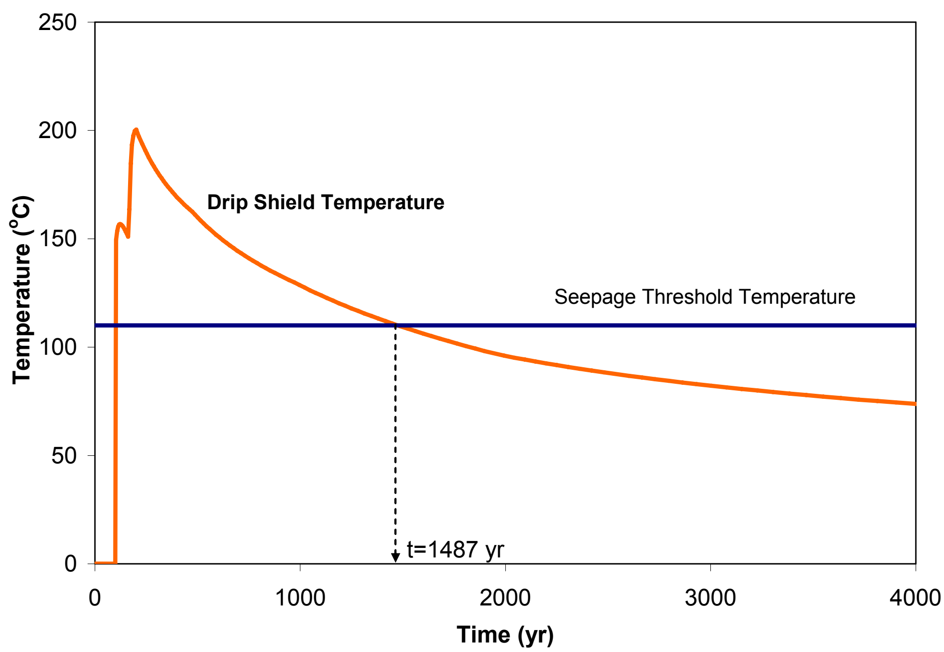


Fig. 13. Time variations in the drip-shield temperature in reference to the seepage threshold temperature for 10Ky. The critical time at which the drip-shield temperature fell below the seepage threshold temperature was 1487 year.

The temperature in the drift wall was above the seepage threshold temperature for t=104yr – 1487 yr. During this period no water should enter waste packages, and hence there should be no releases in this period. Drip/WP from ebsflo.dat shows that the water did not enter waste packages until t=1487 yr (until the drift wall temperature cools down to the seepage threshold temperature). It should be noted that FlowOnsetTemprature (with a mean value of 96°C) has not been implemented in version T or U of TPA. If it were, it would not allow the percolating water contacts waste packages until the waste package temperature falls below FlowOnsetTemperature (this issue has been addressed in SRC673 using BetaW version of the TPA code). Because FlowOnsetTemprature was not implemented in version T or U, deep percolating water contacted waste packages and caused releases as the drip shield temperature fell below the seepage threshold temperature (Figs. 14 and 15). Hence, flow and release rates (recorded in ebsflo.dat and ebssf.dat) indicate the correct implementation of the seepage temperature threshold in the code.

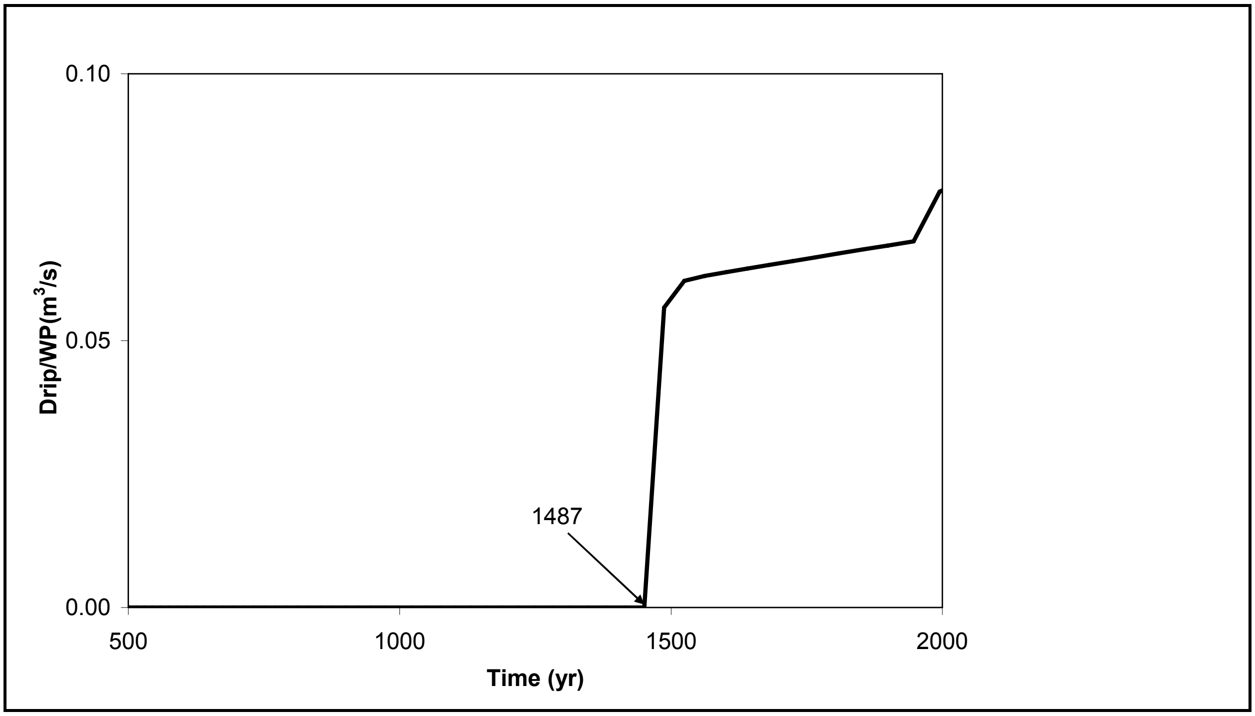


Fig. 14. Time variation in the deep percolating water dripping on waste packages (from ebsflo.dat).

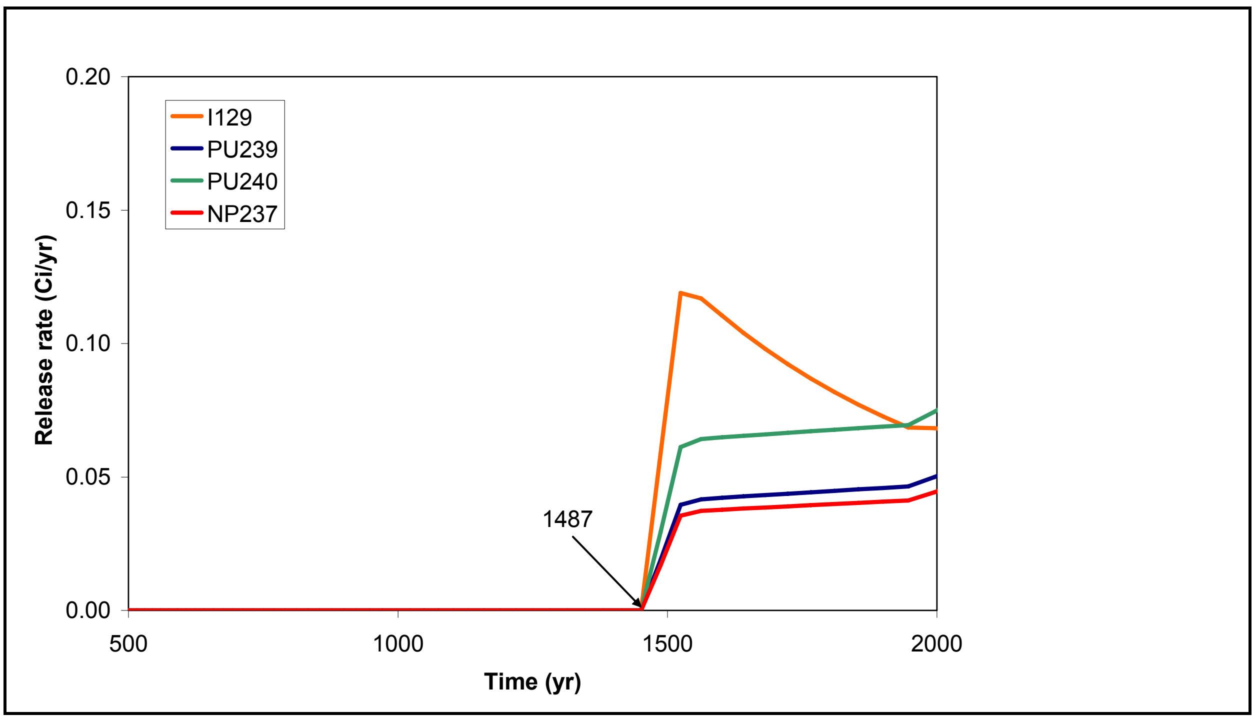


Fig. 15. Release rates of some of radionuclides leaving failed waste packages (from ebsnef2.dat).

Check for correctness of <u>fmult</u> calculations:

F_{mult} calculations were based on the following empirical relation in TPA:

$$F_{mult} = \begin{cases} \dfrac{a}{1 + e^{-\frac{\ln\left[\frac{1000 \frac{\mathrm{yr}}{\mathrm{m}} q_r F_{ow}}{L_{WP} D_{WP}}\right] - x_o}{b}}} & \text{if } t < t_B \\ 1 & \text{if } t > t_B \end{cases} \qquad (1)$$

where

- a — Shape parameter [unitless] (AfmultCoefficient in *tpa.inp*),
- b — Scale parameter [unitless] (BfmultCoefficient in *tpa.inp*),
- x_o — Shift parameter [unitless] (X0FmultCoefficient in *tpa.inp*),
- q_r — Reflux rate in the thermal period or deep percolation rate in post-thermal period [m^3/yr] (Fig. 1.1),
- F_{ow} — Temporal flow focusing factor interpolated from data in *wpflow.def* [unitless],
- L_{WP} — Waste package length [m] (WPLength in *tpa.inp*,),
- D_{WP} — Waste package diameter [m] (WPDiameter in *tpa.inp*),
- t_B — Initial time at which rubble starts accumulating on top of the drip shield [yr].

q_r in Eq. 1 is the Drip/WP (m^3/s) and it is internally calculated and reported in ebsflo.dat. Waste package length and waste package diameter were set to constant values of 5.165m and 1.659 m in TPA, respectively. In mean value data file, AfmultCoefficient = 0.9; BfmultCoefficient = 0.22; and X0FmultCoefficient = 1.49. Temporal variations in F_{mult} is shown in Fig. 16.

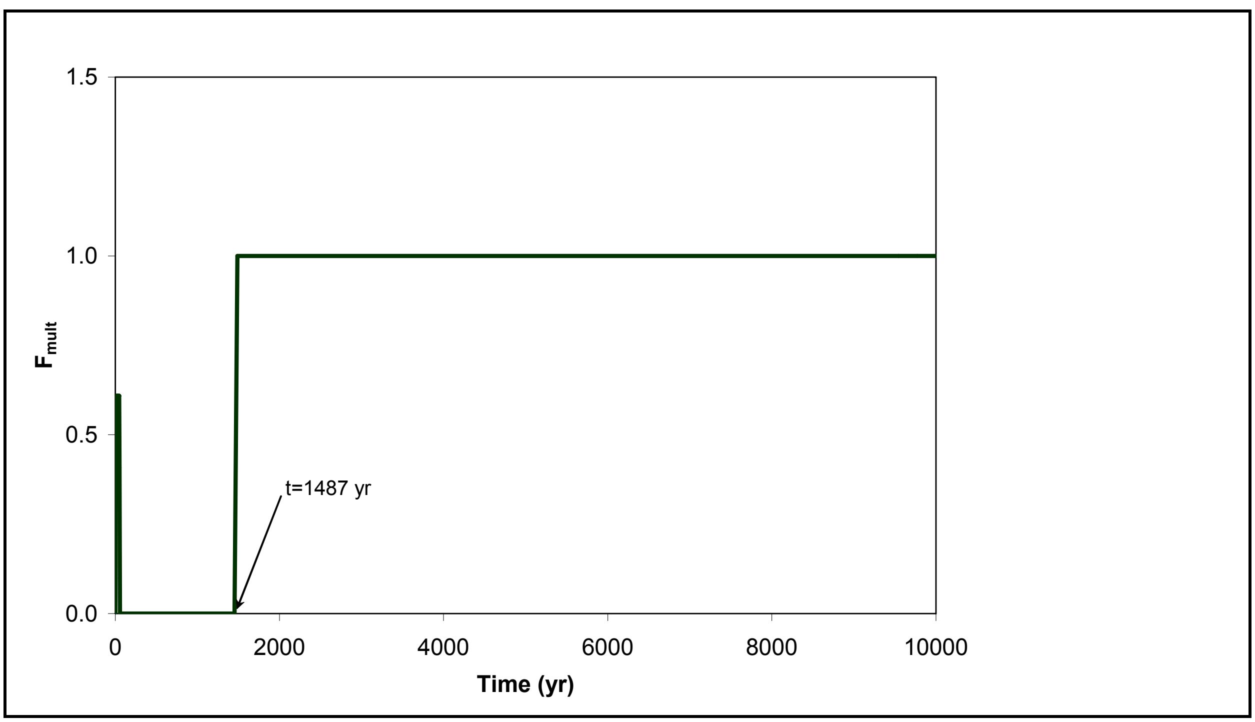


Fig. 16. Temporal variations in F_{mult}.

F_{mult} would take a value of 1 when the rubble starts accumulating on top of the drip shield (in TPA, this time corresponds to filling up the gap between the drip shield and the drift wall by rubble). In TPA, an equivalent time-variant diameter in the horizontal direction, eqBFB, to account for rubble accumulation on top of the drip shield is introduced. When eqBFB is equal to the drift diameter, then F_{mult} should have been equal to 1. In our simulation, this condition occurred at t=168.24 yr (from driftfail.dat) (Fig. 17).

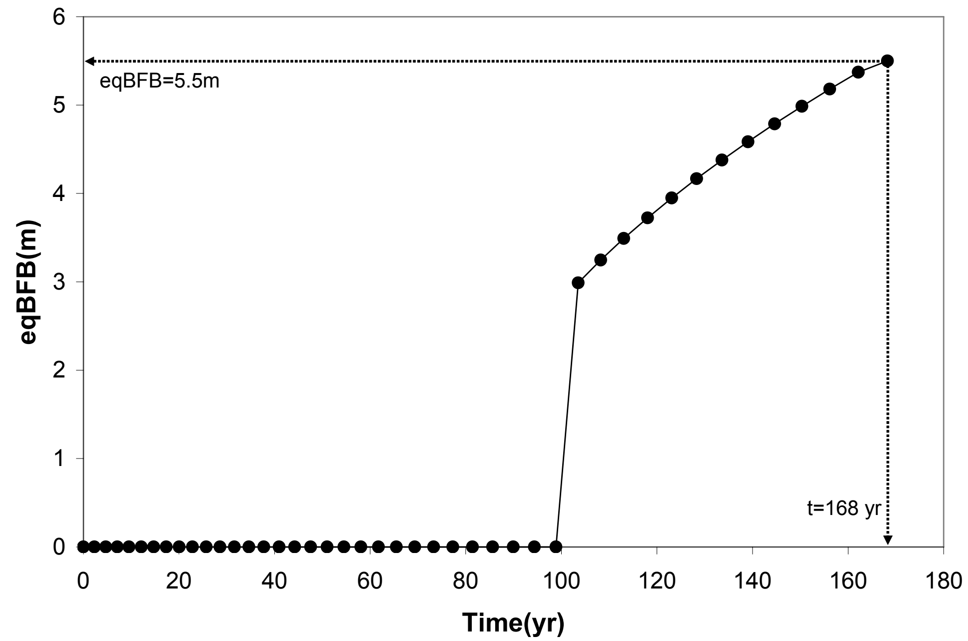


Fig. 17. Temporal variations in equivalent diameter in the horizontal direction, eqBFB.

In Fig. 16, F_{mult} =1 for t>1487 yr. Even though the rubble accumulation occurred at t=168.24 yr, there was no flow until t=1487 yr due to the effect of the Seepage threshold temperature. Hence, in this simulation, the effect of F_{mult} is overwritten by the effect of the seepage threshold temperature.

In Fig. 16, the early time-behavior of F_{mult} is determined by Eq. 1 as a function of deep percolating water, q_r. In order to check the early-time behavior of F_{mult}, we computed F_{mult} as a function of deep percolating water contacting waste packages (from ebsflo.dat) using Eq. 1 outside the code and compared the results against the model computed F_{mult} values reported in ebsflo.dat. The results shown in Fig. 18 reveals that early fluctuations in F_{mult} prior to completion of the drift degradation has been correctly calculated in TPA (based on Eq. 1). Zero values until t=1487 yr are due to the effects of the seepage threshold temperature.

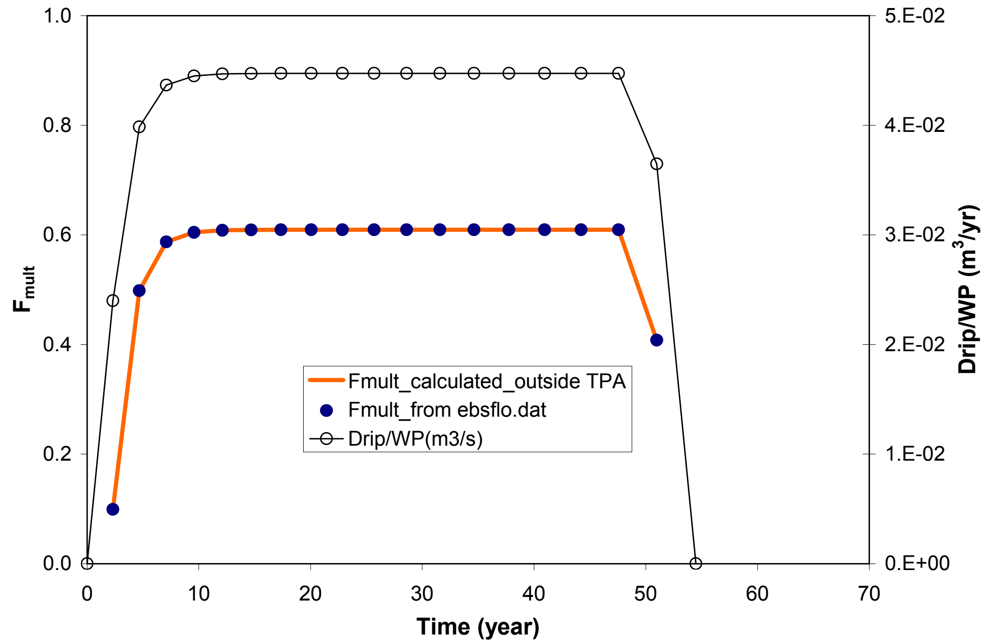


Fig. 18.Fmult values computed by TPA and outside the code using Eq. 1 prior to completion of drift degradation. The right axis is reserved for temporal variations in deep percolating water approaching waste packages.

In order to verify Fmult calculations further, the effect of seepage threshold temperature was suppressed in the next simulation by setting it to 300°C. This would force early arrival of deep percolating water to failed waste packages at earlier times (i.e., earlier than t=1487 yr). In this case, Fmult should take a value of 1 at sometime earlier than 1487 year. Moreover, we increased Time ofRepositoryClosure (a parameter in tpa.inp) from 100 yr to 1000 yr to force delays in rubble accumulations.

Part of the screen output from this simulation is given below:

```
exec: calling uzflow
      Mean Annual Infiltration at Start(AAI0):    5.8327E+00
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
dataFile= dsfailt.dat
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      388.5  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =      582.9  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    ebsfail: time of WP breach by general corrosion =     1077.0  yr
exec: calling mechdriver (waste package)
exec: failed WPs from INITIAL    event =     15 at TPA time =      0.0 yr
exec: failed WPs from LOC CORR   event =    131 at TPA time =    574.9 yr
exec: failed WPs from GEN CORR   event =   2758 at TPA time =   1075.1 yr
 *** failed WPs: all WPs failed ( 2904 ) ***
```

The temporal variations in F_{mult} is shown below:

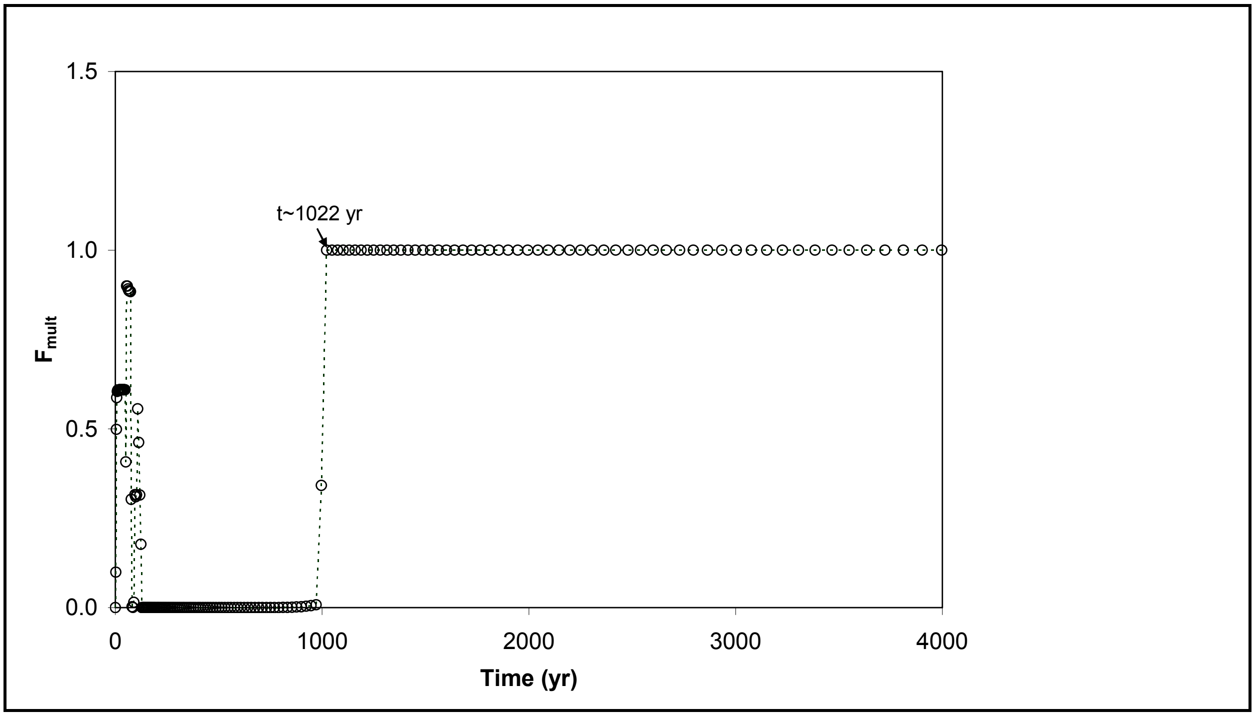


Fig. 19. Temporal variations in F_{mult}.

By eliminating the effect of the seepage threshold temperature (by arbitrarily increasing it to 300°C), the water flux into failed WPs occurred at t=1022 yr instead of t=1487 yr. It was reported in ebsnef2.dat that the releases also occurred for t$\geq$1022 year. The parameter controlling the rubble accumulation, eqBFB, became equal to 5.5 m at t=1022 yr (Fig. 20) (from driftfail.dat), as TimeofRepositoryClosure was increased from 100 yr to 1000 yr. F_{mult}=1 when the rubble accumulation was complete in the absence of seepage threshold temperature, as expected.

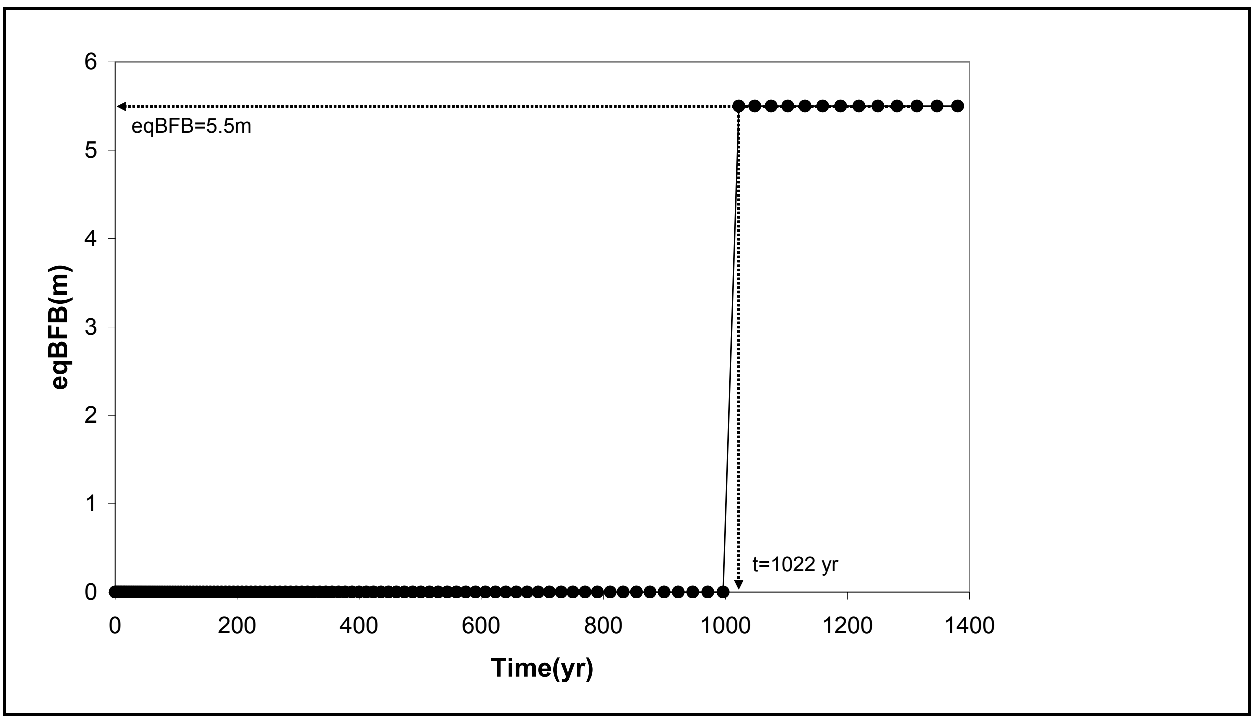


Fig. 20. Temporal variations in equivalent diameter in the horizontal direction, eqBFB.

In Fig. 19, the early time-behavior of F_{mult} is determined by Eq. 1 as a function of deep percolating water, q_r. In order to check the early-time behavior of F_{mult}, we computed F_{mult} as a function of deep percolating water contacting waste packages (from ebsflo.dat) using Eq. 1 outside the code and compared the results against the model computed F_{mult} values reported in ebsflo.dat. The results shown in Fig. 21 reveals that early fluctuations in F_{mult} prior to completion of the drift degradation has been correctly calculated in TPA (based on Eq. 1).

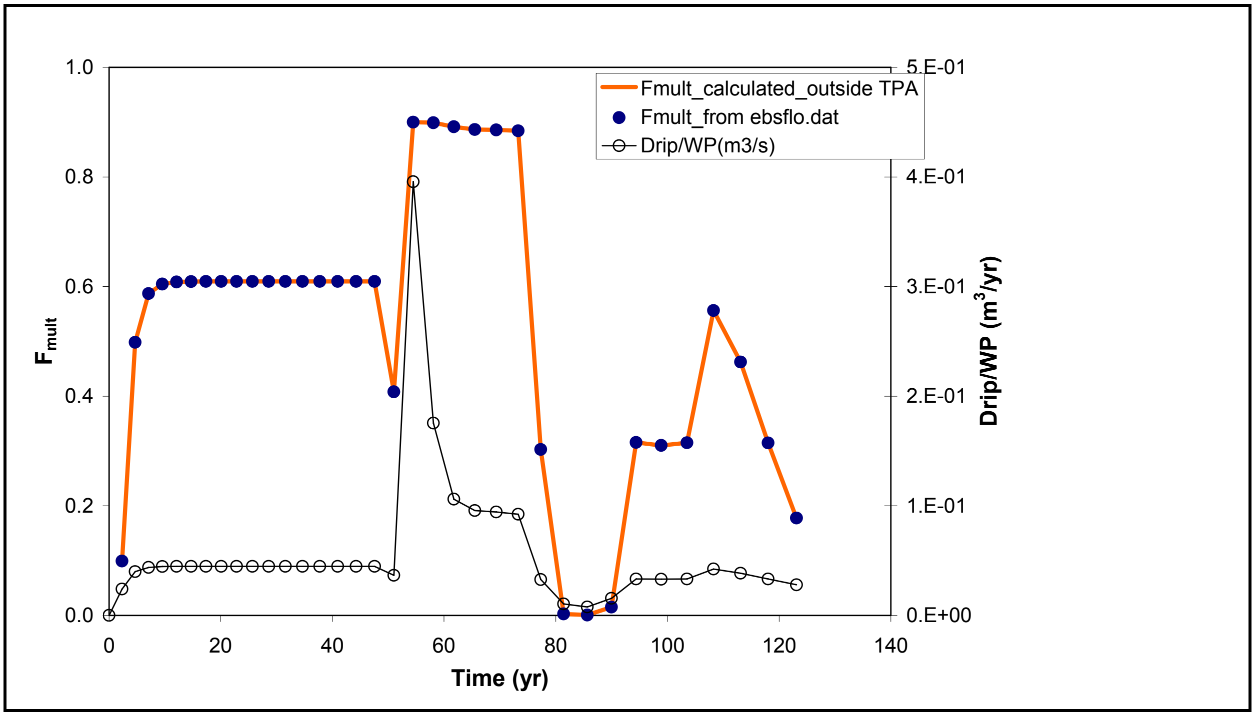


Fig. 21. F_{mult} values computed by TPA and outside the code using Eq. 1 prior to completion of drift degradation. The right axis is reserved for temporal variations in deep percolating water approaching waste packages.

Briefly, both the early and long time behaviors of F_{mult} in the absence or presence of Seepage Threshold Temperature were **correctly** calculated.

Water mass-balance checks:

We checked the water mass-balance using a stand-alone version of the code by employing bathtub and flow through modes for seven failure types, including generalized corrosion. The changes were made in ebsrel.inp for the first six failure types (including initial failure, fault, volcano, mechanical failure 1 and 2, and localized corrosion). Failure type 6 were excluded from these analyses. Because this is a free failure type reserved for future consideration. For general corrosion to start, the flag for general corrosion in ebstrh.dat was switched to 1 and switches for all other failure types in ebsrel.inp were set to 0. In the first six failure types, the number of spent fuel (SF) waste packages was set to 11 (out of 2090 SF waste packages). The waste package number was not specified for generalized corrosion. The results for mass-balance checks were obtained from relcum.out and ebsnef.dat.

<u>Simulations with the bathtub mode:</u>

TPA simulations were conducted for the aforementioned seven failure types.

- **Failure type:** Initial WP Failure

The start and stop time of the failed WPs were recorded in relcum.out.

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	**11**	**1.4900E+03**	**1.5740E+02**	**1.5242E+03**	**1.6816E+03**
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

Start SF Wet time corresponds to the time at which drift wall temperature cools down to the seepage threshold temperature (110^{o}C). This is the time the reflux water breached the dryout zone and reached the failed waste packages. When waste packages are treated as a bathtub, the fill time started at 1524 yr and ended at 1681 yr. So, the fill time was roughly ~157 yr. Because only 11 of SF waste packages underwent flow through due to initial WP failure, the remaining 2079 would be susceptible to general corrosion.

Bathtub filling and ending times are consistent with the results in ebsnef.dat. Part of the results in ebsnef.dat are given below:

………

1.3808E+03	0.0000E+00	0	0.0000E+00	0.0000E+00	0.0000E+00
1.4154E+03	0.0000E+00	0	0.0000E+00	0.0000E+00	0.0000E+00
1.4508E+03	0.0000E+00	0	0.0000E+00	0.0000E+00	0.0000E+00
1.4871E+03	0.0000E+00	0	0.0000E+00	5.9158E-05	0.0000E+00
1.5242E+03	0.0000E+00	0	0.0000E+00	6.4421E-05	0.0000E+00
1.5622E+03	0.0000E+00	0	0.0000E+00	6.5474E-05	0.0000E+00
1.6011E+03	0.0000E+00	0	0.0000E+00	6.6105E-05	0.0000E+00
1.6409E+03	0.0000E+00	0	0.0000E+00	6.6842E-05	0.0000E+00
1.6816E+03	1.3348E-04	0	1.4129E-01	6.7579E-05	6.7604E-05
1.7233E+03	1.8764E-03	0	1.4282E-01	6.8316E-05	6.8334E-05
1.7660E+03	1.8212E-03	0	1.4413E-01	6.9053E-05	6.8961E-05

………..

The first column above is the time, the second column is the release rate of a particular radionuclide (CM246 in this case) from the EBS, the third column is the flag for the solubility limit, the fourth column is the total water outflow, and the fifth and six columns represent the total water inflow and outflow averaged over the total number of failed waste packages.

When failed waste packages were treated as a bathtub, they were contacted by water at t=1487 yr. Until the bathtub was full, there was no outflow. When the bathtub was full, the first outflow occurred at t=1681 yr. After t=1681 yr, the flow mode switched from ‘bathtub’ to ‘flow through’ mode, as expected. These results are consistent with the results reported in relcum.out.

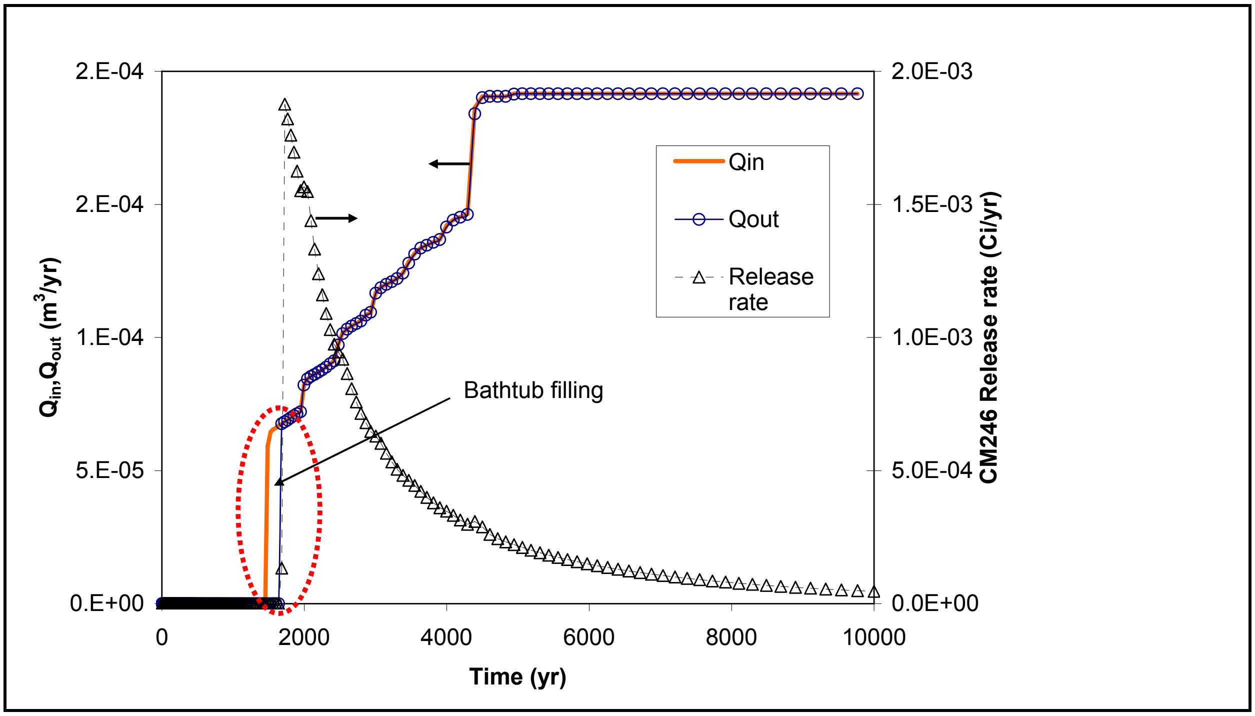


Fig. 22. Inflow and outflow rates from a failed waste package as a result of initial waste package failure. A bathtub flow mode was implemented. The right axis is reserved for release rates of CM246 from the EBS. This figure is representative for all failure modes, except for general corrosion, discussed in this section.

Radionuclide releases started when the bathtub was full. The results for the first failure type are shown in Fig. 22. The left axis in this figure is reserved for the inflow and outflow rates, and the right axis is reserved for release rate of CM246. The figure indicates that (a) no releases took place until the bathtub was full, and (b) once the bathtub was filled-up, inflow and outflow rates were practically equal, hence the mass-balance was conserved and flow switched from bathtub mode to the flow through mode. The "maximum" mass-balance error for water flux was observed at t=4394 yr, where the inflow rate was 0.00018632 m^3/yr and outflow rate was 0.00018403 m^3/yr. The rest of the time the mass-balance error for water flux was less than ~0.5%. Considering potential round off errors in calculations in TPA, and absence of a specific algorithm (or iterative schemes) for checking and correcting the mass-balance error internally in the code, the "maximum" water mass-balance error of 0.5-1% is deemed acceptable.

- Failure type: Fault, Volcano, mechanical failures 1 and 2, and localized corrosion. The results from these failure types are identical to the results from the initial waste package failure type (regarding Q_{in}, Q_{out}, and release rates and time of CM246). Therefore, we included below only a part of relcum.out for these failure types.

- Fault:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	**11**	**1.4900E+03**	**1.5740E+02**	**1.5242E+03**	**1.6816E+03**
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+

- Valcano:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	**11**	**1.4900E+03**	**1.5740E+02**	**1.5242E+03**	**1.6816E+03**
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

- Mechanical Failure 1:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	**11**	**1.4900E+03**	**1.5740E+02**	**1.5242E+03**	**1.6816E+03**
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

- Mechanical Failure 2:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	**11**	**1.4900E+03**	**1.5740E+02**	**1.5242E+03**	**1.6816E+03**
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

- Local Corrosion:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	**11**	**1.4900E+03**	**1.5740E+02**	**1.5242E+03**	**1.6816E+03**
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

- General Corrosion:

We turned on the flag for the general corrosion in ebstrh.dat, and changed the general corrosion start time from a default value of ~100ky to a number less than 10 Ky to force the general corrosion within 10Ky simulation period.

---

1 **1.0769564397E+02** | WP Breach by General Corrosion Flag (1 = failure), Time of WP Breach by General Corrosion[yr]

The results from relcum.out:

1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	**2090**	**1.4900E+03**	**1.5740E+02**	**1.5242E+03**	**1.6816E+03**

The time for waste packages contacted by water was determined by the seepage threshold temperature as for the other failure types. The results are identical, but the volume of Q_{in} and Q_{out}, and the release rates were higher for the general corrosion case, because more waste packages were failed by general corrosion than by other failure modes . In the tabulated results above, all 2090 SF waste packages underwent flow through when general corrosion took place. The results are shown in Fig. 23.

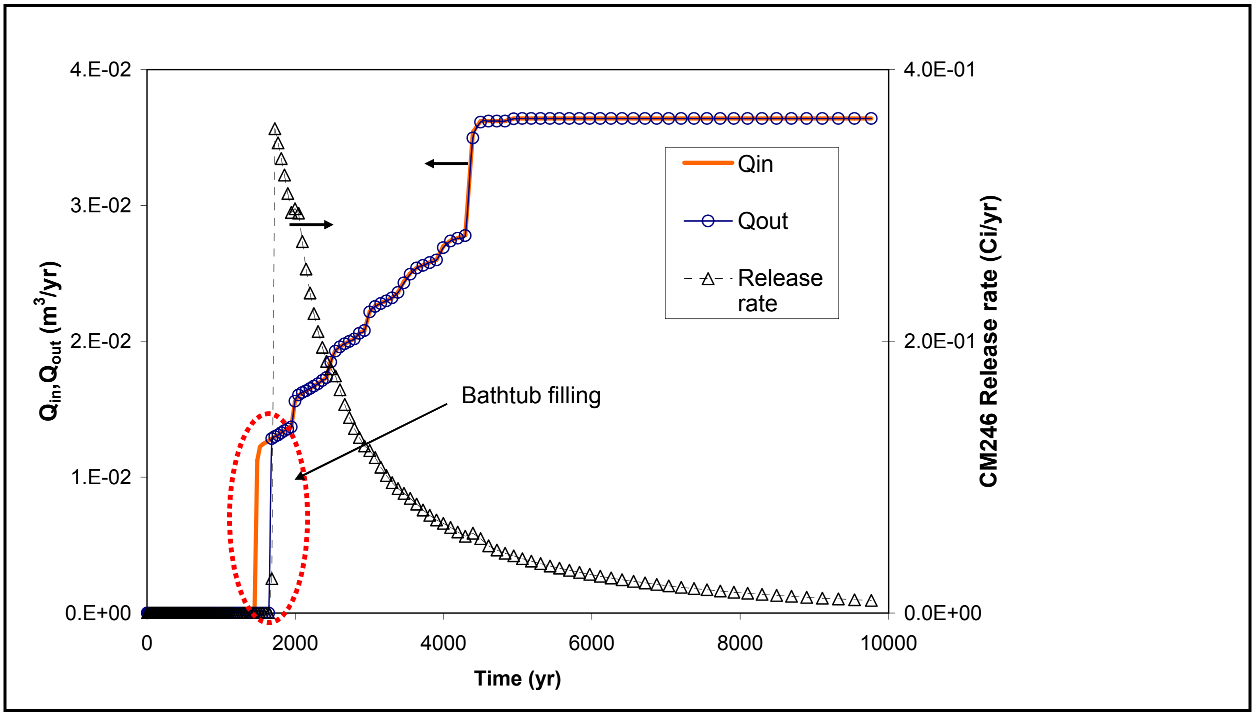


Fig. 23. Inflow and outflow rates from a failed waste package as a result of general corrosion. A bathtub flow mode was implemented. The right axis is reserved for release rates of CM246 from the EBS.

Simulations with the flow through mode:

- **Failure type:** Initial WP Failure

The start and stop time of the failed WPs were recorded in relcum.out.

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	**11**	**1.4900E+03**	**0.0000E+00**	**1.5242E+03**	**1.5242E+03**
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

Start SF Wet time corresponds to the time at which drift wall temperature cools down to the seepage threshold temperature (110°C). This is the time the reflux water reached the failed WPs. Unlike the bathtub mode, the fill time was 0. Again, the total number of SF WPs in Subarea were 2090, and only 11 of them underwent initial WP failure, and the remaining 2079 were susceptible to general corrosion, if general corrosion takes place within 10Ky period (only one failure mode was activated in each simulation).

These results are consistent with the results in ebsnef.dat. Part of the results in ebsnef.dat are given below:

....

1.4154E+03	0.0000E+00	0	0.0000E+00	0.0000E+00	0.0000E+00
1.4508E+03	0.0000E+00	0	0.0000E+00	0.0000E+00	0.0000E+00
1.4871E+03	0.0000E+00	0	0.0000E+00	5.9158E-05	0.0000E+00
1.5242E+03	1.8102E-04	0	1.3469E-01	6.4421E-05	6.4447E-05
1.5622E+03	5.0929E-04	0	1.3686E-01	6.5474E-05	6.5483E-05
1.6011E+03	7.6849E-04	0	1.3814E-01	6.6105E-05	6.6095E-05

....

The first column above is the time, the second column is the release rate of a particular radionuclide (CM246 in this case) from the EBS, the third column is the flag for the solubility limit, the fourth column is the total water outflow, and the fifth and six columns represent the total water inflow and outflow averaged over the total number of failed WPs.

When failed WPs were treated as a flow through system with no storage, they were contacted by water first at t=1487 yr. After water contacted the WP, all inflow (weighted by the number of waste packages) left the failed waste packages in the same time-step. The radionuclides release time coincided with the nonzero outflow time. Thus, the model performed as expected. The results are shown in for the initial WP failure type in Fig. 24.

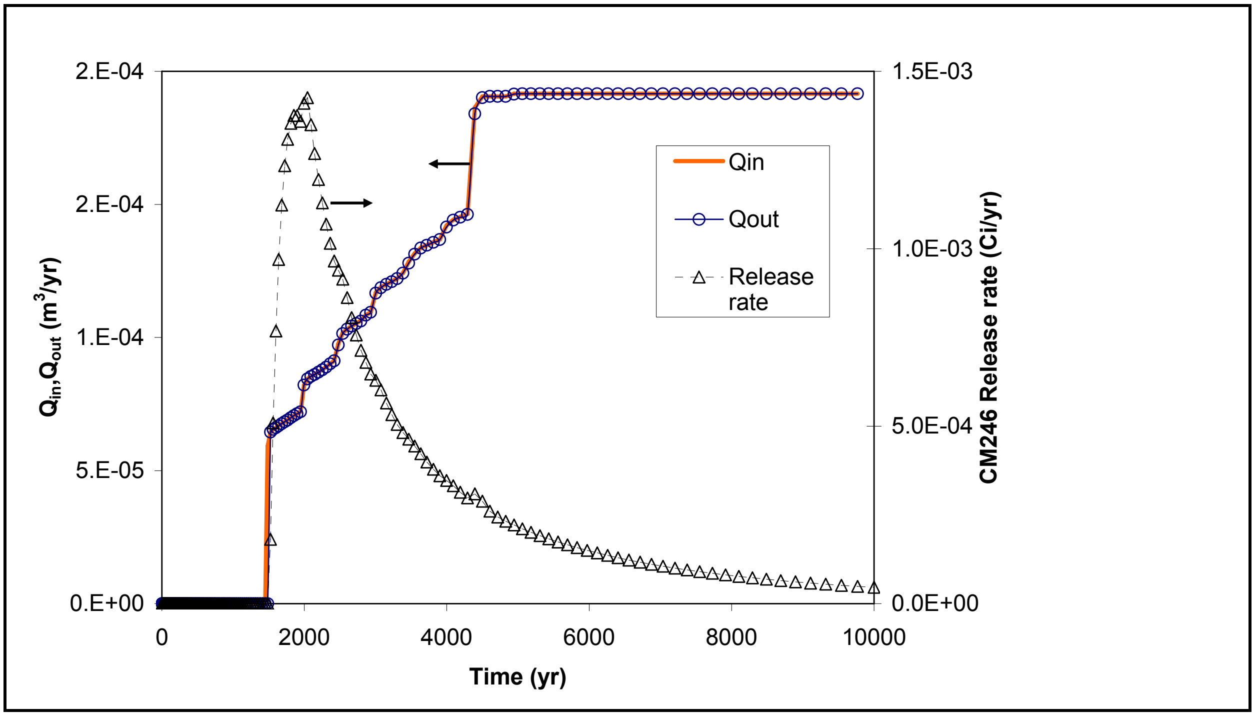


Fig. 24. Inflow and outflow rates from a failed waste package as a result of initial waste package failure. A flow through mode was implemented. The right axis is reserved for release rates of CM246 from the EBS. This figure is representative for all failure modes, except for general corrosion, discussed in this section.

As in the bathtub mode, the maximum mass-balance for water flux was achieved within 1%. “Maximum” mass-balance error for water flux was observed at t=4394 yr, where the inflow rate was 0.00018632 m^3/yr and outflow rate was 0.00018403 m^3/yr. The rest of the time the mass-balance error for water flux was less than ~0.5%. Considering potential round off errors in calculations in TPA, and absence of a specific algorithm (or iterative schemes) for checking and correcting the mass-balance error internally in the code, the “maximum” water mass-balance error of 0.5-1% is deemed acceptable.

The results (Q_{in}, Q_{out}, and release time and rates) for the rest of the failure modes, except for generalized corrosion, were the same; therefore, we provided only results from relcum.out in the subsequent section.

- Fault:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	**11**	**1.4900E+03**	**0.0000E+00**	**1.5242E+03**	**1.5242E+03**
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

- Valcano:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	**11**	**1.4900E+03**	**0.0000E+00**	**1.5242E+03**	**1.5242E+03**
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

- Mechanical Failure 1:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	**11**	**1.4900E+03**	**0.0000E+00**	**1.5242E+03**	**1.5242E+03**
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+0-

Mechanical Failure 2:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	**11**	**1.4900E+03**	**0.0000E+00**	**1.5242E+03**	**1.5242E+03**
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

- Local Corrosion:

1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	**11**	**1.4900E+03**	**0.0000E+00**	**1.5242E+03**	**1.5242E+03**
8	2079	1.0000E+04	0.0000E+00	1.0000E+04	1.0000E+04

- General Corrosion:

We turned on the flag for the general corrosion in ebstrh.dat, and changed the general corrosion start time from a default value of ~100ky to a number less than 10 Ky to force the general corrosion within 10Ky simulation period.

----

1 1.0769564397E+02 | WP Breach by General Corrosion Flag (1 = failure), Time of WP Breach by General Corrosion[yr]

The results from relcum.out:

1	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
2	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	0	1.4900E+03	0.0000E+00	0.0000E+00	0.0000E+00
8	**2090**	**1.4900E+03**	**0.0000E+00**	**1.5242E+03**	**1.5242E+0**

The results are identical, but the volume of Q_{in} and Q_{out}, and the release rates were higher for the general corrosion case, because more waste packages were failed by general corrosion. The time for waste packages contacted by water was determined by the seepage threshold temperature as for the other failure types. In the tabulated results above, all 2090 SF waste packages (as opposed 11 waste packages for other failure modes) underwent flow through when general corrosion took place. The results are shown in Fig. 25.

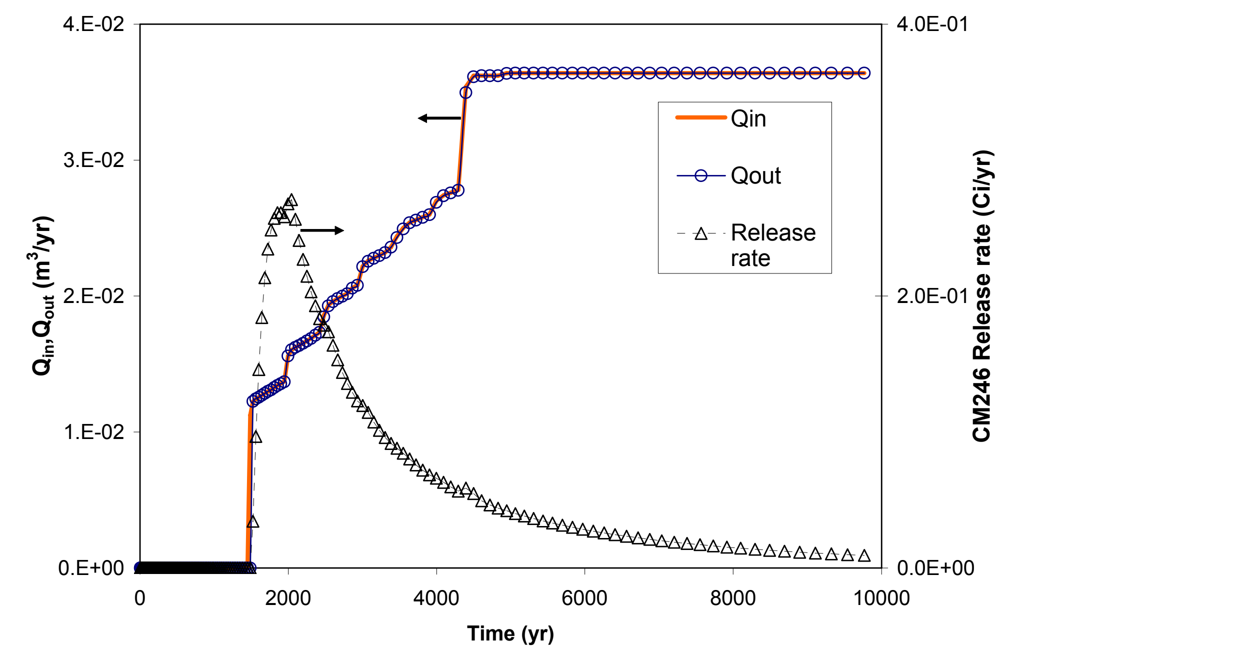


Fig. 25. Inflow and outflow rates from a failed waste package as a result of general corrosion. A flow through mode was implemented. The right axis is reserved for release rates of CM246 from the EBS.

In summary, WP-averaged inflow flow and outflow rates were correctly calculated for all failure types. For the bathtub mode, the outflow did not start until the bathtub was full, and the fill time was correctly calculated. For both bathtub and flow through modes, the mass-balance for water flux was accurate within 1%. The radionuclides released from failed waste packages as soon as outflow from failed waste packages became non-zero. Hence, flow modes (bathtub and flow through) are correctly implemented in TPA, and Q_{in} and Q_{out} are correctly calculated.

Check for general and localized corrosion failure times and the weld failure time

We looked at the results from TPA simulations with the mean value data. The failure times were recorded in failt.out. Portion of the results is shown below:

! SECTION 2 ; WELD CORROSION RESULTS
!
! This section contains weld corrosion failure data,
! or it indicates that weld corrosion failure did not occur

5.82869E+02 ! Weld failure time (year)

! SECTION 3 ; WASTE PACKAGE CORROSION RESULTS
!
! This section contains waste package corrosion failure data,
! or it indicates that waste package corrosion failure did
! not occur

1.07696E+03 ! General corrosion failure time (year)

These values are consistent with the information printed out on the screen, as shown below:

----

exec: calling mechdriver (drip shield)
exec: time of **drip shield mechanical failure** = 388.5 yr
*** No Drip Shield Failure by General Corrosion ***
exec: calling nfenv
exec: calling ebsfail
ebsfail: time of **corrosion breach on welded areas** = 582.9 yr
*** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
ebsfail: time of WP breach by general corrosion = 1077.0 yr
exec: calling mechdriver (waste package)
exec: failed **WPs from INITIAL event** = 15 at TPA time = 0.0 yr
exec: failed **WPs from LOC CORR** event = 131 at TPA time = 574.9 yr
exec: failed **WPs from GEN CORR** event = 2758 at TPA time = 1075.1 yr
*** failed WPs: all WPs failed (2904) ***
exec: calling ebsrel

These failure times are also consistent with failure times recorded in ebstrh.dat read by releaset.f. The failure times written in ebstrh.dat is,

----

1 5.8286850000E+02 | Weld Failure Flag (1 = failure), Weld Failure Time[yr]
1 1.0769564397E+03 | WP Breach by General Corrosion Flag (1 = failure), Time of WP Breach by General Corrosion[yr]

Failure time by localized corrosion is close to corrosion breach on welded areas. The difference, ~8 years, is due to a different time-stepping considered in TPA simulations.

Check for the number of WPs failed by failure mode

We reviseited the simulation results on P-10 E-10. The summary was:

----

exec: calling mechdriver (drip shield)
    exec: time of **drip shield mechanical failure** =   388.5 yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling nfenv
exec: calling ebsfail
    ebsfail: time of **corrosion breach on welded areas** =   582.9 yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    ebsfail: time of WP breach by general corrosion =   1077.0 yr
exec: calling mechdriver (waste package)
exec: failed **WPs from INITIAL   event** =   15 at TPA time =   0.0 yr
exec: failed **WPs from LOC CORR**   event =   131 at TPA time =   574.9 yr
exec: failed **WPs from GEN CORR**   event =   2758 at TPA time =   1075.1 yr
 *** failed WPs: all WPs failed (2904) ***
exec: calling ebsrel

The results from **wpsfail.res**:

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	3	0.00000E+00	3.05000E+02	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	5.74897E+02	0.00000E+00	**2.90400E+03**	0.00000E+00	0.00000E+00	0.00000E+00

The results from **wpsfail2.res**:

vector unitless	subarea unitless	time yr	#initial unitless	#gencorr unitless	#loccorr unitless	#mechanical unitless	#fault unitless	#ign_act unitless
1	3	0.00000E+00	**1.50000E+01**	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	5.74897E+02	0.00000E+00	0.00000E+00	**1.31000E+02**	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.07512E+03	0.00000E+00	**2.75800E+03**	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

wpsfail.res reports the total number of failed waste packages susceptible to initial WP failures (which was 305) and corrosion (which was 2904) without differentiating them with respect to the aforementioned failure modes. Wpsfail2.dat reports the number of failed waste packages by initial failure, localized corrosion, and general corrosion.

The relation between the results in wpsfail.res and wpsfail2.res is given by the product of the two probability terms describing the probability of a waste package to be contacted by water and the probability of contacting water to cause waste form mobilization. Both of these probability terms are user-defined parameters and vary with the failure type. In tpa.inp,

For the failure by initial defects:

----

constant
Probability_WPWaterContact_InitialDefects
1.0
**
constant

```
Probability_WPWaterAllowance_InitialDefects
 5.050000000000000E-02
**
----------------------------------------------------------------------------------------------------------
```

Hence, $P_{allowance} \times P_{contact}$=0.05, indicating that 5% of the waste packages that failed due to initial defects would be contacted by water capable of mobilizing waste forms. The number of waste packages susceptible to failure by initial defects was given as 305 in wpsfail.res. Hence, the number of waste packages to fail due to initial defect is 305×0.05=15.25~15. This number is consistent with the number of waste packages failed by initial defects as reported in wpsfail2.res.

The total number of waste packages in subarea 3 is 2904. The number of waste packages susceptible to failure by localized corrosion is 2904-305=2599. For failures by localized corrosion (from tpa.inp):

```
----------------------------------------------------------------------------------------------------------
**
constant
Probability_WPWaterContact_LC
 5.050000000000000E-02
**
constant
Probability_WPWaterAllowance_LC
1.0
**
----------------------------------------------------------------------------------------------------------
```

Hence, $P_{allowance} \times P_{contact}$=0.0505, indicating that 5% of the remaining waste packages that failed due to localized corrosion would be contacted by water capable of mobilizing waste forms , 2599×0.0505=131.25 ~131. This number is consistent with the number of waste packages failed by localized corrosion as reported in wpsfail2.res at t = 575 yr.

If general corrosion occurs, the rest of the waste packages (that were not failed yet) are susceptible to general corrosion. Hence, 2904-(15+131)=2758 are susceptible to general corrosion.

For the failure type by general corrosion (from tpa.inp),

```
----------------------------------------------------------------------------------------------------------
constant
Probability_WPWaterContact_GC-Flt-Ig
1.0
**
constant
Probability_WPWaterAllowance_GC-Flt-Ig
1.0
**
----------------------------------------------------------------------------------------------------------
```

Hence, $P_{allowance} \times P_{contact}=1$, indicating that 100% of the remaining WPs failed by general corrosion would be contacted by water capable of mobilizing waste forms, and this number is 2758. This number is consistent with the number of waste packages failed by general corrosion as reported in wpsfail2.res.

<u>Check that the last two columns of infilper.res file contain WP-weighted average flow rates.</u>

We looked at the results from ebsnef.dat (from a standalone run of ebsrel.f) and infilper.res (because ebsnef.dat is overwritten when TPA is run). The last two columns in ebsnef.dat correspond to the WP-weighted average flow rates; therefore they should be consistent with the WP-weighted average flow rates in infilper.res.

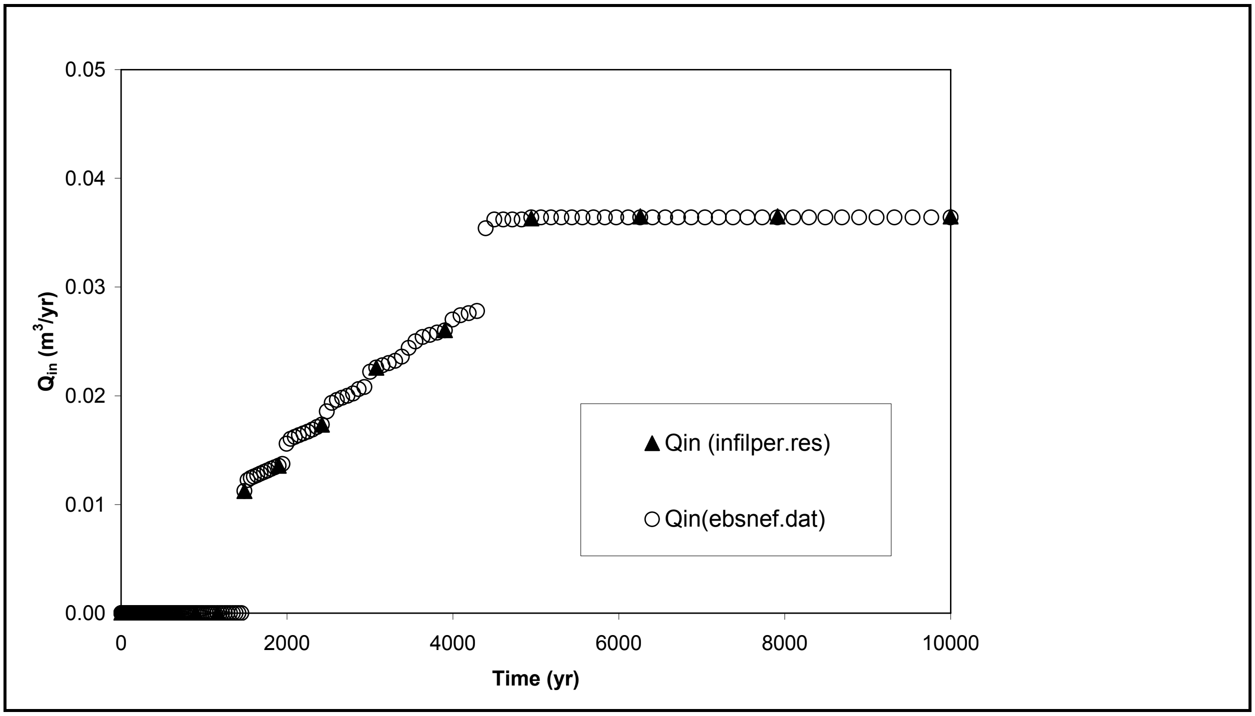


Fig. 26. Inflow rates reported in infilper.res and ebsnef.dat. Flow through mode was implemented.

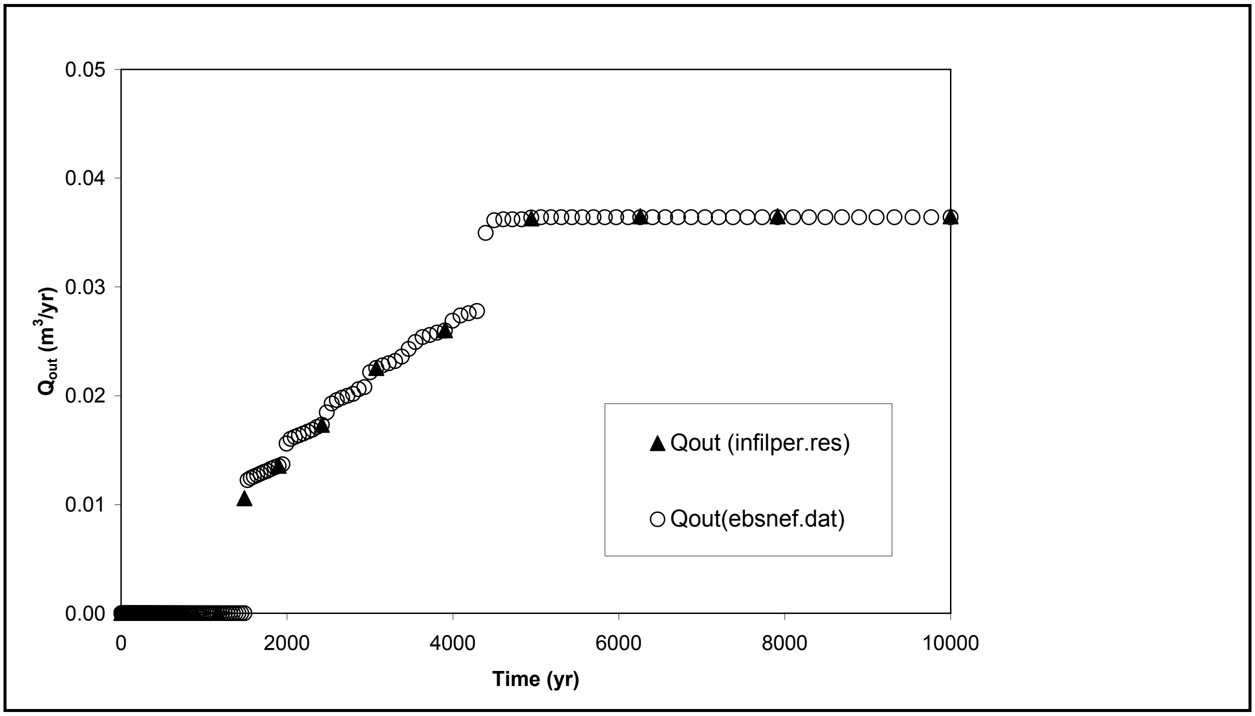


Fig. 27. Outflow rates reported in infilper.res and ebsnef.dat. Flow through mode was implemented.

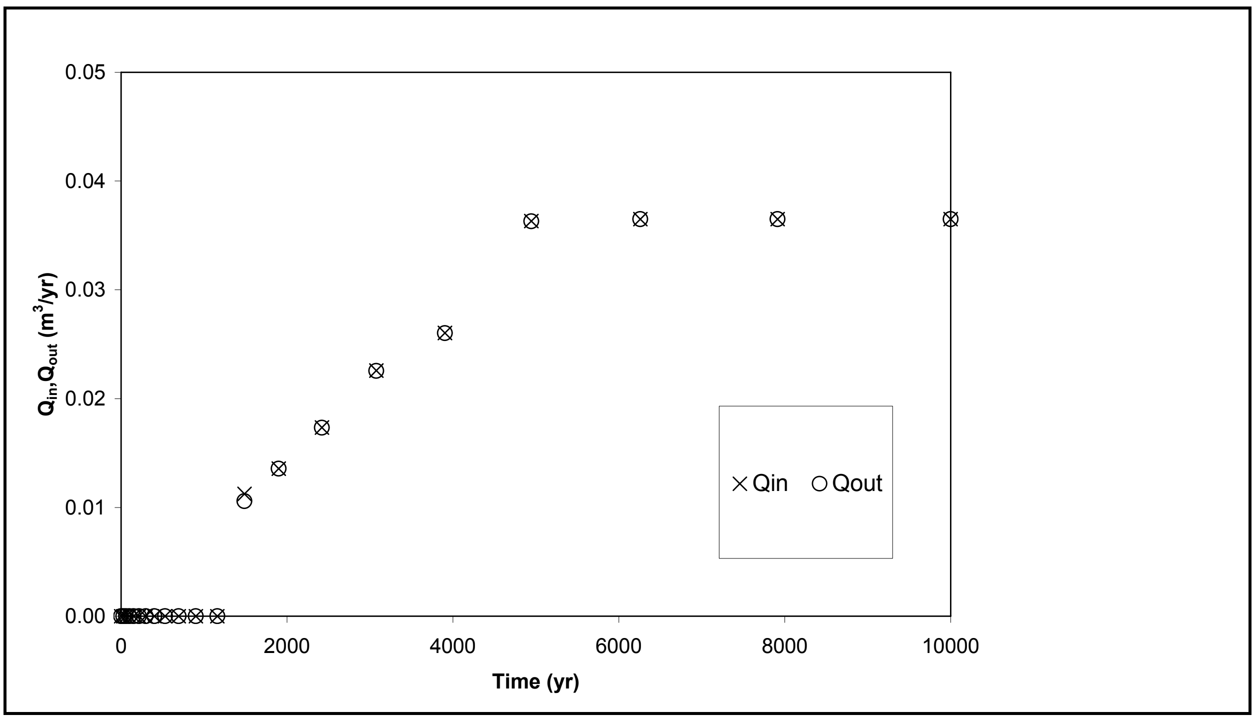


Fig. 28. Inflow and outflow rates reported in infilper.res. Flow through mode was implemented.

Figs. 26 and 27 reveal that the last two columns in infilper.res are WP-averaged flow rates. Fig. 28 shows that WP averaged inflow and outflow also meet the mass-balance requirement.

Test 5 Evaluation (Pass/Fail): PASS

Attachment F
TPA Version 5.1 Validation Task P-10
Test 6 Description

Test Method	
code inspection	spreadsheet
x output inspection	graphical
hand calculation	comparison with external code results

Test Objective: Verify the functionalities implemented in RELEASET.

Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): XP

Input Data (files, data base, mode settings): See the attachment.

Assumptions, constraints, and/or scope of test: (none)

Test Procedure:
Execute the TPA code mean value data file for 10,000 yr for Subarea 3. Verify that *ebsrel.inp* is written for SF and glass in the *ebsrelsf.inp* and *ebsrelglass.inp* files.

Test Results

Location: P10\TPA_Validation\Test6

Test Criterion or Expected Results: *ebsrel.inp* would be written for SF and glass in the *ebsrelsf.inp* and *ebsrelglass.inp* files.

Test Evaluation (Pass/Fail): **Pass**

Notes: See following pages of this attachment for analysis of results.

Tester: Hakan Basagaoglu Robert Rice	Date: April 27, 2007

Results:

Because a run using the mean value data file did not result in releases from the EBS, the input file from Test 5 was used for Test 6.

ebsrel.inp was a temporary file in TPA calculations. In the TPA run, ebrselsf.inp was saved initially as ebsrel.inp and calculations for spent fuel (sf) were carried out. Once all calculations for sf were completed, then ebsrel.inp was overwritten by ebsrelgass.inp, and the calculations for glass were carried out by using the updated ebsrel.inp. The original files, ebsrelsf.inp and ebsrelglass.inp, remained unchanged in the main directory.

Hence, after the completion of the model run, ebsrelglass.inp and ebsrel.inp would be the same the same, but ebsrelsf.inp and ebsrel.inp are different. This was shown below using small portions of these files.

from **ebsrel.inp**

```
 …….
8.14000E+02 ! xcon
 5.00000E-01 ! sawetfrac
 0.00000E+00 ! defect
          4 ! idefect
 0.00000E+00 ! sftimef
 …….
```

---

from **ebsrelglass.inp**

```
…….
 8.14000E+02 ! xcon
 5.00000E-01 ! sawetfrac
 0.00000E+00 ! defect
          4 ! idefect
 0.00000E+00 ! sftimef
 ………
```

---

from **ebsrelsf.inp**

```
 …….
2.09000E+03 ! xcon
 5.00000E-01 ! sawetfrac
 0.00000E+00 ! defect
         11 ! idefect
 0.00000E+00 ! sftimef
 ………
```

The total number of waste packages failed is **2904** (814 from ebsrelglass.inp; and 2090 from ebsrelsf.inp). This number is consistent with the information printed on the screen.

```
   exec: time of drip shield mechanical failure =      388.5  yr
   *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
   ebsfail: time of corrosion breach on welded areas =      582.9  yr
   *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
```

ebsfail: time of WP breach by general corrosion = 1077.0 yr
exec: calling mechdriver (waste package)
exec: failed WPs from INITIAL event = 15 at TPA time = 0.0 yr
exec: failed WPs from LOC CORR event = 131 at TPA time = 574.9 yr
exec: failed WPs from GEN CORR event = 2758 at TPA time = 1075.1 yr
*** failed WPs: all WPs failed (**2904**) ***

These information were correctly reported in the output files.

From relcumsf.out:

Type#	Failed	Start SF Wet[yr]	Fill Time[yr]	Fill Start[yr]	Fill Stop[yr]
1	11	1.4871E+03	0.0000E+00	1.4871E+03	1.4871E+03
2	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	94	1.4871E+03	0.0000E+00	1.4871E+03	1.4871E+03
8	1985	1.4871E+03	0.0000E+00	1.4871E+03	1.4871E+03

2090 Waste packages subject to immediate flow through

From relcumglass.out

1	4	1.4871E+03	0.0000E+00	1.4871E+03	1.4871E+03
2	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
3	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
4	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
5	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
6	0	1.4871E+03	0.0000E+00	0.0000E+00	0.0000E+00
7	37	1.4871E+03	0.0000E+00	1.4871E+03	1.4871E+03
8	773	1.4871E+03	0.0000E+00	1.4871E+03	1.4871E+03

814 Waste packages subject to immediate flow through

Test 6 Evaluation (Pass/Fail): PASS

Attachment G
TPA Version 5.1 Validation Task P-10
Test 7 Description

Test Method

code inspection	x spreadsheet
x output inspection	x graphical
hand calculation	comparison with external code results

Test Objective: Verify the functionalities implemented in RELEASET.

Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): XP

Input Data (files, data base, mode settings): See the attachment.

Assumptions, constraints, and/or scope of test: (none)

Test Procedure:

Execute the TPA code mean value data file for 10,000 yr for Subarea 3. Verify that *ebspac.nuc* is written for SF and glass in the *ebspacsf.nuc* and *ebspacglass.nuc* files. Additionally, verify all release rates in the RELEASET file *ebsnef.dat* are positive. Verify in RELEASET calculations there are no diffusive releases and there is instantaneous waste form release. These conditions were accomplished by setting *tpa.inp* input parameters FractionOfWPsWithDiffusionTilt[] and FuelRodHalfLength[m] equal to 0.

Test Results

Location: P10\TPA_Validation\test7

Test Criterion or Expected Results: *ebspac.nuc* would be written for SF and glass in the *ebspacsf.nuc* and *ebspacglass.nuc* files. All releases should be nonnegative. FuelRodHalfLength[m]>0 (non-zero cladding effect) should result in slower releases due to the enhanced diffusion process, and small unphysical releases prior to failure times should be eliminated by setting FractionOfWPsWithDiffusionTilt[] to 0.

Test Evaluation (Pass/Fail): Pass

Notes: See following pages of this attachment for analysis of results.

Tester: Hakan Basagaoglu Robert Rice	Date: April 27, 2007

Results:

Because a run using the mean value data file did not result in releases from the EBS, the modified mean value data from Test #5 was used for Test #7.

ebspacsf.nuc was saved initially as ebspac.nuc and calculations for spent fuel were carried out. Then, ebspacglass.nuc was saved as ebspac.nuc and calculations for glass were carried out. Therefore, ebspacglass.nuc and ebspac.nuc (after completion of the model run) are the same, but ebspacsf.nuc and ebspacglass.nuc are different. The original files, ebspacsf.nuc and ebspacglass.nuc were retained. This was shown below using small portions of these files.

from ***ebspacsf.nuc***

…….

	Radionuclide	Half-life	Inventory	Gap Fraction
246.0	CM246	4.731E+03	1.617E+00	0.000E+00
238.0	U238	4.468E+09	**2.619E+00**	**0**.000E+00
245.0	CM245	8.499E+03	**4.734E+00**	0.000E+00
241.0	AM241	4.322E+02	**2.967E+04**	0.000E+00

…….

from ***ebspacglass.nuc***

…….

	Radionuclide	Half-life	Inventory	Gap Fraction
246.0	CM246	4.731E+03	0.000E+00	0.000E+00
238.0	U238	4.468E+09	**8.639E-02**	0.000E+00
245.0	CM245	8.499E+03	**0.000E+00**	0.000E+00
241.0	AM241	4.322E+02	**1.399E+02**	0.000E+00

………

from ***ebspac.nuc***

…….

	Radionuclide	Half-life	Inventory	Gap Fraction
246.0	CM246	4.731E+03	0.000E+00	0.000E+00
238.0	U238	4.468E+09	**8.639E-02**	0.000E+00
245.0	CM245	8.499E+03	**0.000E+00**	0.000E+00
241.0	AM241	4.322E+02	**1.399E+02**	0.000E+00

………

In summary, the input files were processed in the right order, and they were all saved separately. The release rates were obtained from ebsnef2.dat and non-negative release rates from the EBS are shown in Figs. 29-34 .

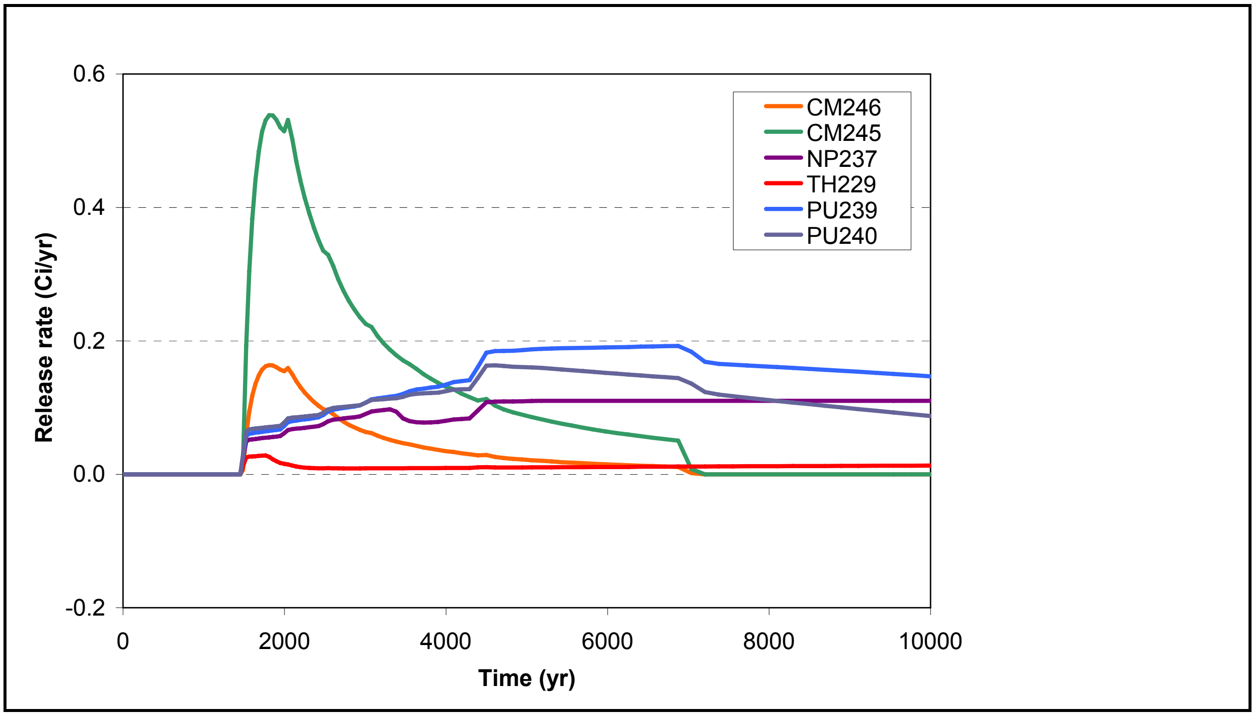


Fig. 29. Non-negative release rate of radionuclides from the EBS.

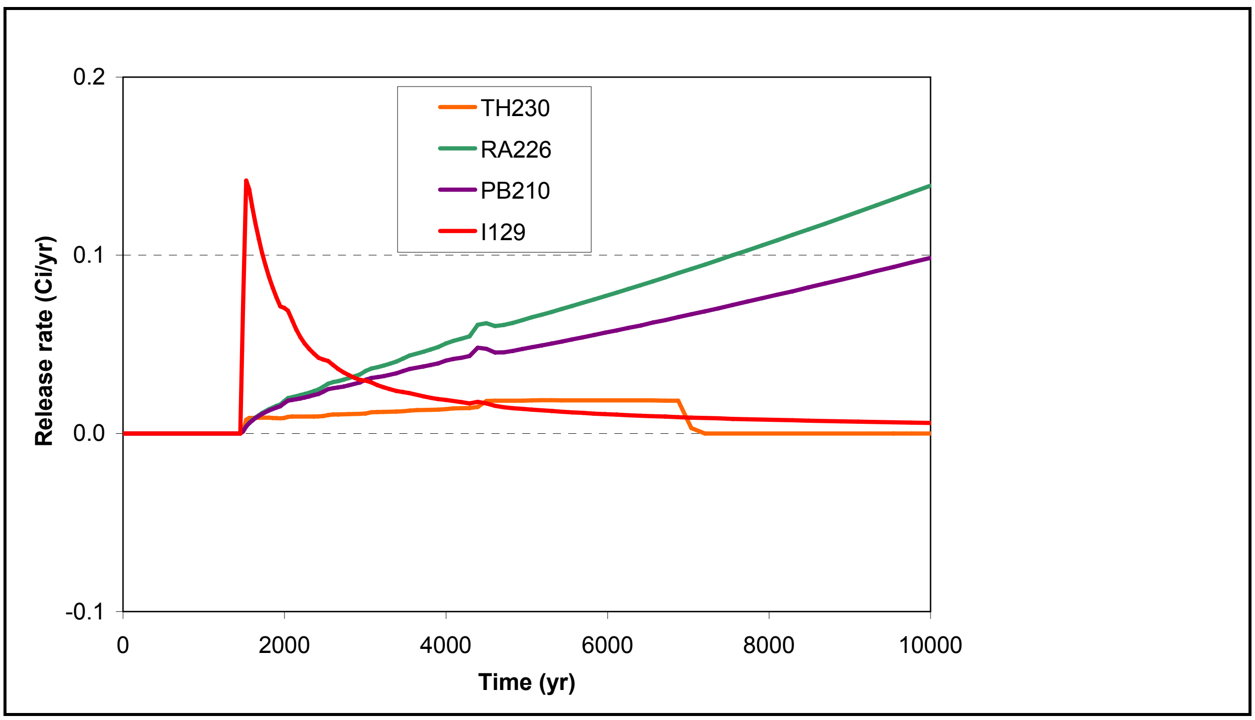


Fig. 30. Non-negative release rate of radionuclides from the EBS.

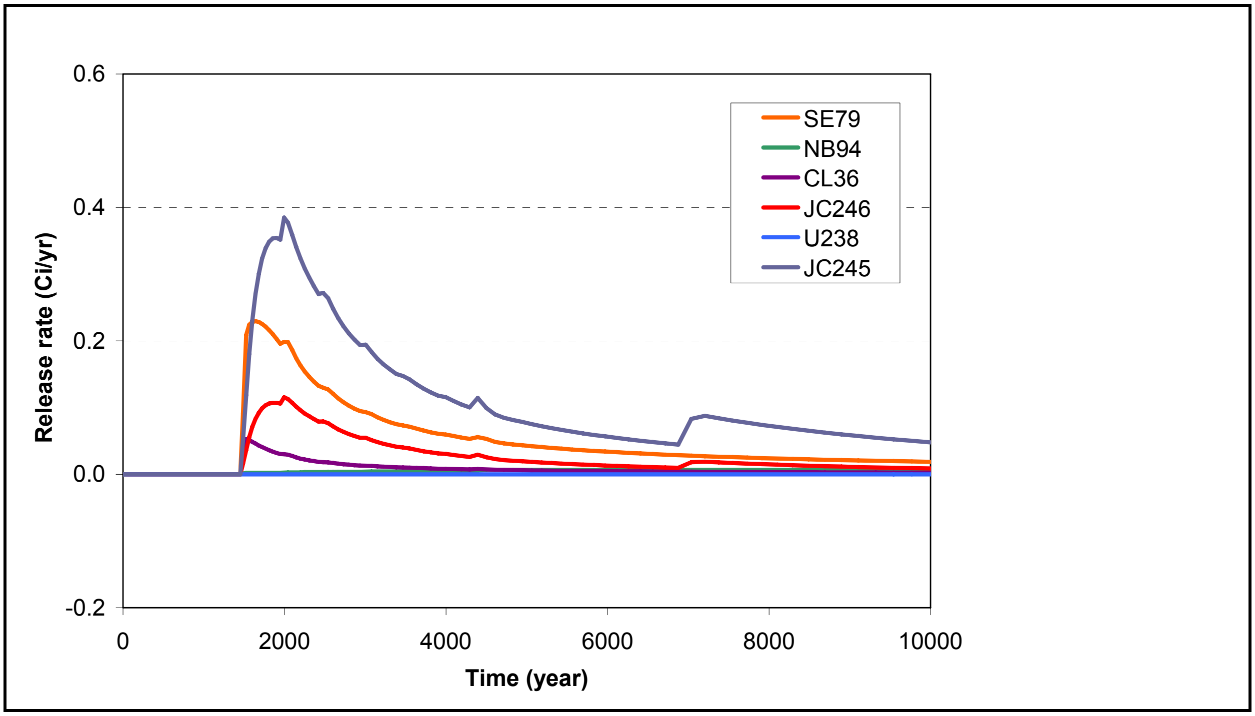


Fig. 31. Non-negative release rate of radionuclides from the EBS.

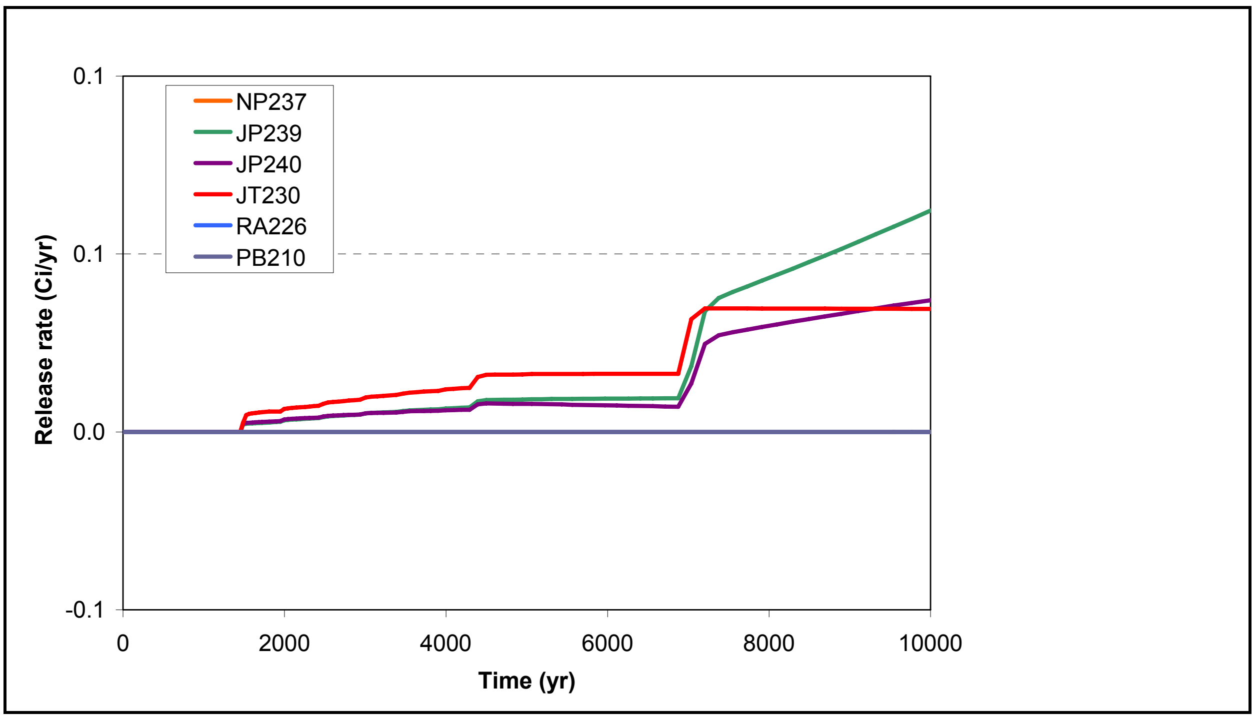


Fig. 32. Non-negative release rate of radionuclides from the EBS.

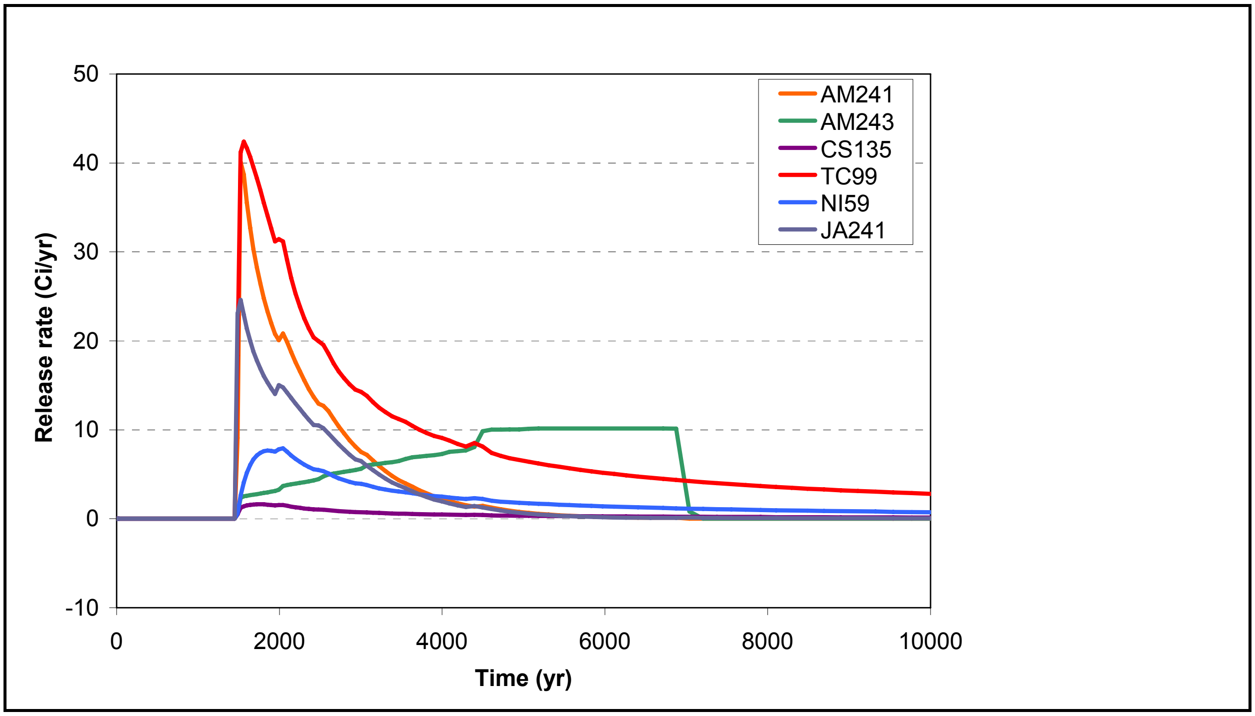


Fig. 33 Non-negative release rate of radionuclides from the EBS.

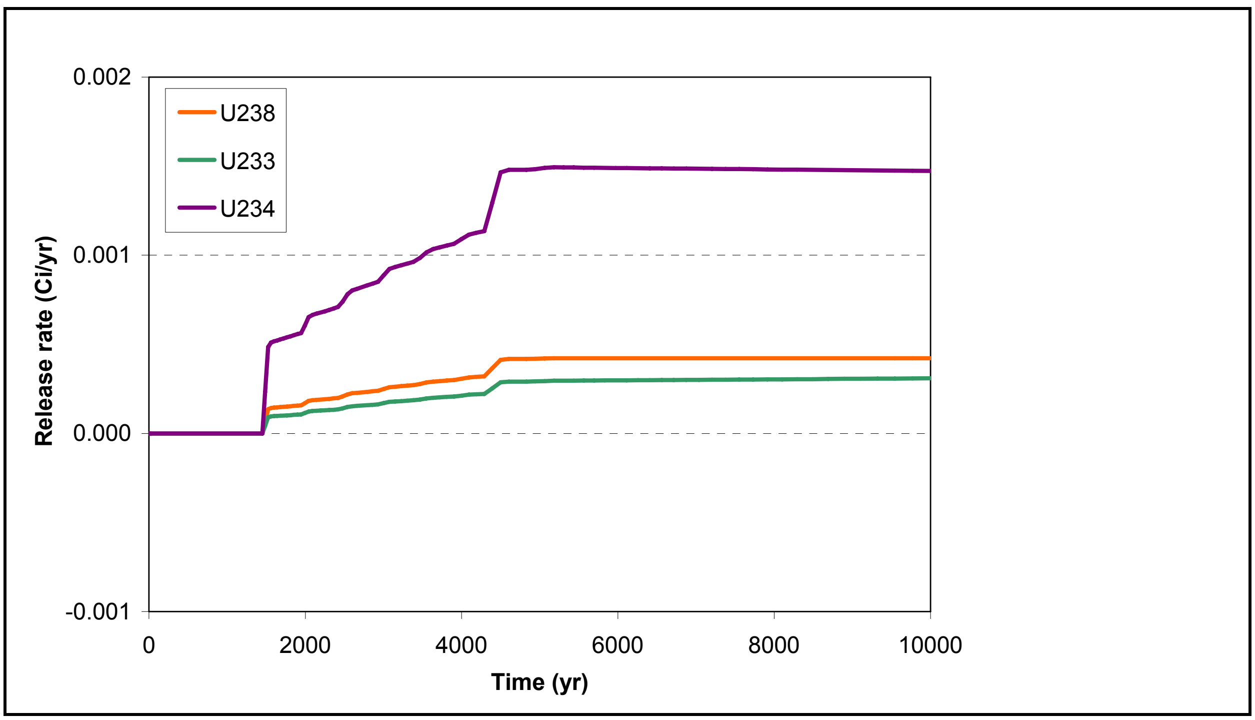


Fig. 34 Non-negative release rate of radionuclides from the EBS.

Reference case values for FractionOfWPsWithDiffusionTilt and FuelRodHalfLength were 0 in the mean value data file. The latter accounts for the cladding protection. To force diffusive releases, FractionOfWPsWithDiffusionTilt was set to 0.7 and FuelRodHalfLength was set to 0.3 and 0.8. If the diffusive releases are calculated correctly, then we should expect a smaller peak but a longer tail from simulations with FuelRodHalfLength=0.3 than for FuelRodHalfLength=0.8 (and FuelRodHalfLength= FractionOfWPsWithDiffusionTilt =0) in the breakthrough curves.

Two radionuclides were arbitrarily chosen, Cm245 and Tc99 for this analysis and release rates (from ebsnef2.dat) are shown in Figs. 35-36. Flow-through mode was employed in these simulations. Figs. 35-36. indicate that diffusive releases were achieved by setting FuelRod HalfLength to a non-zero value (i.e., non-zero cladding effect). FractionOfWPsWithDiffusionTilt does not seem to have an effect on the release rates (the second curve in green and the last curve traced by +). These results further indicate that as the cladding increased from 0 to 0.3 and to 0.8 (an increase in the diffusion path), the peak value of the breakthrough curve decreased while the tail of the breakthrough curve stretched further. The longer tailing with an increase in the diffusional path was clear for CM245. Hence slower releases due to longer diffusion paths across the cladding have been reasonably well captured in these simulations.

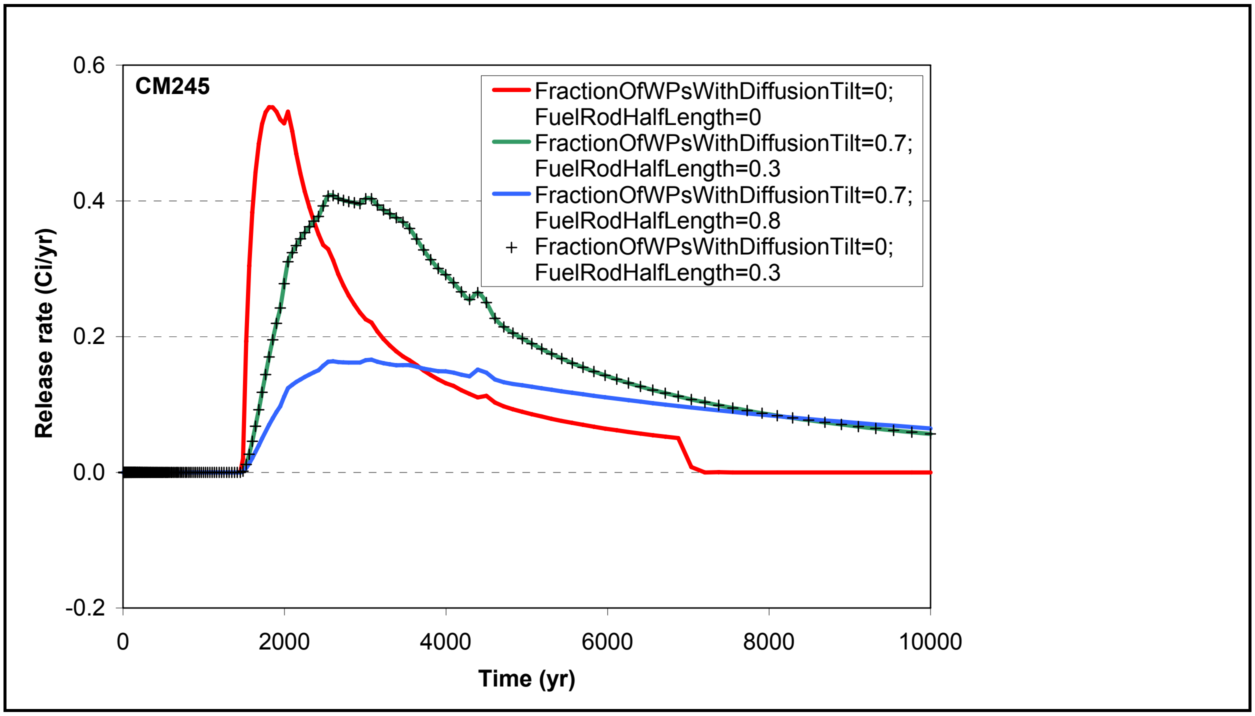


Fig. 35. Release rate of Cm245 as a function of two tpa.inp parameters, FuelRodHalfLength and FractionOfWPsWithDiffusionTilt.

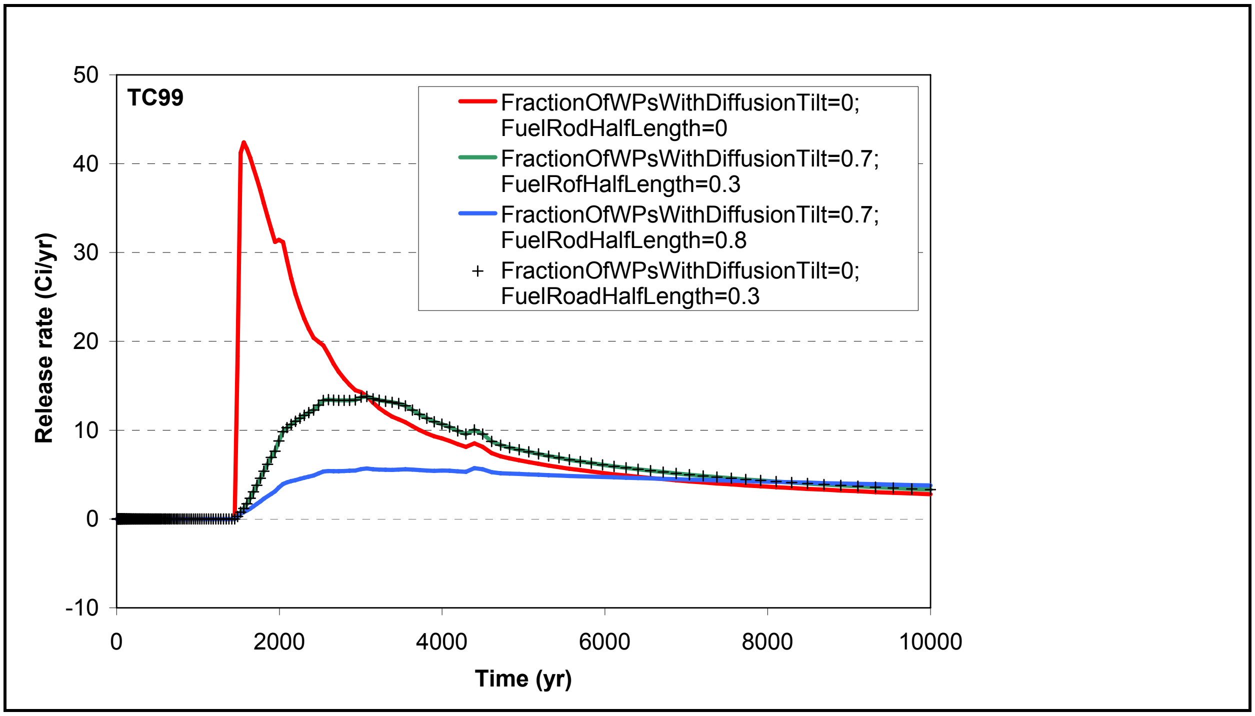


Fig. 36. Release rate of Tc99 as a function of two tpa.inp parameters, FuelRodHalfLength and FractionOfWPsWithDiffusionTilt.

Next, all the seepage factors reported in ebsflo.dat were plotted. These seepage factors should not vary with whether releases are instantaneous or diffusion controlled. This has been verified by Figs. 37-46. All these flow factors were discussed in depth on P10 E-2 through P10 E-5.

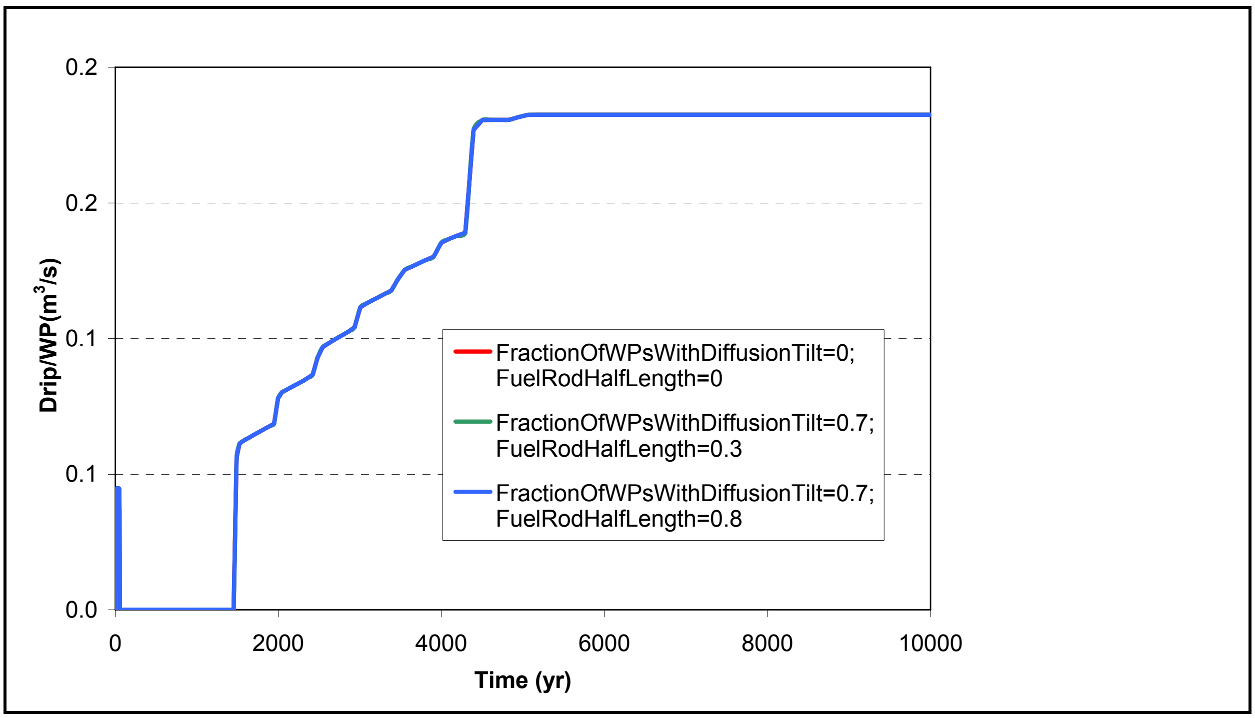


Fig. 37. Temporal variations in Drip/WP as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

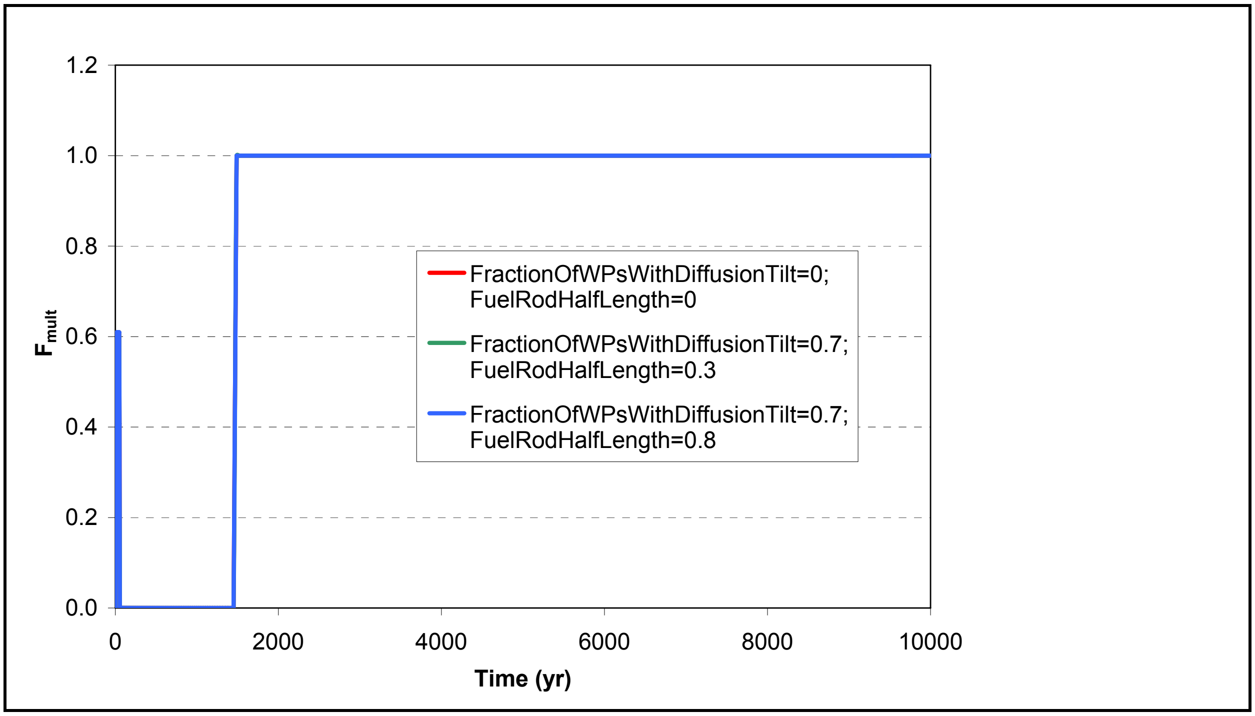


Fig. 38.Temporal variations in F_{mult} as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

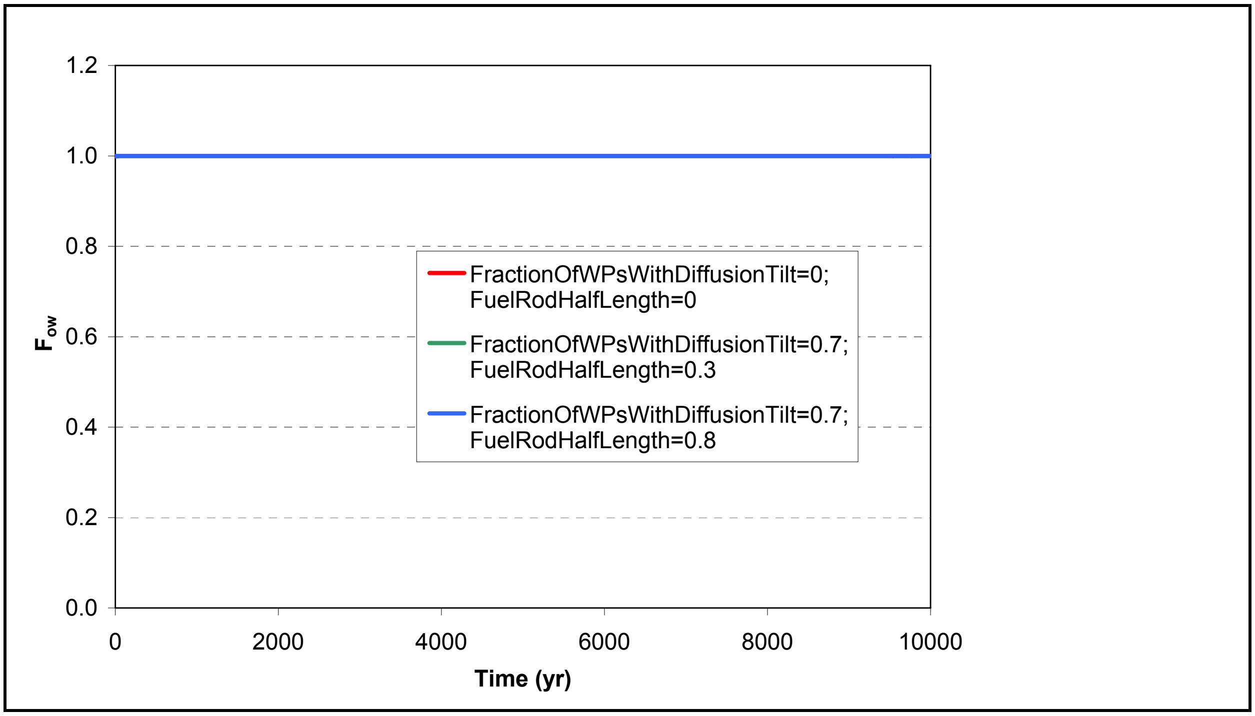


Fig. 39. Temporal variations in F_{ow} as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

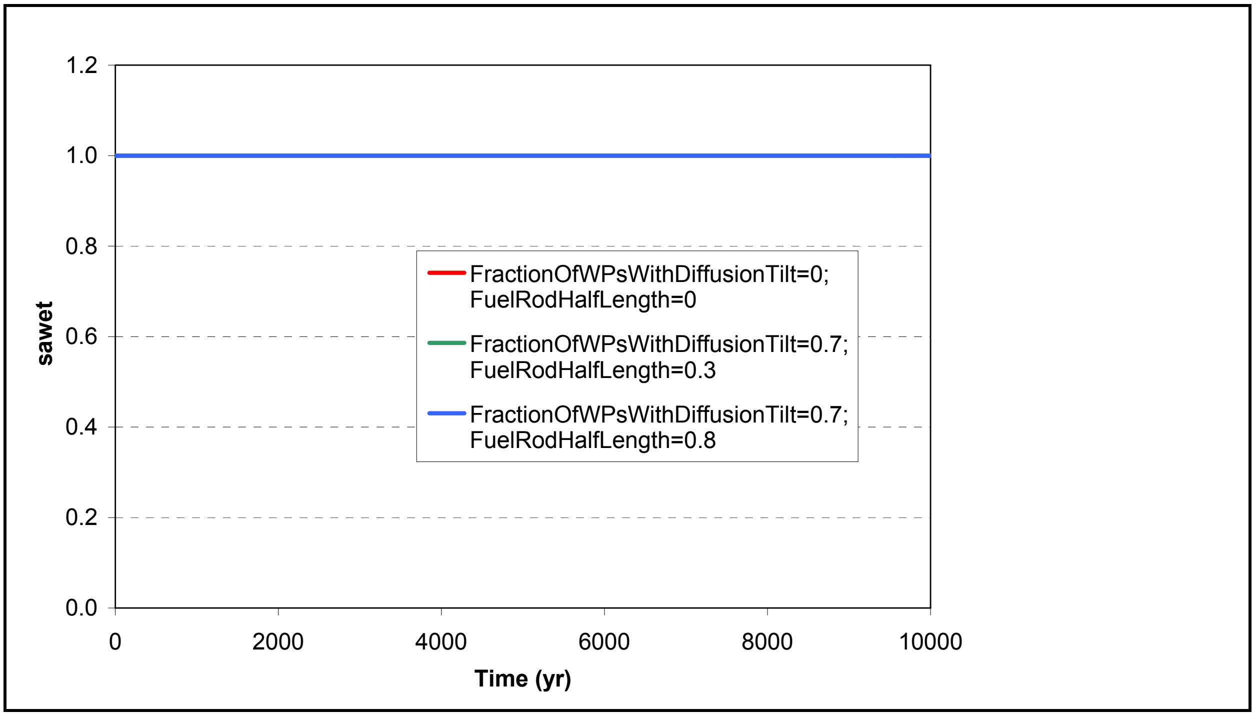


Fig. 40. Temporal variations in sawet as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

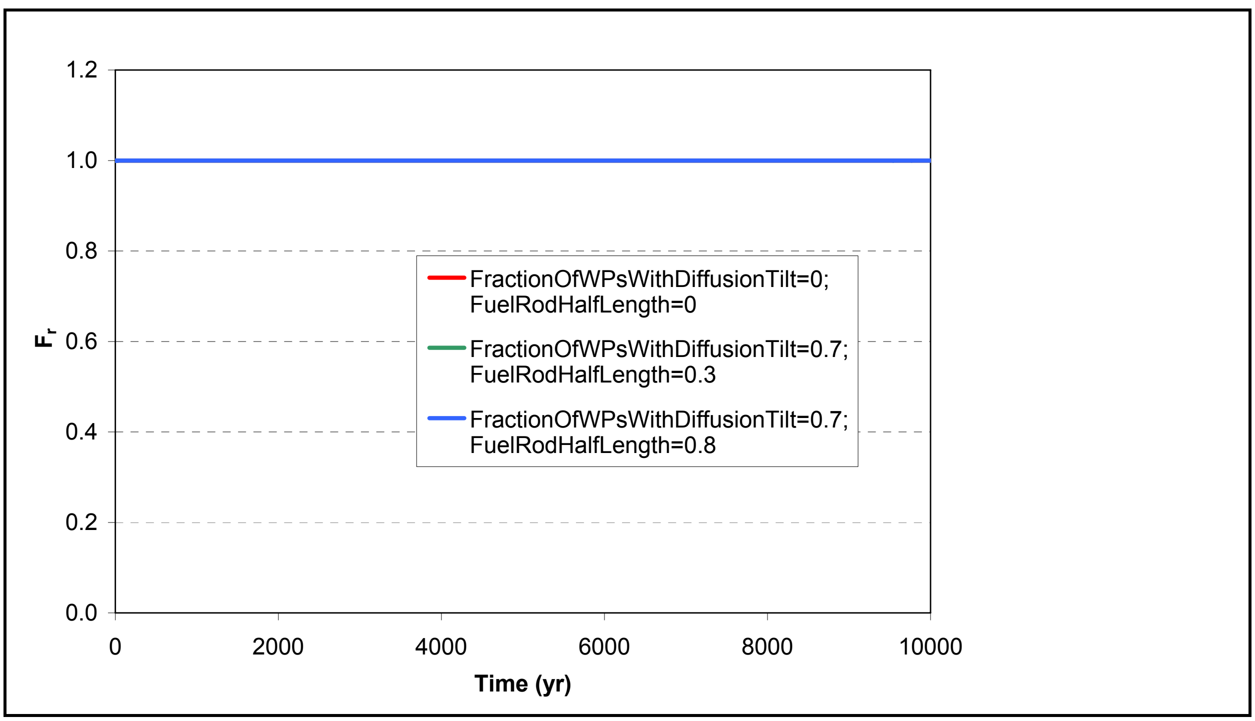


Fig. 41. Temporal variations in F_r as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

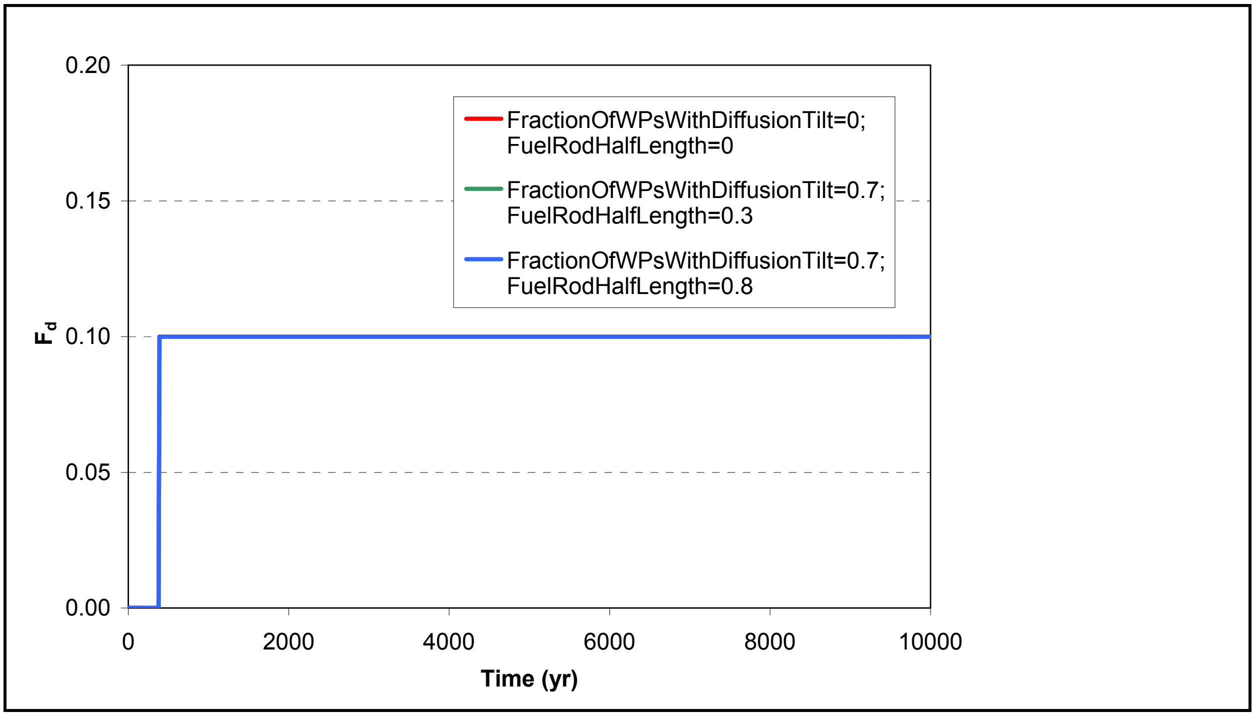


Fig. 42. Temporal variations in F_d as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

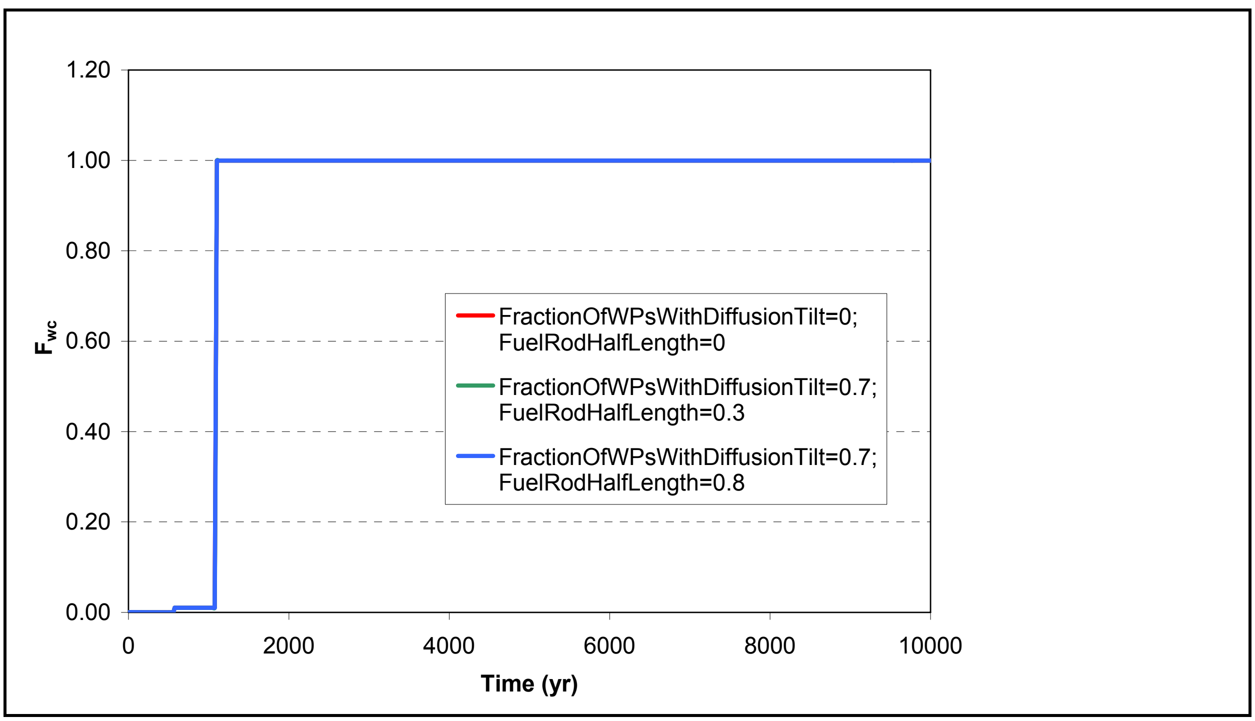


Fig. 43. Temporal variations in F_{wc} as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

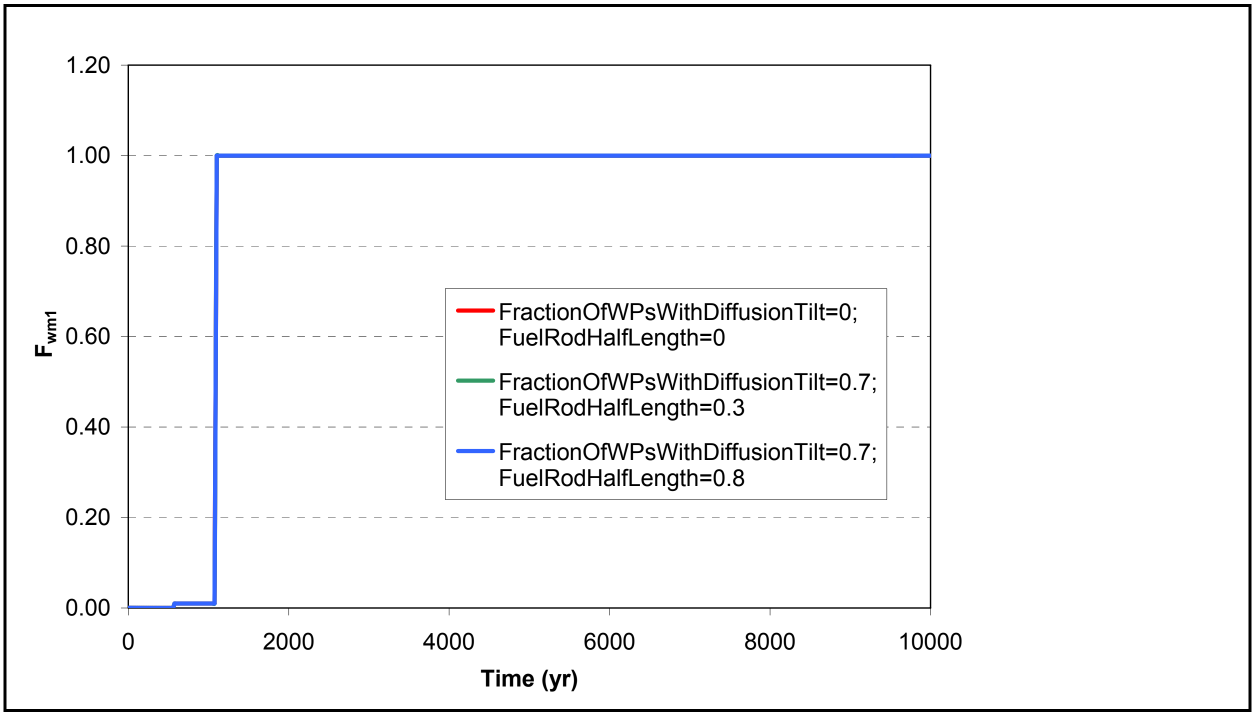


Fig. 44. Temporal variations in F_{wm1} as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

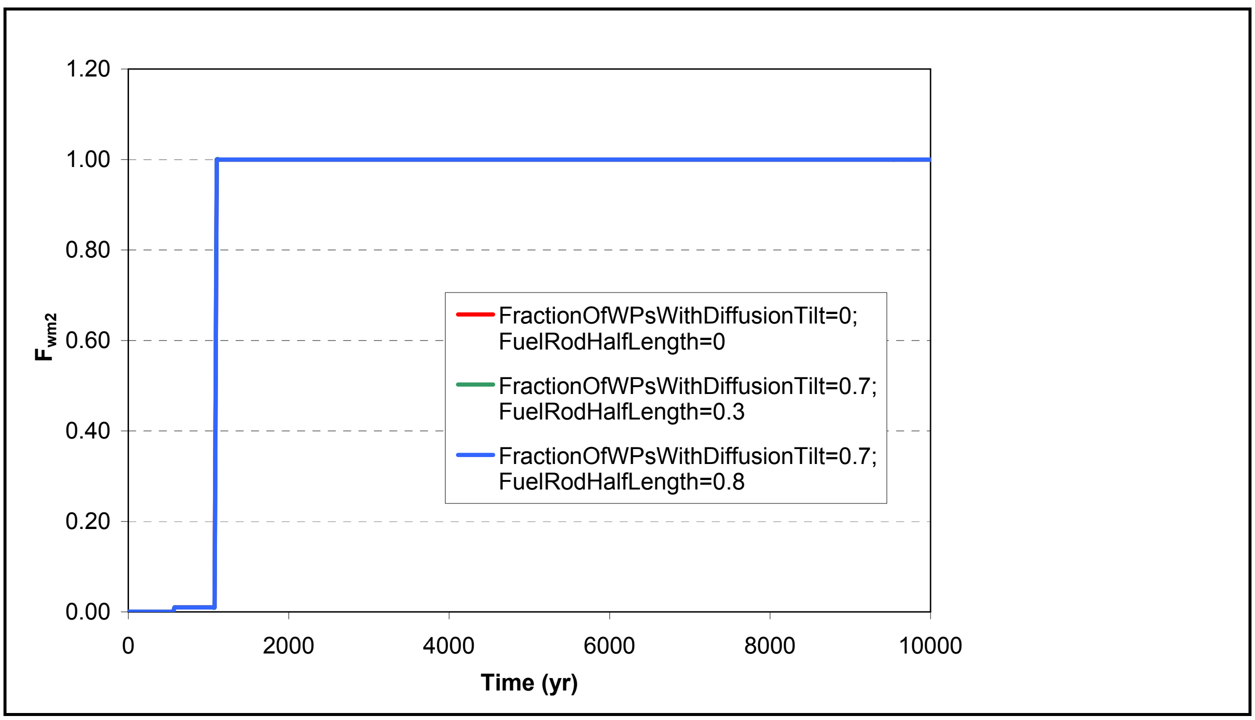


Fig. 45. Temporal variations in F_{wm2} as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

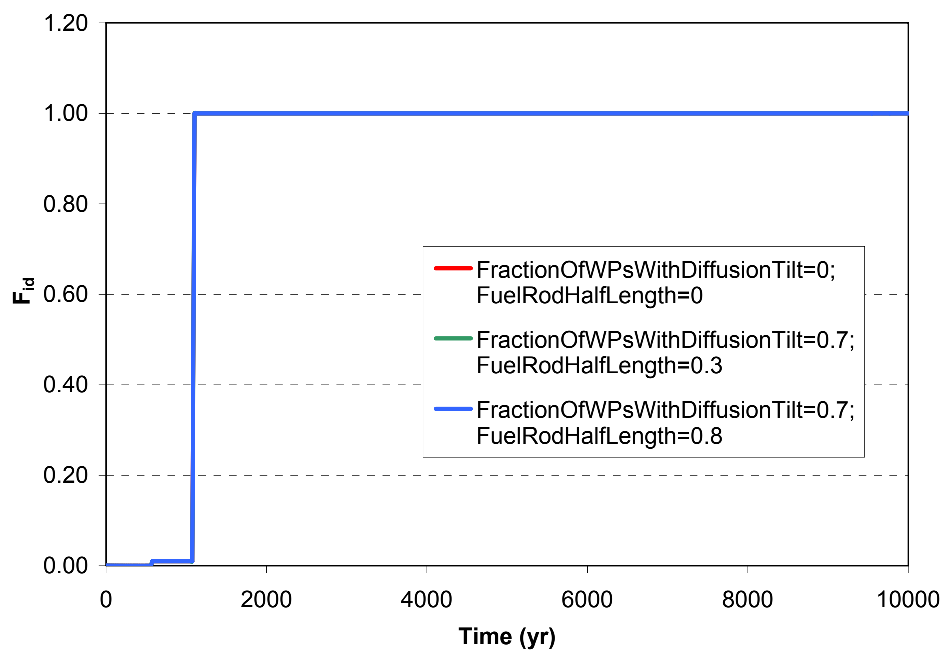


Fig. 46. Temporal variations in F_{id} as a function of FuelRodHalfLength and FractionOfWps WithDiffusionTilt.

Next, we repeated the same simulations with using a stand alone version of the code in the bathtub mode. We forced a longer bathtub filling period by decreasing the flow factor in the first row of ebsflo.dat from 2.0 to 0.1, and the results are shown in Figs. 47-50.

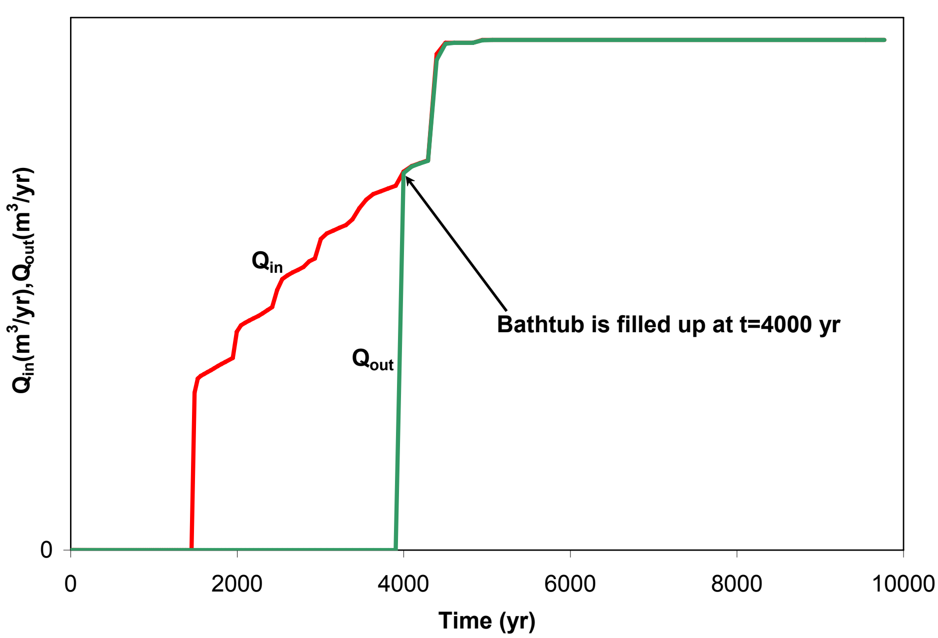


Fig. 47. Temporal variations in inflow and outflow rates. Bathtub mode was implemented.

In this simulation, the bathtub filling started at t~1490 yr and was completed at t~4000 yr. Two simulations were carried out with FractionOfWPsDiffusionTilt=0 or 0.1. The releases for Tc99 and Cm245 from these simulations are shown below:

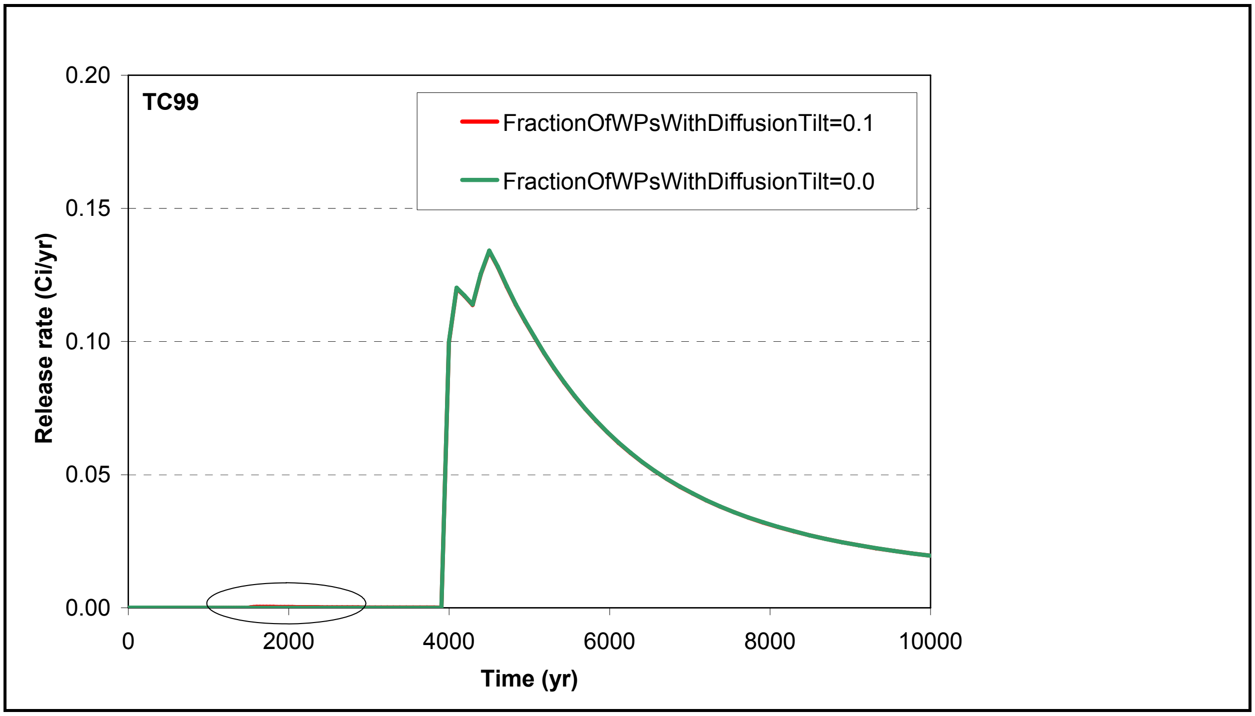


Fig. 48. Temporal variations in release rates of Tc99 from the EBS as a function of FractionOf WPsWithDiffusionTilt. Bathtub mode was implemented.

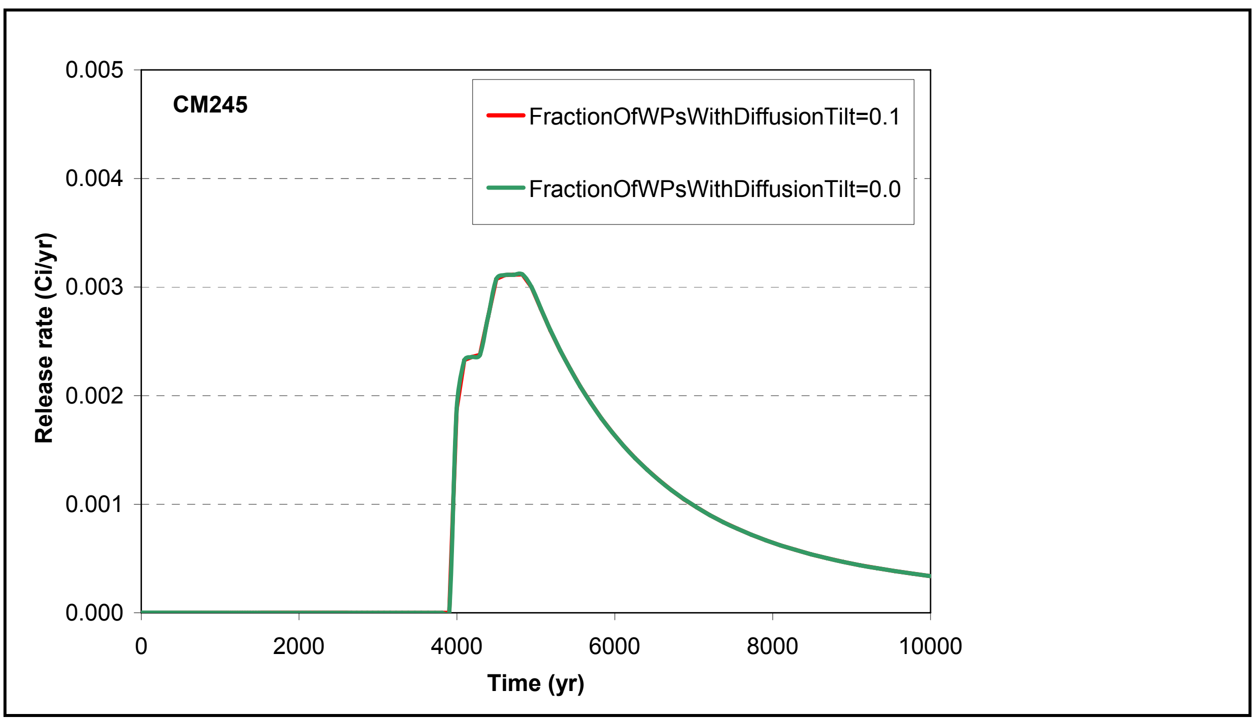


Fig. 49. Temporal variations in release rates of Cm245 from the EBS as a function of FractionOf WPsWithDiffusionTilt. Bathtub mode was implemented.

The results look reasonable except for a small blip encircled in Tc99 releases in fig. 48, which reveals small releases prior to completion of bathtub filling for FractionOfWPsDiffusionTilt = 0.1. This section of the breakthrough curve is expanded below:

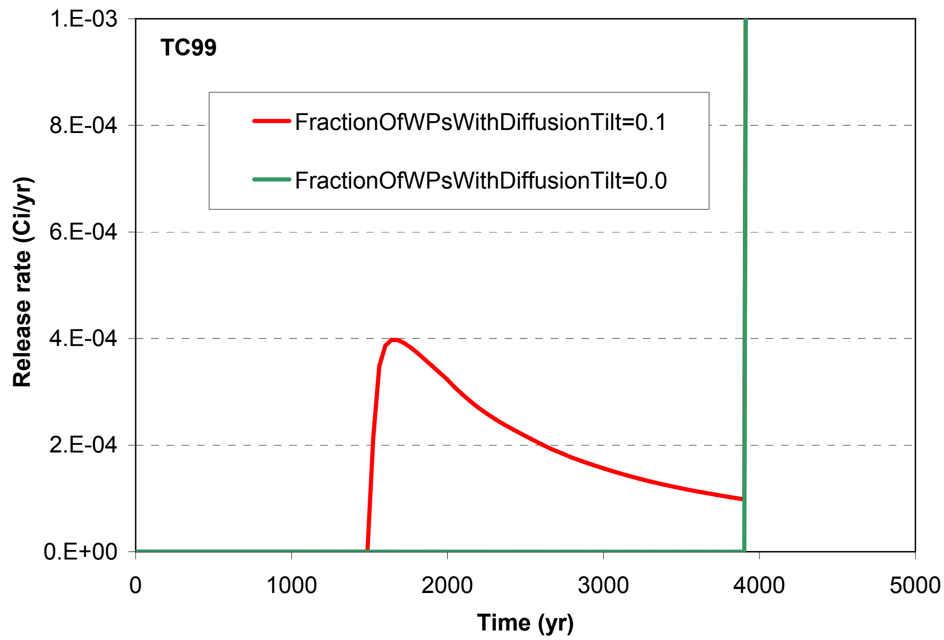


Fig. 50. Temporal variations in release rates of Tc99 from the EBS prior to completion of bathtub filling as a function of FractionOf WPsWithDiffusionTilt.

This plot indicates that the small releases prior to bathtub filling have been removed by setting FractionOfWPsWithDiffusionTilt to zero.

Test 7 Evaluation (Pass/Fail): PASS

Attachment H
TPA Version 5.1 Validation Task P-10
Test 8 Description

Test Method

	code inspection	x	spreadsheet
x	output inspection	x	graphical
	hand calculation		comparison with external code results

Test Objective: Verify the functionalities implemented in RELEASET.

Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): XP

Input Data (files, data base, mode settings): See the attachment.

Assumptions, constraints, and/or scope of test: (none)

Test Procedure:

Execute the TPA code mean value data file for 10,000 yr for Subarea 3. Force only localized corrosion failures (i.e., no other failure types) and verify the releases are correctly transferred from RELEASET output files and the timing of the release is correct. The occurrence of localized corrosion will be forced by adjusting critical relative humidities, while a delay in the occurrence of weld corrosion will be forced by setting the weld thickness equal to a large value. Also, the information in the file *ebsnef2.dat* will be evaluated to determine whether release rates are correct (i.e., have not been zeroed out).

Test Results

Location: P10\TPA_Validation\Test8

Test Criterion or Expected Results: Timing of releases should be correctly transferred to output files (ebsnef2.dat, ebsflo.dat, relcum.out). No releases should occur prior to WPs failures by localized corrosion and WPs contact by deep percolating water. Releases must be non-negative. An increase in the weld thickness should delay the occurrence of localized corrosion.

Test Evaluation (Pass/Fail): **Pass**

Notes: See following pages of this attachment for analysis of results.

Testers: Hakan Basagaoglu Robert Rice	Date: April 27, 2007

Results:

Critical relative humidity for air and water (CriticalRelativeHumifityHumidAirCorrosion and CriticalRelativeHumidityAqueousCorrosion in tpa.inp) was set to 0.01 (it was equal to 0.15 for air and 0.20 for aqueous in the reference case). The weld thickness (WPWeldThickness in tpa.inp) was increased from 0.02 to 0.05 m. Seepage threshold temperature was set to 1000°C in tpa.inp to eliminate its potential effect on delays in seepage. Part of the screen output file listing failure types is shown below.

```
        .......
exec: calling  nfenv
exec: calling ebsfail
   ebsfail: time of corrosion breach on welded areas =      371.1  yr
   *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
   *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    147 at TPA time =    366.5 yr
 *** failed WPs:  147   out of  2904  ***      .......
```

Hence, localized corrosion on failed waste packages and welds was enforced in this simulation. Because waste packages failed at t=366.5 yr, there should not be any releases prior to t=366.5 yr, and nonzero releases should be expected after WP failure by localized corrosion. The release rates are shown in Figs. 51- 56 (the arrows indicated which axis the breakthrough curve belongs to in these plots). The source file for these plots were ebsnef2.dat.

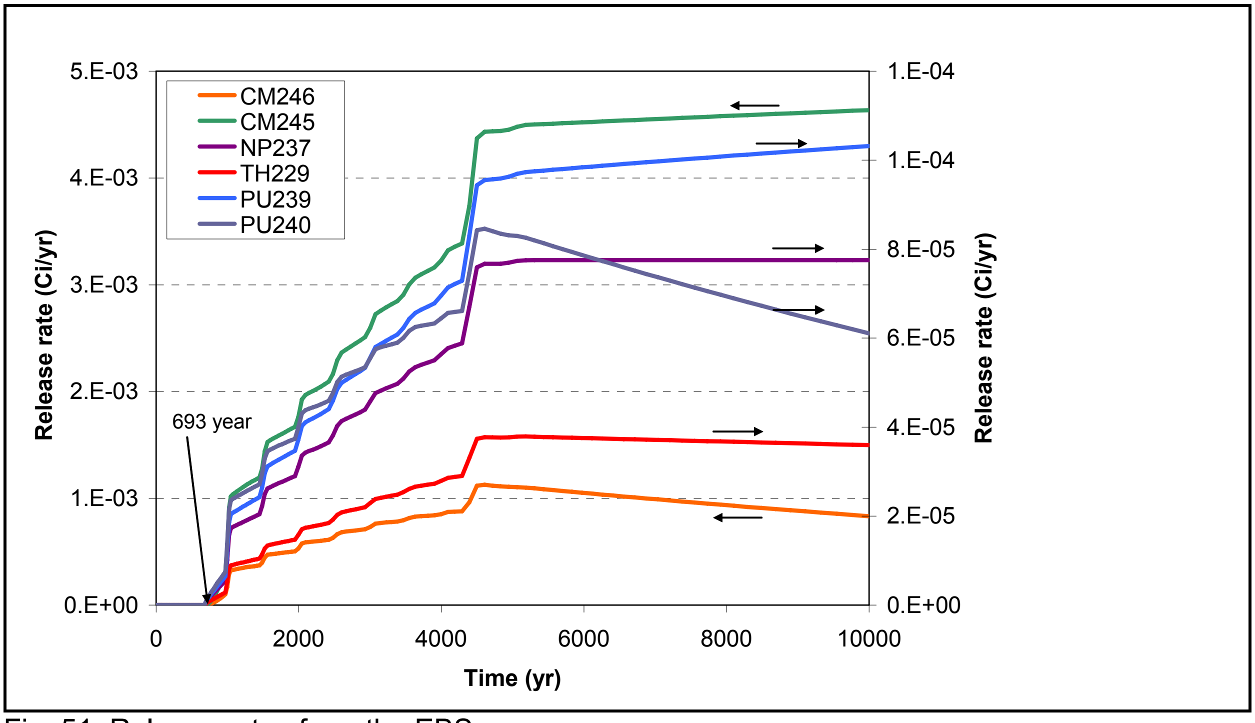


Fig. 51. Release rates from the EBS.

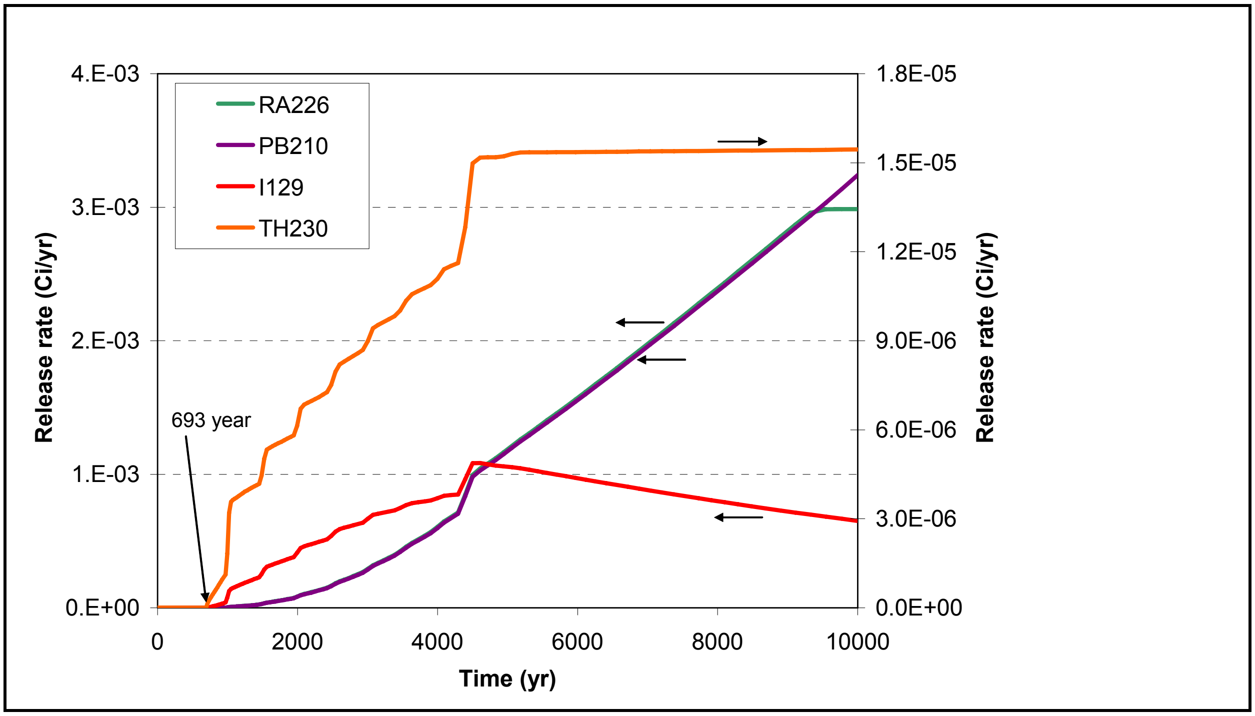


Fig. 52. Release rates from the EBS.

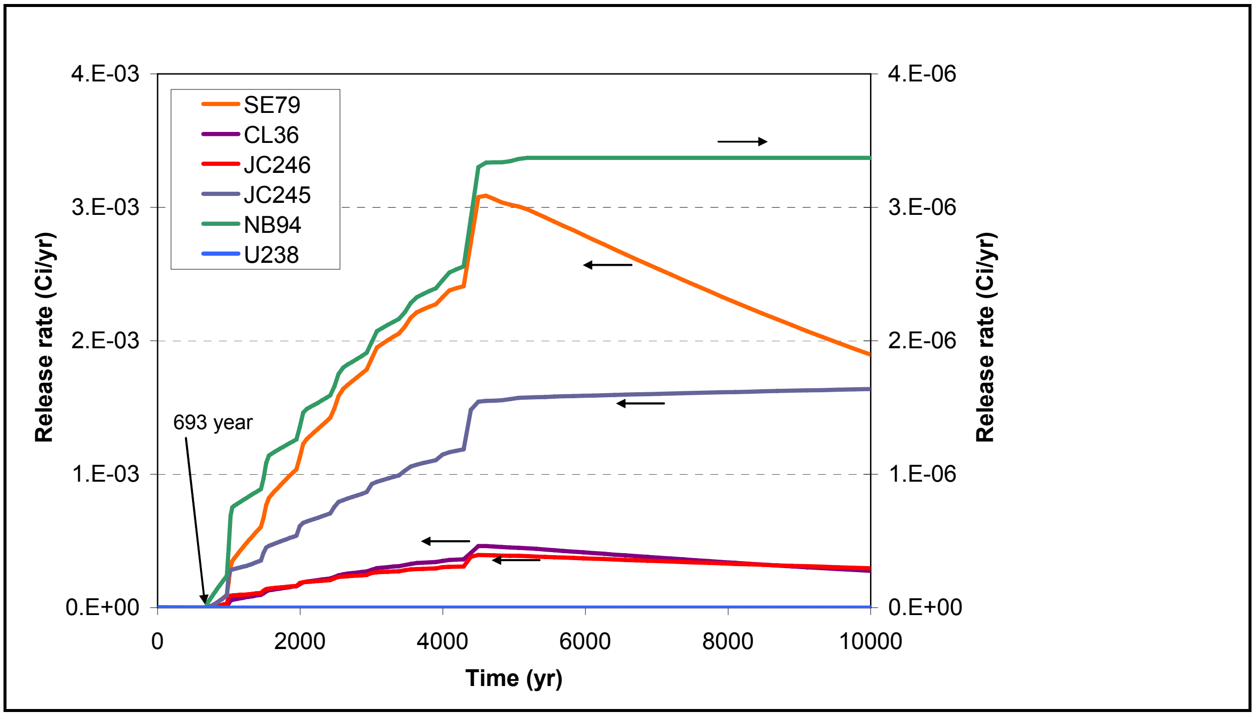


Fig. 53. Release rates from the EBS.

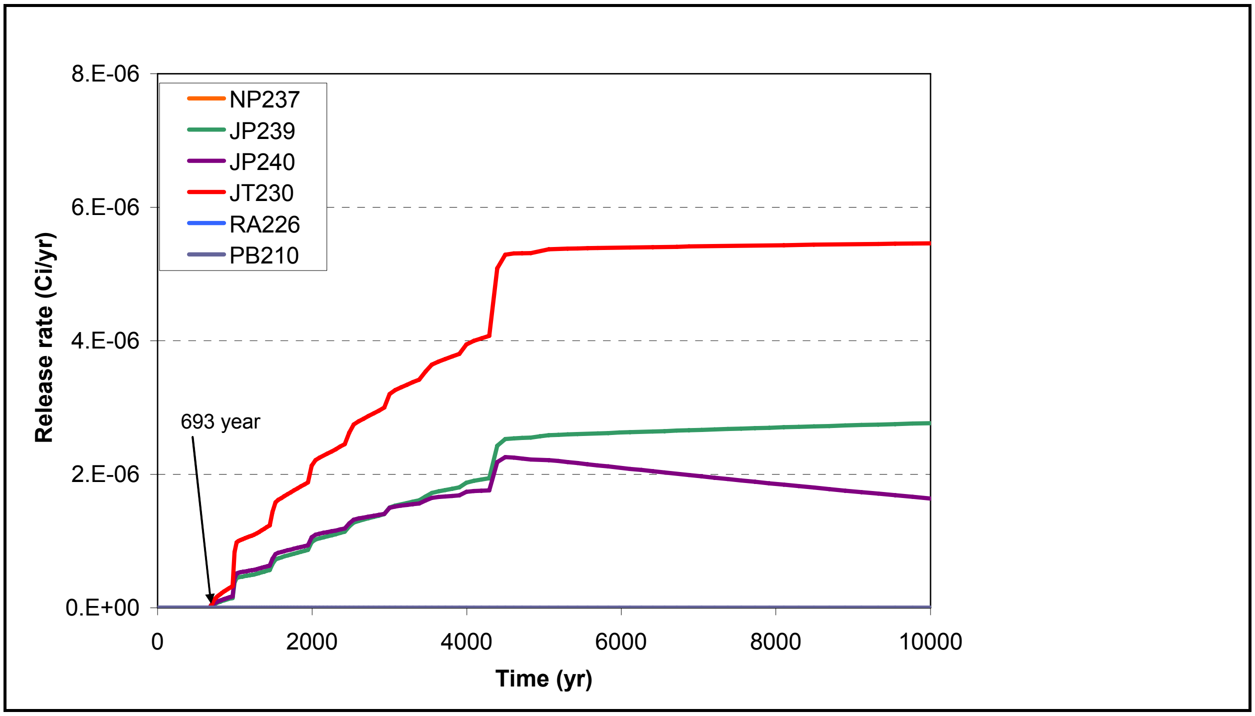


Fig. 54. Release rates from the EBS.

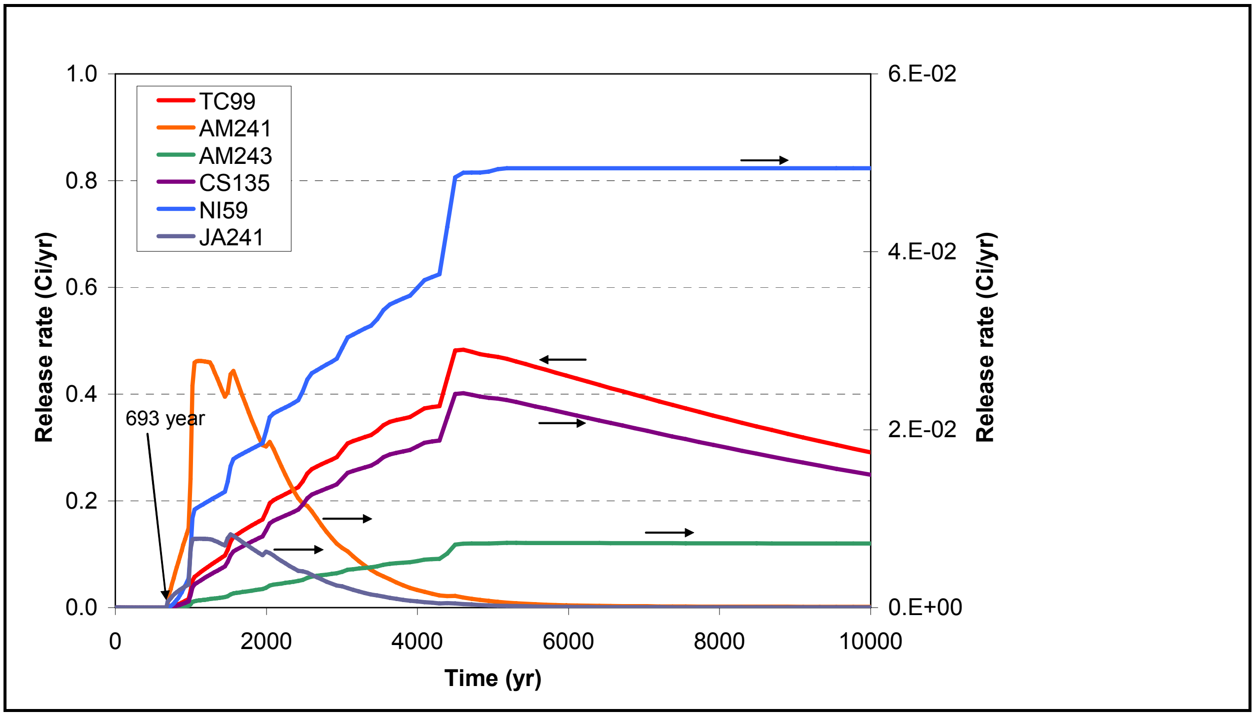


Fig. 55. Release rates from the EBS.

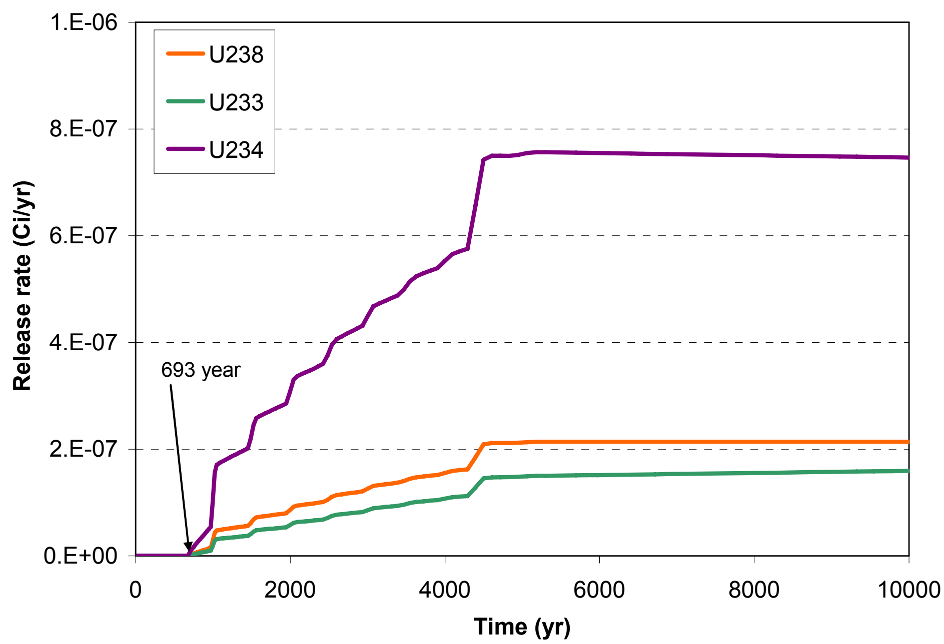


Fig. 56. Release rates from the EBS.

Hence, all releases occurred at t≥693 yr, about ~350 yr after WPs failed by localized corrosion. Except for a few radionuclides (e.g., NP237, RA226, PB210), all radionuclides released from failed WPs, as expected. The delay (~350 yr) in releases following the WP failure by localized corrosion is because deep percolating water did not contact failed waste packages until t=693 yr (Fig. 57).

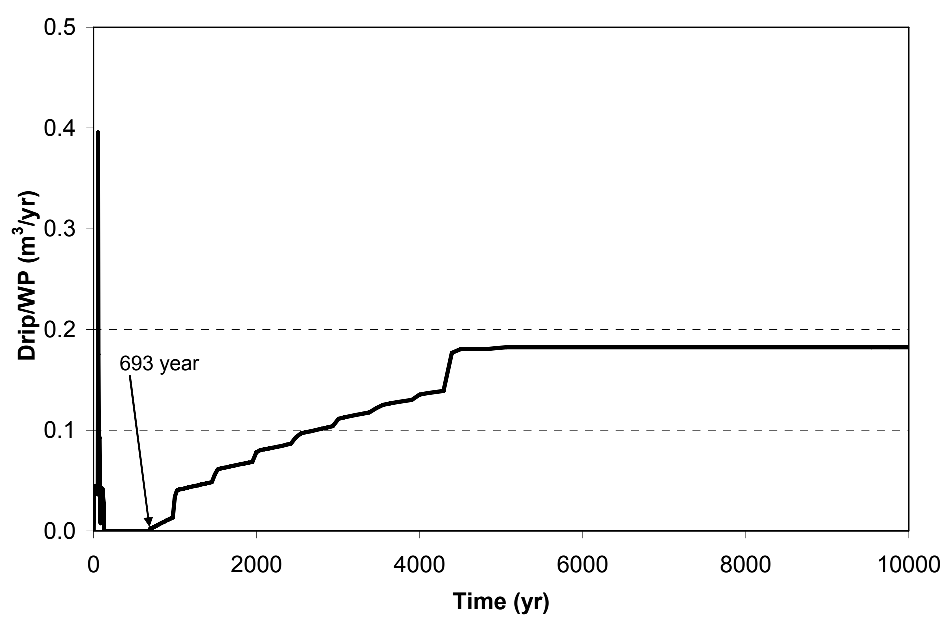


Fig. 57. Temporal variations in deep percolating water contacting failed waste packages (from ebsflo.dat).

The timing of releases was also transferred other output files correctly:

relcum.out:

```
     1.00000E+04     Simulation Time

     Type# Failed    Start SF Wet[yr]       Fill Time[yr]      Fill Start[yr]       Fill Stop[yr]
       1       0         6.9334E+02          0.0000E+00          0.0000E+00          0.0000E+00
       2       0         6.9334E+02          0.0000E+00          0.0000E+00          0.0000E+00
       3       0         6.9334E+02          0.0000E+00          0.0000E+00          0.0000E+00
       4       0         6.9334E+02          0.0000E+00          0.0000E+00          0.0000E+00
       5       0         6.9334E+02          0.0000E+00          0.0000E+00          0.0000E+00
       6       0         6.9334E+02          0.0000E+00          0.0000E+00          0.0000E+00
       7      41         6.9334E+02          0.0000E+00          6.9335E+02          6.9335E+02
       8     773         1.0000E+04          0.0000E+00          1.0000E+04          1.0000E+04
```

We also test the effects of the weld thickness on the localized corrosion start time by reducing its value from 0.05 m to 0.01 m. Part of the screen output file was included below. When this summary file is compared the summary file on P10 H2 (with a weld thickness of 0.05 m), a five-fold increase in the weld thickness caused a ~59 yr delay in the occurrence of weld corrosion.

```
dataFile= dsfailt.dat
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      388.5  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =      211.1  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    147 at TPA time =    208.0 yr
 *** failed WPs:  147   out of  2904  ***
```

In summary,

- An increase in weld thickness resulted in delays in occurrence of localized corrosion,
- Timing of releases was correctly transferred to output files. No releases occurred before WPs failed by localized corrosion. No releases occurred from failed WPs before failed WPs were contacted by water,
- No negative releases were observed.

Test 8 Evaluation (Pass/Fail): PASS

Attachment I
TPA Version 5.1 Validation Task P-10
Test 9 Description

<table>
<tr><td colspan="2" align="center">Test Method</td></tr>
<tr><td>code inspection
x output inspection
hand calculation</td><td>x spreadsheet
x graphical
comparison with external code results</td></tr>
<tr><td colspan="2">Test Objective: Verify the functionalities implemented in RELEASET.</td></tr>
<tr><td colspan="2" align="center">Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): XP

Input Data (files, data base, mode settings): See the attachment.</td></tr>
<tr><td colspan="2">Assumptions, constraints, and/or scope of test: (none)</td></tr>
<tr><td colspan="2">Test Procedure:

Execute the TPA code mean value data file for 10,000 yr for Subarea 3. Set the flow multiplication factors in wpflow.def to large values to give early and large releases. For a conservative and highly-soluble radionuclides (e.g., Tc-99 and I-129), determine whether mass is conserved .</td></tr>
<tr><td colspan="2" align="center">Test Results

Location: P10\TPA_Validation\Test9

Test Criterion or Expected Results: Mass-balance requirement for Tc99 and I129 would be met within ~1% .

Test Evaluation (Pass/Fail): Passed</td></tr>
<tr><td colspan="2">Notes: See following pages of this attachment for analysis of results.</td></tr>
<tr><td>Testers: Hakan Basagaoglu
Robert Rice</td><td>Date: April 27, 2007</td></tr>
</table>

Results:

The TPA run using the mean value data file did not result in any releases. Therefore, the input file used for Test 5 (reported on P10 E-2) was used for this test. The flow multiplication factor, Fow, were set to 1 for the base case and to 2 for high-flow case in wpflow.def under a subdirectory "tpa51betaU\data" for t = 0-10,000 year. The release rates for Tc99 and I129 are shown in Fig. 58 and 59 (the source data for these plots was ebsnef2.dat).

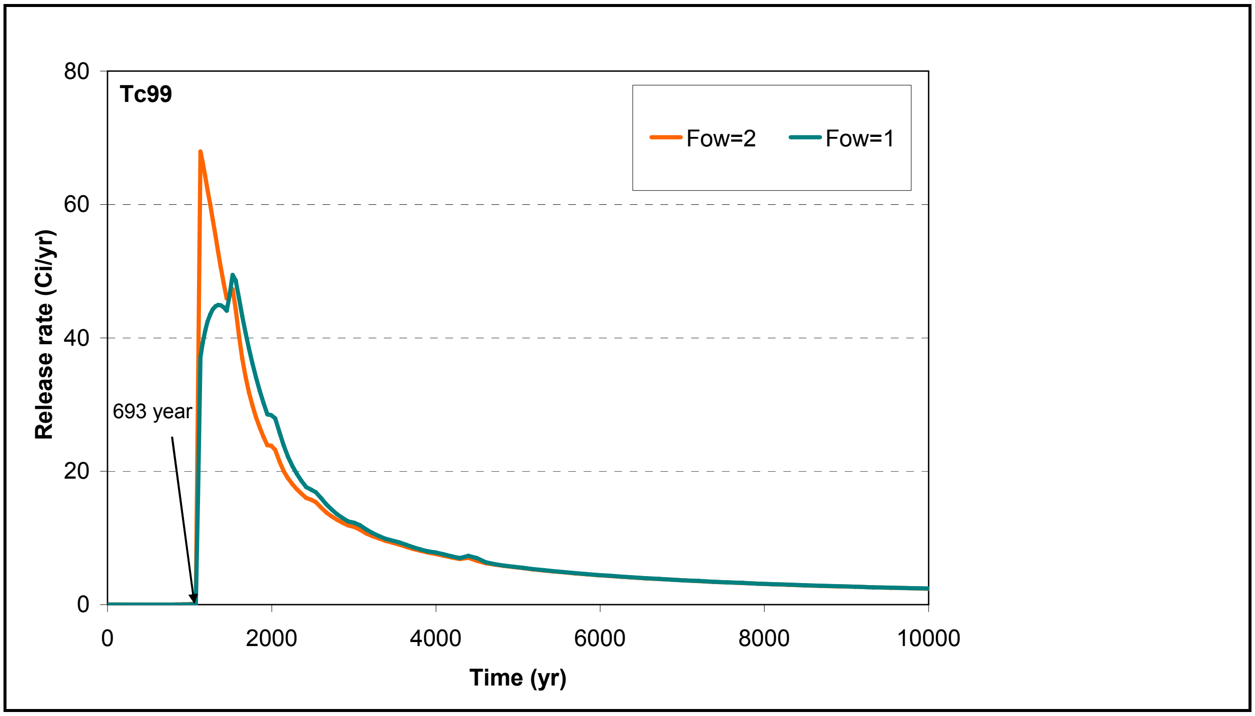


Fig. 58. Temporal variations in Tc99 releases.

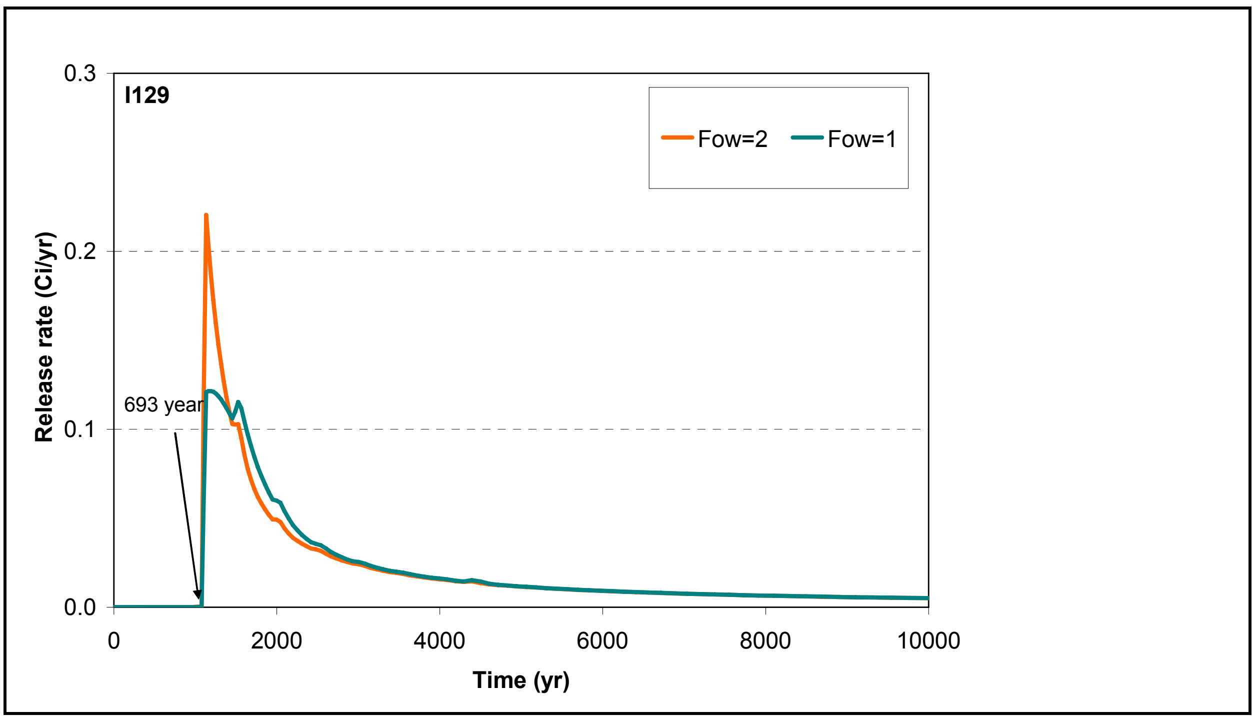


Fig. 59. Temporal variations in Tc99 releases.

The main concern with these plot was that I129 and Tc99 did not completely leave the EBS after 10Ky; therefore, they can not be directly used for mass-balance computations. To enforce, a complete releases of these radionuclides, we set in tpa.inp:

Preexponential_SFDissolutionModel2 = 6000000
GapFractionforI129=0,
GapFractionforTc99=0.

The resulting breakthrough curves for I129 and Tc99 are shown in Figs. 60 and 61. These plots indicate that both redionuclides were flushed out within a 10Ky simulation period.

The releases in each time step can be approximately calculated by multiplying the release time interval between two consecutive time steps by the average release rates over two consecutive time steps (i.e., calculating the area under breakthrough curves using a trapezoid approximation) (in ebsnef2.dat). Then, by adding the releases in each time-step over the entire simulation length (10Ky in this simulation), the total releases can be approximately computed.

In order to test the mass-balance error for radionuclides, the total releases should also be compared with the initial inventories. Initial inventories were computed by multiplying the number of failed waste packages (obtained from ebsrelsf.inp and ebsrelglass.inp) by the release rates per waste package for spent fuel (SF) and glass (obtained from ebspacsf.nuc and ebspacglass.nuc) and by summing up the products over failed SF and glass WPs . The results is then multiplied by the subareawetfraction to calculate the initial inventory. The subareawetfraction in these simulations was set to 0.5.

From ebsrelsf.inp:

```
2.09000E+03 ! xcon
5.00000E-01 ! sawetfrac
```
(Number of WPs for SF)
(SubareawetFraction)

From ebsrelglass.inp:

```
8.14000E+02 ! xcon
5.00000E-01 ! sawetfrac
```
(Number of WPs for Glass)

From ebspacsf.nuc

```
I129   3.061E-01
TC99   1.278E+02
```
(Ci/WP)
(Ci/WP)

From ebspacglass.nuc

```
I129   1.366E-02
TC99   1.870E+01
```
(Ci/WP)
(Ci/WP)

Hence, the initial inventories for I129 = 0.5 × (0.3061 × 2090 +0.01366 ×814) = 325.4341 ci
Hence, the initial inventories for Tc99 = 0.5 × (127.8 × 2090 +18.7 ×814) = 141161.9 ci.

The total releases calculated in the end of 10Ky using the trapezoid approximation for I129 and Tc99 were 329.22 ci and 142146 ci
(the calculations were reported in \Test9\10Ky\Low_flow_prexp_GapFraction\I129
\Test9\10Ky\Low_flow_prexp_GapFraction\Tc99).

Alternatively, the total releases of I129 and Tc99 from the EBS were reported in cumrel.res:

I129	3.2922E+02	Ci
Tc99	1.4205E+05	Ci

Hence, the total releases computed using trapezoid approximation or obtained directly from cumrel.res are within ~1% initial inventories computed from ebsrelsf.inp, ebsrelglass.inp, ebspacsf.nuc, and ebspacglass.nuc.

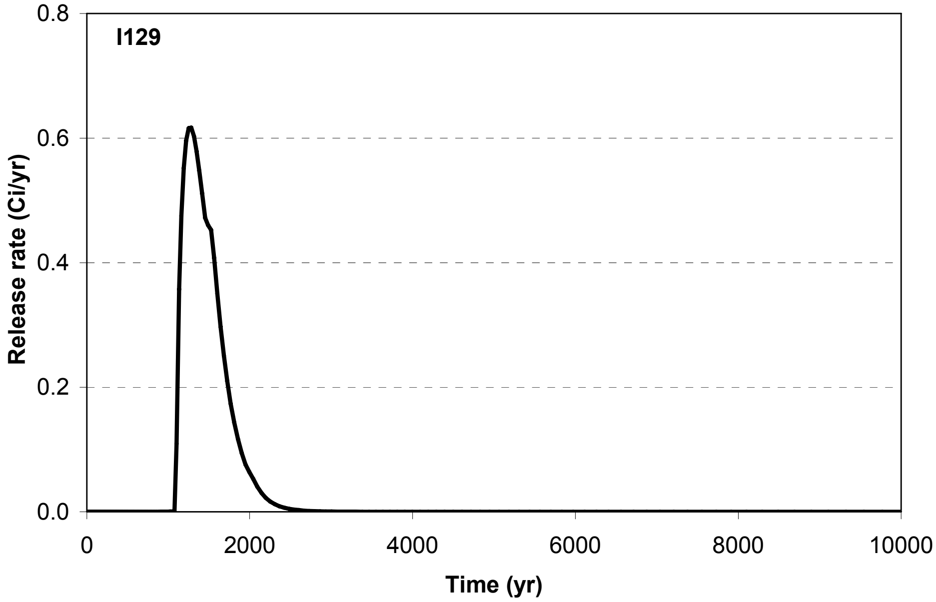


Fig. 60. Temporal variations in Tc99 releases.

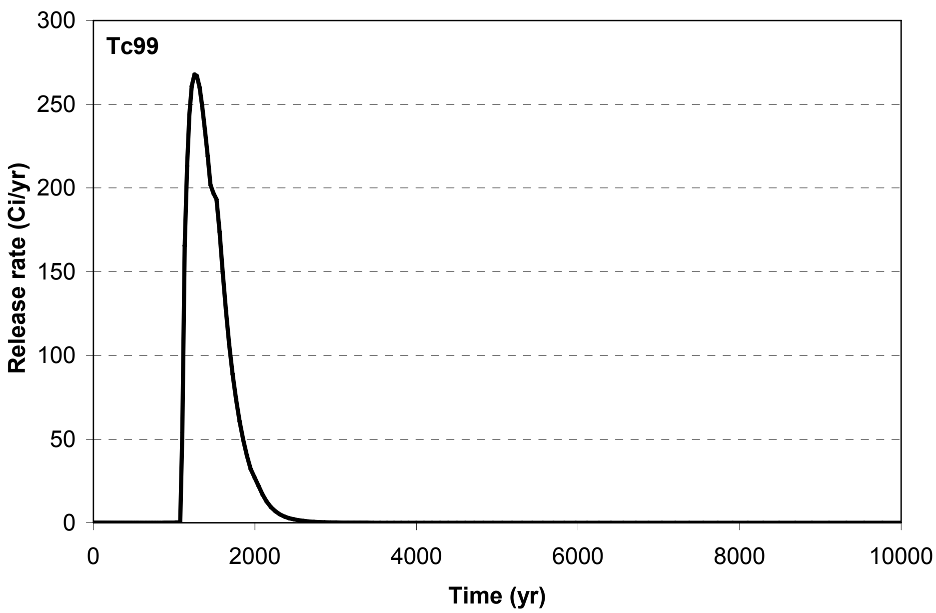


Fig. 61. Temporal variations in Tc99 releases.

These results suggest that when the early and large releases were forced, the mass-balance was accomplished within 1% for Tc99 and 1.2% for I129. Hence, the mass-balance error for Tc99 and I129 was ~1%.

Test 9 Evaluation (Pass/Fail): PASS

SOFTWARE VALIDATION REPORT (SVR)

SVTR#:	Project#: 20.06002.01.354	
Software Name: TPA		Version: 5.1betaX
Test ID: Task P-11	Test Series Name: Colloid Facilitated Releases from the Engineered Barrier System	

Test Method

x code inspection
x output inspection
hand calculation

x spreadsheet
graphical
comparison with external code results

Test Objective: Verify the release functionality for radionuclides irreversibly attached to colloids

Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): Microsoft Windows XP

Input Data (files, data base, mode settings): See below.

Assumptions, constraints, and/or scope of test: Scope is limited to evaluating functionality of the irreversible colloid function of the EBSREL module and its outputs to UZFT.

Test Procedure: See Attachments A–F.

Test Results

Location: See CD labeled “TPA Version 5.1 Validation Task P-11" for associated input and output files.

Test Criterion or Expected Results: See Attachments A–F.

Test Evaluation (Pass/Fail): Pass

Notes:

Tester: O. Osidele, D. Pickett	Date: 05/29/2007

Attachment A

Task P-11 Test Plan
Objectives, Assumptions, Tests

OBJECTIVES
In addition to the functionality described for Task 10, the *ebsrel.f* module and *releaset.f* and *ebsfilt.f* codes have been modified to account for irreversible colloid attachment of radionuclides released from the engineered barrier subsystem. Irreversible attachment is simulated by specifying a fraction of the release for a particular radionuclide. This fraction is assigned to a set of new (artificial) radionuclides, referred to as J-species, to represent colloidal species that possess transport properties appropriate for colloids. The four elements allowed to bind irreversibly to colloids are plutonium, americium, thorium, and curium. Mass loading of these elements to colloids is calculated based on competitive sorption among the four plus uranium. The modified abstraction enables adjustment of solubility limits for plutonium and americium so that dissolved radionuclides can still be released at their solubility limits after the colloidal fraction is allotted. Although uranium is not associated with the J-species, the uranium solubility limit is also enhanced to fully enable its colloid sorption competitive effects. Because the effective solubility limit is an estimate of what is needed to account for competitive colloid sorption, it is possible that final output aqueous concentration may exceed the sampled solubility limit for U, Pu, and Am.

Scope: Review SCRs indicated in Table 6.1-1 and conduct additional testing as necessary to verify the following:

1. Adjustments to effective solubility of U, Am, and Pu to account for competitive irreversible sorption to colloids are appropriately implemented.
2. Finite sorption capacity of colloids is appropriately implemented and calculations for competitive sorption on colloids correctly accounts for the sorption affinities of the different nuclides.
3. Colloid-facilitated releases can be turned off to permit comparison of scenarios with and without colloids.

The validation team also may conduct any additional testing deemed appropriate to provide confidence that the colloid source term functions are implemented as intended.

TESTS
The following five tests address the objectives of this SVR. Summaries of test results are provided in Attachments B–F.

1. Repeat SCR 611 process-level acceptance test PL-1, which used a spreadsheet to test appropriate calculation of effective solubility limits for americium, plutonium, and uranium.

2. Repeat SCR 611 process-level acceptance test PL-2, which used a spreadsheet to test appropriate calculation of release concentrations and affinity-weighted concentrations.

3. Repeat SCR 611 process-level acceptance test PL-3, which used a spreadsheet to test appropriate calculation of colloidal J-species concentrations.

4. Execute the TPA code for 10 reference case realizations covering 10 subareas over 10,000 years. From files *ebsnef.dat* and *ebsnef2.dat* for each of the 100 subarea realizations, use a script to extract the maximum concentration of released uranium, plutonium, and americium over the time series. This will involve, for each of these three elements, conversion of the Ci/yr release rates to kg/m^3 concentrations (using the corresponding water flux) for each aqueous species isotope, summation of the calculated isotope mass concentrations, and selection of the maximum element

concentration among all time steps for the realization. Testers may devise other means (e.g., inspection) for selecting the time step with maximum concentration if this can be done with reasonable assurance. Note that maximum concentration does not necessarily correspond to maximum release rate.

For each realization, compare the maximum released concentration for each element with the sampled solubility limit. The maximum concentration should not exceed the solubility limit by more than 50 percent.

5. In tpa.inp, set IrreversibleColloidModel[0=no,1=yes] to a value of 0. Execute the TPA code for one reference case realization covering 10,000 years. Check EBSREL output files to ensure that zero releases are reported for all J-species.

CRITERIA

The criteria for each of the above five tests are described in the following Attachments B–F.

Attachment B

Task P-11 Test 1

Test 1 repeats process-level acceptance test PL-1 for SCR 611. A spreadsheet is used to test appropriate calculation of effective solubility limits for americium, plutonium, and uranium. The results and all associated files are contained on the CD named "TPA 5.1 Validation Task P-11."

Criterion

The screen print output should give the same value of effective solubility limit for each radionuclide as the spreadsheet calculations.

Test 1 Procedure and Analysis of Results

The TPA 5.1betax code was modified by adding print statements to *ebsrel.f* to display the solubility limit for each radionuclide before (`sol`) and after (`effsol`) executing the `calc_EffectiveSolLimit` subroutine. The results were written to *tpa.out*. The print statement was enabled for only one isotope of a given element, because these calculations are element-specific and are the same for all isotopes of an element. Using the reference case *tpa.inp*, the code was run for one realization in Subarea 3 (substituted for Subarea 2, specified in SCR-611, because Subarea 2 had no releases).

The equation used for calculating the effective solubility limit is shown in Section 4 of Attachment A of SCR 611. This equation was performed for americium, plutonium, and uranium in an Excel spreadsheet (*P-11_1-3_results.xls*) using the sampled values (from *samplpar.res*) for solubility limits, relative affinities, and sorption capacity. These values were compared with those reported in *tpa.out*, which are shown in this excerpt:

```
U238
 sol = 6.593307000000000E-02
 effsol = 6.611584601605558E-02
Am241
 sol = 1.274698000000000E-04
 effsol = 2.970874990205505E-04
Pu239
 sol = 1.057580000000000E-04
 effsol = 1.185007649238688E-04
```

Table B-1 below shows the compared values. The values all match. It was also noted in *tpa.out* that, appropriately, no other elements had effective solubility limits that differed from the sampled value.

Table B-1. Comparison of effective solubility limits calculated by spreadsheet and by EBSREL

Element	Sampled Solubility Limit	Effective Solubility Limit: Spreadsheet	Effective Solubility Limit: TPA
americium	1.275E-04	2.971E-04	2.971E-04
plutonium	1.058E-04	1.185E-04	1.185E-04
uranium	6.593E-02	6.612E-02	6.612E-02

Test Evaluation (Pass/Fail): Pass.

Attachment C

Task P-11 Test 2

Test 2 repeats process-level acceptance test PL-2 for SCR 611. A spreadsheet is used to test appropriate calculation of release concentrations and affinity-weighted concentrations. The results and all associated files are contained on the CD named "TPA 5.1 Validation Task P-11." This test used the same simulation as was used for Test 1.

Criterion

The screen print should give the same value of concentration and total affinity-weighted concentration as obtained from the spreadsheet calculation.

Test 2 Procedure and Analysis of Results

The TPA 5.1betax code was modified by adding print statements to *ebsrel.f* to save a copy of *ebsnef.dat* to *ebsnef_int.dat* immediately after running the *releaset* standalone code . Print statements were added to *ebsrel.f* to display the radionuclide concentration calculated from the release (*releaset*) and the sum of the affinity-weighted cocncentrations for Pu, Am, Th, Cm and U (`totalAffCon`). The results were written to *tpa.out*. Only the results for the last time step are displayed.

Values for radionuclide half-life and atomic weight were extracted from *nuclides.dat*. Values for flow rate and release rates were extracted from *ebsnef_int.dat*. In Excel spreadsheet *P-11_1-3_results.xls,* release rates were converted to concentrations for CM246, U238, CM245, AM241, U233, TH229, AM243, PU239, PU240, U234, and TH230 using the equation in Section 6 of Attachment A of SCR 611. Isotopes were combined to give total element concentrations for Pu, Am, Th, Cm, and U.

In the spreadsheet, total affinity-weighted concentrations for Pu, Am, Th, Cm, and U were calculated using the denominator of the equation in Section 7 of Attachment A. The term "affinity-weighted concentration" refers to the total element concentration multiplied by the affinity factor, cumulatively increased as each element is added in the order Am, Pu, U, Cm, and Th. In other words, the value for Th is equal to the summation in the denominator of the equation in Section 7 of Attachment A.

These values were compared to outputs in the *tpa.out* file, the relevant portions of which are shown here:

```
CM246
concentration = 1.624366808107054E-05
totalelementconc = 1.624366808107054E-05
U238
concentration = 5.497695828362212E-02
totalelementconc = 5.497695828362212E-02
CM245
concentration = 1.616919756663057E-04
totalelementconc = 1.779356437473762E-04
AM241
concentration = 2.245100652197504E-07
totalelementconc = 2.245100652197504E-07
NP237
concentration = 5.741618649257425E-02
totalelementconc = 0.000000000000000E+00
U233
concentration = 1.436424861816728E-06
totalelementconc = 5.497839470848394E-02
TH229
concentration = 2.968214478154497E-05
totalelementconc = 2.968214478154497E-05
```

AM243
concentration = 2.321278229433787E-04
totalelementconc = **2.323523330085984E-04**
PU239
concentration = 8.488793828004330E-05
totalelementconc = 8.488793828004330E-05
PU240
concentration = 1.366067471509901E-05
totalelementconc = **9.854861299514231E-05**
U234
concentration = 1.031319407854270E-05
totalelementconc = **5.498870790256248E-02**
TH230
concentration = 1.811406234426568E-04
totalelementconc = **2.108227682242017E-04**

Am
colloidAffinity = 11.04367000000000
colloidSolubility = 1.274698000000000E-04
totalAffCon = 1.407734406166000E-03
Pu
colloidAffinity = 1.000000000000000
colloidSolubility = 1.057580000000000E-04
totalAffCon = 1.506283019161142E-03
_U
colloidAffinity = 2.300729000000000E-02
colloidSolubility = 6.593307000000000E-02
totalAffCon = 2.771424168600689E-03
Cm
colloidAffinity = 11.89902000000000
colloidSolubility = 3.139903000000000E-02
totalAffCon = 4.888683952263594E-03
Th
colloidAffinity = 7.161611000000000
colloidSolubility = 2.535013000000000E-04
totalAffCon = 6.398514608228488E-03

In the first portion of this file excerpt above, the term "concentration" refers to the radionuclide concentration in kg/m^3. The term "totalelementconc" is the element concentration accounting for all isotopes, but note that it is cumulative for each element, such that the true total is shown only for the last listed isotope. This final concentration for the elements of interest is denoted by bold text. The second portion of the file excerpt above shows the affinity-weighted concentration in kg/m^3 as "totalAffCon."

Table C-1 shows a comparison between the radionuclide concentrations from TPA ("concentration" in the *tpa.out* excerpt above) and those reported in the Excel file *P-11_1-3_results.xls*. The values match.

Table C-2 compares the total element concentrations ("totalelementconc" of final listed isotope in the excerpt above) and affinity-weighted concentrations ("totalAffCon" in the excerpt above) from TPA and those reported in the Excel file *P-11_1-3_results.xls*. The values match.

Test Evaluation (Pass/Fail): Pass.

Table C-1. Comparison of EBSREL radionuclide concentration calculations (kg/m^3) with spreadsheet results.

	CM246	U238	CM245	AM241	U233	TH229	AM243	PU239	PU240	U234	TH230
Spreadsheet	1.62E-05	5.50E-02	1.62E-04	2.25E-07	1.44E-06	2.97E-05	2.32E-04	8.49E-05	1.37E-05	1.03E-05	1.81E-04
TPA	1.62E-05	5.50E-02	1.62E-04	2.25E-07	1.44E-06	2.97E-05	2.32E-04	8.49E-05	1.37E-05	1.03E-05	1.81E-04

Table C-2. Comparison of EBSREL element concentration calculations (kg/m^3) with spreadsheet results.

		Am	Pu	U	Cm	Th
Total concentration	Spreadsheet	2.32E-04	9.85E-05	5.50E-02	1.78E-04	2.11E-04
	TPA	2.32E-04	9.85E-05	5.50E-02	1.78E-04	2.11E-04
Affinity-weighted concentration	Spreadsheet	1.41E-03	1.51E-03	2.77E-03	4.89E-03	6.40E-03
	TPA	1.41E-03	1.51E-03	2.77E-03	4.89E-03	6.40E-03

Attachment D

Task P-11 Test 3

Test 3 repeats process-level acceptance test PL-3 for SCR 611. A spreadsheet is used to test appropriate calculation of colloidal J-species concentrations. The results and all associated files are contained on the CD named "TPA 5.1 Validation Task P-11." This test used the same simulation as was used for Test 1.

Criterion

The concentrations and releases calculated for the J-species should be the same as those written by the code to *ebsnef.dat*..

Test 3 Procedure and Analysis of Results

The EBSREL J-species release rates (Ci/yr) and concentrations (kg/m^3) were read from the final time step from *ebsnef2.dat* as follows. The release rate is from the second column of the file, while the concentration is in the fifth column. The radionuclide identities in parentheses were added.

```
JC246 (Cm-246)
 1.0000E+04   3.2877E-06   0   9.6960E-04   1.1030E-05
JC245 (Cm-245)
 1.0000E+04   1.8292E-05   0   9.6960E-04   1.0979E-04
JA241 (Am-241)
 1.0000E+04   2.5852E-07   1   9.6960E-04   7.7622E-08
JA243 (Am-243)
 1.0000E+04   1.5525E-05   1   9.6960E-04   8.0256E-05
JP239 (Pu-239)
 1.0000E+04   2.9224E-07   1   9.6960E-04   4.8442E-06
JP240 (Pu-240)
 1.0000E+04   1.7237E-07   1   9.6960E-04   7.7956E-07
JT230 (Th-230)
 1.0000E+04   1.4501E-06   1   9.6960E-04   7.4029E-05
```

The concentrations and release rates of the corresponding dissolved species were likewise reported in *ebsnef2.dat* for the final time step as follows:

```
CM246
   1.0000E+04   1.5541E-06   0   9.6960E-04   5.2138E-06
CM245
   1.0000E+04   8.6464E-06   0   9.6960E-04   5.1899E-05
AM241
   1.0000E+04   4.8921E-07   1   9.6960E-04   1.4689E-07
AM243
   1.0000E+04   2.9378E-05   1   9.6960E-04   1.5187E-04
PU239
   1.0000E+04   4.8289E-06   1   9.6960E-04   8.0044E-05
PU240
   1.0000E+04   2.8482E-06   1   9.6960E-04   1.2881E-05
TH230
   1.0000E+04   2.0981E-06   1   9.6960E-04   1.0711E-04
```

In Excel spreadsheet *P-11_1-3_results.xls*, the colloid J-species concentrations were calculated as follows. First, the equation in Section 7 of Attachment A of SCR 611 was used to calculate elemental J-species concentrations. Then, the element mass was apportioned to isotopes. For example, for Pu-239, the J-species concentration is

$$C_{JPu-239} = C_{JPu} \frac{C_{Pu-239}}{C_{Pu-239} + C_{Pu-240}}$$

where

$C_{JPu\text{-}239}$	—	preliminary Pu-239 J-species concentration [kg/m^3]
C_{JPu}	—	total plutonium J-species concentration [kg/m^3]
$C_{Pu\text{-}239}$	—	concentration of total released Pu-239 [kg/m^3]
$C_{Pu\text{-}240}$	—	concentration of total released Pu-240 [kg/m^3]

Next, mass balance was checked:

$$C_{JFPu-239} = Min(C_{Pu-239}, C_{JPu-239})$$

where

$C_{JFPu\text{-}239}$	—	final Pu-239 J-species concentration [kg/m^3]
$C_{JPu\text{-}239}$	—	Pu-239 J-species concentration from previous equation [kg/m^3]
$C_{Pu\text{-}239}$	—	concentration of total released Pu-239 [kg/m^3]

Next, the dissolved released radionuclide concentrations were calculated by mass balance; for example:

$$C_{DissPu-239} = C_{Pu-239} - C_{JFPu-239}$$

In the spreadsheet, the colloid and dissolved concentrations were converted back to release rates using the converse of the equation in Section 6 of Attachment A of SCR 611.

Table D-1 compares TPA and spreadsheet values for the colloidal and dissolved release rates and concentrations for all radionuclides for which J-species are modeled. The values match.

Test Evaluation (Pass/Fail): Pass.

Table D-1. Comparison of TPA and spreadsheet release rates (Ci/yr) and concentrations (kg/m^3) for J-species and corresponding dissolved species

		Cm-246	Cm-245	Am-241	Am-243	Pu-239	Pu-240	Th-230
Dissolved release rate	TPA	1.55E-06	8.65E-06	4.89E-07	2.94E-05	4.83E-06	2.85E-06	2.10E-06
	Spreadsheet	1.55E-06	8.65E-06	4.89E-07	2.94E-05	4.83E-06	2.85E-06	2.10E-06
Dissolved concentration	TPA	5.21E-06	5.19E-05	1.47E-07	1.52E-04	8.00E-05	1.29E-05	1.07E-04
	Spreadsheet	5.21E-06	5.19E-05	1.47E-07	1.52E-04	8.00E-05	1.29E-05	1.07E-04
J-species release rate	TPA	3.29E-06	1.83E-05	2.59E-07	1.55E-05	2.92E-07	1.72E-07	1.45E-06
	Spreadsheet	3.29E-06	1.83E-05	2.59E-07	1.55E-05	2.92E-07	1.72E-07	1.45E-06
J-species concentration	TPA	1.10E-05	1.10E-04	7.76E-08	8.03E-05	4.84E-06	7.80E-07	7.40E-05
	Spreadsheet	1.10E-05	1.10E-04	7.76E-08	8.03E-05	4.84E-06	7.80E-07	7.40E-05

Attachment E

Task P-11 Test 4

Test 4 is intended to ensure that the effective solubility limit calculation, which depends on an estimate of the appropriate factor to apply, does not result in unreasonably high released concentrations. Released dissolved concentrations for americium, plutonium, and uranium were compared to the sampled solubility limit to see if removal of mass for the J species led to excessive concentrations, i.e., if solubility limit enhancement was excessive. The results and all associated files are contained on the CD named "TPA 5.1 Validation Task P-11."

Criterion

In general, the maximum released dissolved concentrations for americium, plutonium, and uranium should not exceed the solubility limit by more than 50 percent. To the extent that any radionuclides in any of the test realizations exceed this arbitrary criterion, results should be evaluated to ensure there is will be no significant bias to release rates of dissolved species.

Test 4 Procedure and Analysis of Results

Ten reference case realizations were performed for all subareas over 10,000 years. Because releases did not occur for all subareas and realizations (100 combinations), this resulted in 31 cases in which releases were calculated. For each subarea and realization, the maximum released elemental concentration for americium, plutonium, and uranium was selected from the time series. Selection of the maximum was sufficient, because the concentrations for a realization are all compared to the same sampled solubility limit. Then, for each element, the maximum released concentration among the subareas in a realization was compared to the sampled solubility limit.

Table E-1 shows a spreadsheet excerpt (*P-11_4_results.xls*) containing the maximum dissolved elemental concentrations per subarea and realization. A zero means that releases did not occur. The final column shows a percentage comparison between the released dissolved concentration and the sampled solubility limit. The test criterion - that the maximum concentration should not exceed the solubility limit by more than 50 percent - translates to a value here of 150 percent.

Of the 30 concentrations compared (three elements in ten realizations), the 150 percent criterion was exceeded in only one case - 173 percent for americium in Realization 1. No other values were even above 100 percent. The 173 percent result is considered acceptable because (i) it occurred in only one realization for one element, (ii) the 150 percent criterion was arbitrary, and (iii) solubility limit probability distributions have multiple order-of-magnitude ranges that dwarf this exceedance. Moreover, releasing dissolved americium at a concentration in excess of the sampled solubility limit will not lead to a significant overestimate of dose because americium isotope doses are expected to be dominated by the more mobile colloidal species.

The occurrence in Table E-1 of values markedly less than 100 percent does not necessarily imply that solubility limits were under-enhanced. It may be that release was not solubility-limited in these cases.

Test Evaluation (Pass/Fail): Pass.

Table E-1. Comparing released dissolved concentration (kg/m^3) for americium, plutonium, and uranium with sampled solubility limit.

Realization #		Solubility Limit	subarea 1	subarea 2	subarea 3	subarea 4	subarea 5	subarea 6	subarea 7	subarea 8	subarea 9	subarea 10	% Solub. Limit
1	Am	1.27E-04	2.21E-04	0	2.08E-04	0	2.14E-04	0	0	0	0	0	173%
	Pu	1.06E-04	1.00E-04	0	1.00E-04	0	1.00E-04	0	0	0	0	0	95%
	U	6.59E-02	5.50E-02	0	5.50E-02	0	5.50E-02	0	0	0	0	0	83%
2	Am	2.07E-05	0	0	0	4.11E-06	0	0	0	0	0	0	20%
	Pu	1.83E-05	0	0	0	4.90E-06	0	0	0	0	0	0	27%
	U	2.16E-01	0	0	0	5.52E-02	0	0	0	0	0	0	26%
3	Am	7.89E-04	0	0	0	0	1.79E-04	0	1.76E-04	1.80E-04	0	1.80E-04	23%
	Pu	1.01E-05	0	0	0	0	3.26E-06	0	3.26E-06	3.26E-06	0	3.26E-06	32%
	U	9.28E-01	0	0	0	0	2.85E-01	0	2.85E-01	2.85E-01	0	2.85E-01	31%
4	Am	2.40E-02	0	0	7.77E-03	7.93E-03	0	0	0	5.60E-03	2.29E-03	6.91E-03	33%
	Pu	4.46E-06	0	0	3.97E-06	3.95E-06	0	0	0	3.90E-06	3.86E-06	4.00E-06	90%
	U	1.03E-02	0	0	8.39E-03	8.39E-03	0	0	0	8.39E-03	8.39E-03	8.39E-03	81%
5	Am	6.43E-04	0	1.99E-04	0	1.76E-04	0	2.52E-04	0	0	0	0	39%
	Pu	1.71E-05	0	8.76E-06	0	8.72E-06	0	8.89E-06	0	0	0	0	52%
	U	1.67E-03	0	8.50E-04	0	8.50E-04	0	8.50E-04	0	0	0	0	51%
6	Am	3.70E-05	1.27E-05	0	1.72E-05	1.84E-05	0	0	0	0	0	1.51E-05	50%
	Pu	2.54E-05	9.24E-06	0	9.35E-06	9.36E-06	0	0	0	0	0	9.32E-06	37%
	U	5.50E-03	1.49E-03	0	1.49E-03	1.49E-03	0	0	0	0	0	1.49E-03	27%
7	Am	3.49E-03	0	0	2.97E-03	2.17E-03	0	0	2.51E-03	2.65E-03	0	0	85%
	Pu	1.24E-04	0	0	9.69E-05	9.58E-05	0	0	9.56E-05	9.66E-05	0	0	78%
	U	5.92E-03	0	0	4.25E-03	4.25E-03	0	0	4.25E-03	4.25E-03	0	0	72%
8	Am	3.32E-05	0	0	0	0	0	1.94E-05	0	0	0	0	59%
	Pu	2.85E-04	0	0	0	0	0	9.61E-05	0	0	0	0	34%
	U	9.97E-03	0	0	0	0	0	2.56E-03	0	0	0	0	26%
9	Am	3.39E-05	0	0	0	0	2.97E-05	0	0	2.97E-05	0	0	88%
	Pu	4.79E-05	0	0	0	0	3.27E-05	0	0	3.27E-05	0	0	68%
	U	4.68E-02	0	0	0	0	2.94E-02	0	0	2.94E-02	0	0	63%
10	Am	5.58E-04	0	3.10E-04	0	0	3.30E-04	0	3.05E-04	0	3.43E-04	0	61%
	Pu	5.64E-05	0	3.15E-05	0	0	3.16E-05	0	3.15E-05	0	3.16E-05	0	56%
	U	1.84E-02	0	9.81E-03	0	0	9.81E-03	0	9.81E-03	0	9.81E-03	0	53%

Attachment F

Task P-11 Test 5

Test 5 is designed to ensure that colloid species concentrations are zero or are not calculated when the user has elected to disable the irreversible colloid model.

Criterion
When the *tpa.inp* input parameter IrreversibleColloidModel[0=no,1=yes] is set to 0, no J-species releases should be calculated.

Test 5 Procedure and Analysis of Results

One realization was performed with the *tpa.inp* parameter IrreversibleColloidModel[0=no,1=yes] set to 0. The TPA code was modified so that the *ebsnef2.dat* results for each subarea would be saved in separate files rather than being overwritten each time a new subarea was simulated. The new files were named *ebsnef2_rlz01_sa01.dat* and so on. These files contain radionuclide engineered barrier system release rates. The results and all associated files are contained on the CD named "TPA 5.1 Validation Task P-11."

All ten output files were inspected. None contained data on J species radionuclides.

Test Evaluation (Pass/Fail): Pass.

SOFTWARE VALIDATION REPORT (SVR)

<table>
<tr><td>SVR#:</td><td colspan="2">Project#: 06002.01.354</td></tr>
<tr><td colspan="2">Software Name: Total-system Performance Assessment (TPA)</td><td>Version: 5.1betaU, 5.1betaW, 5.1betaY</td></tr>
<tr><td>Test ID: P-12</td><td colspan="2">Test Series Name: Unsaturated Zone Flow and Transport</td></tr>
<tr><td colspan="3">Test Method
☐ code inspection
Xoutput inspection
X hand calculation
X spreadsheet
☐ graphical
☐ comparison with external code results</td></tr>
<tr><td colspan="3">Test Objective: See Attachment A</td></tr>
<tr><td colspan="3">Test Environment Setup
Hardware (platform, peripherals): Desktop PC
Software (OS, compiler, libraries, auxiliary codes or scripts): Microsoft Windows 2000 (Tests P12-1, P12-3, P12-4); Microsoft Windows XP (Test P12-2)
Input Data (files, data base, mode settings): See Attachment A for each test case.
Environment variable:
Test case P12-1: TPA_DATA=..\tpa51betaY ; TPA_TEST=..\tpa51betaY
Test case P12-2: TPA_DATA=..\tpa51betaU; TPA_TEST=..\tpa51betaU
Test case P12-3: TPA_DATA=..\tpa51betaY ; TPA_TEST=..\tpa51betaY
Test case P12-4: TPA_DATA=..\tpa51betaW; TPA_TEST=..\tpa51betaW
Path for archive of results:
Test case P12-1: [CD:folder titled P12 Testing]: \SVT_P12\test1
Test case P12-2: [CD:folder titled P12 Testing]: \SVT_P12\test2
Test case P12-3: [CD:folder titled P12 Testing]: \SVT_P12\test3
Test case P12-4: [CD:folder titled P12 Testing]: \SVT_P12\test4</td></tr>
<tr><td colspan="3">Assumptions, constraints, and/or scope of test: Scope is limited to evaluating functionality of UZFT module and its outputs to SZFT. It is assumed for purposes of this test that information passed as input to UZFT by EXEC or EBSREL modules is correct.</td></tr>
<tr><td colspan="3">Test Procedure: See details in Attachment A for tests P12-1, P12-2, P12-3, and P12-4.</td></tr>
<tr><td colspan="3">Test Results
Location: See attached CD labeled “TPA Version 5.1 Validation Task P-12"
Test Criterion and Analysis of Results: See Attachment A
Test Evaluation (Pass/Fail): PASS</td></tr>
<tr><td colspan="3">Notes:</td></tr>
<tr><td>Testers: Jude McMurry, James Winterle</td><td colspan="2">Date: 05/23/2007</td></tr>
</table>

Attachment A

TPA Version 5.1 Validation
Task P-12 Tests and Results

The UZFTmodule executes the NEFTRAN II code to calculate the transport of released radionuclide species from the unsaturated zone to the water table. Changes to this abstraction include code modifications to account for both reversible and irreversible colloid-facilitated transport, colloid filtration, addition of new repository subareas with new input values, modifications to the layer-selection algorithm to prevent skipping of unsaturated zone transport calculations, creation of new *uz_kdrd.out* and *uz_revers.out* intermediate output files for traceability of retardation coefficient calculations, modifications to include at least one matrix transport layer in every transport calculation, and changes to the fast-flow bypass calculation so that only the portion of flow that cannot be accommodated by the most permeable matrix layer is bypassed.

Objectives: The objective of Software Validation Report (SVR) #12 is to verify the process level calculations performed by the TPA module UZFT. Confirm the following results:

1. In each subarea, the layer present (i.e., non-zero thickness) with the most permeable matrix is assigned matrix layer properties and is used for the transport calculations.
2. The thickness of the most permeable matrix layer is increased if necessary to provide an average groundwater travel time of at least 20 years in that layer. (Note that this adjustment is made for computational efficiency, but setting a minimum travel time of 20 years for unsaturated zone transport is reasonable; justification for this approach will be provided in TPA Version 5.1 User Guide; this approach applies only to the fraction that does not bypass unsaturated zone transport).
3. The mass fraction of the release term allowed to bypass the unsaturated zone transport calculation is equal to the portion of flow that cannot be accommodated in the most permeable matrix layer.
4. Colloid filtration is appropriately applied based on the layer, of those present (i.e., non-zero thickness) in the subarea, that has the highest filtration factor value.
5. Calculated sorption coefficients and retardation factors for the actinides Am, Np, Pu, Th, U, and Cm are correctly reported in *uz_kdrd.out*.
6. Retardation factors are correctly adjusted to account for reversible colloid transport and are correctly reported in *uz_revers.out*.
7. For average and for time-dependent groundwater velocities, the repository leg properties in *nefiiuz.inp* are correctly calculated based on the properties of the first kept layer (leg) selected for use in the transport calculations.

During the testing, the validation teams may conduct additional tests as needed, to be documented in the SVR, to understand and verify software performance related to the UZFT module.

Test 12-1: Matrix-Fracture Flux Splitting and Adjusted Matrix Layer Thickness

Special diagnostic code modifications required:
Print statements are added to *uzft.f* to display: (i) the media type (matrix or fracture) assigned to each UZ layer, (ii) the matrix conductivity calculated for each existing (non-zero thickness) layer; (iii) the layer with the highest matrix conductivity; (iv) the "infil" value and fracture fraction at each time step; (v) the layer kept for the NEFTRAN input file and the travel time in the kept layer; (vi) the reset layer thickness; (vii) the total UZ travel time; and (viii) the travel times in the layers included in the NEFTRAN input file.

Test 12-1 Description: Verify that the hydrostratigraphic layer with the highest saturated matrix conductivity is (i) assigned matrix layer properties and kept for inclusion in the NEFTRAN input file; (ii) used to calculate the fraction used for splitting flux between matrix and bypass ("fracture") fraction; and (iii) assigned a greater thickness if its average groundwater travel time otherwise is less than 20 years.

Test 12-1 Objectives: The objectives are to confirm the following results:
1. In each subarea, the layer present (i.e., non-zero thickness) with the most permeable matrix is assigned matrix layer properties and is selected for use in the transport calculations.
2. The thickness of the most permeable matrix layer is increased if necessary to provide an average groundwater travel time of at least 20 years in that layer. (Note that this adjustment is made for computational efficiency, but setting a minimum travel time of 20 years for unsaturated zone transport is reasonable; justification for this approach will be provided in TPA Version 5.1 User Guide; this approach applies only to the fraction that does not bypass unsaturated zone transport).
3. The mass fraction of the release term allowed to bypass the unsaturated zone transport calculation is equal to the portion of flow that cannot be accommodated in the most permeable matrix layer.

Test 12-1 Output files to compare or examine: Screen print (*tpa.out*) with diagnostic print statements. Matrix properties are identified as "type 1" in the output, and fracture properties are "type 2".
The hydrostratigraphic layers are designated by number as:

layer # 1	Topopah Spring welded (Tsw)
layer # 2	Calico Hills nonwelded vitric (CHnv)
layer # 3	Calico Hills nonwelded zeolitic (CHnz)
layer # 4	Prow Pass welded (PPw)
layer # 5	Upper Crater Flat (UCF)
layer # 6	Bullfrog welded (BFw)
layer # 7	Unsaturated Fault Zone (UFZ)

Test 12-1 Step-by-step test procedure to be used:
1. Execute ten realizations (start at realization 15 and stop at realization 24) of the test code with the specified modifications using the reference case *tpa.inp* file and capture the screen print in the *tpa.out* file.
2. Set the CHnv layer thickness to zero in *tpa.inp*.
3. Repeat Step 1 to force selection of a different layer with the highest matrix conductivity.

4. Compare the *tpa.out* files generated from Steps 1 and 3.

Test 12-1 Pass/Fail criteria:

1. The kept matrix layer (indexed by its sequence number) should match the layer determined to have the highest matrix conductivity.
2. The "fracture" (bypass) fraction printed to the screen should equal 1 minus the ratio of the highest saturated matrix conductivity to the "infil" value at each time step. If the highest saturated matrix conductivity exceeds the "infil" value, then the "fracture" (bypass) fraction at that time step should be zero.
3. If the travel time for this kept leg is less than 20 years, then a reset statement should follow, indicating the augmented layer thickness.

Test 12-1 Execution and Results of Test

Step 1 was implemented by executing ten realizations of the test code with the specified print statement modifications. Calculations were performed for only one subarea (Subarea 6) in each realization. Subarea 6 was selected because the reference case *tpa.inp* assigns non-zero thicknesses in this subarea for all hydrostratigraphic layers except UFZ, the hypothetical fault zone. In the test case, values in *tpa.inp* (with a copy saved as *v1_tpa.inp*) were set as follows:

Reference Case Parameter	Changes in *v1_tpa.inp*	Remarks

`iconstant`
`StartAtSubarea`
`1`
	`iconstant`
	`StartAtSubarea`
	`6`	

`iconstant`
`StopAtSubarea`
`0`
	`iconstant`
	`StopAtSubarea`
	`6`	

`iconstant`
`StartAtRealization`
`1`
	`iconstant`
	`StartAtRealization`
	`15`	

`iconstant`
`StopAtRealization`
`1`
	`iconstant`
	`StopAtRealization`
	`24`	

`loguniform`
`DefectiveFractionOfWPs/cell`
`1.0e-4,  1.0e-2`
	`constant`
	`DefectiveFractionOfWPs/cell`
	`0.5`
		Change ensures some releases from EBSREL so that UZFT is called

`uniformCHnvThickness_6SubAr`
`ea[m]`
`49, 60`
	`constant`
	`CHnvThickness_6SubArea[m]`
	`10.0`
		Set to a constant so it can be changed to zero in Step 2 without affecting the sampled values of other parameters

Step 2 was executed by changing the CHnv layer thickness to zero in subarea 6 in *tpa.inp* (copy saved as *v2_tpa.inp*):

```
constant
CHnvThickness_6SubArea[m]
0.0
```

Test P12-1 Results

Part of the modified print statement from *v1_tpa.out* is shown for Realization 15:

```
layer #  1  is type  2
layer #  2  is type  1
layer #  3  is type  2
layer #  4  is type  2
layer #  5  is type  2
layer #  6  is type  2
layer #  7  is type  2
Layer #  1  matrix conductivity =  8.268961680000000E-05
Layer #  2  matrix conductivity =  8.262565416000001
Layer #  3  matrix conductivity =  1.885834717200000E-03
Layer #  4  matrix conductivity =  5.794654005000000E-03
Layer #  5  matrix conductivity =  1.081521189000000E-03
Layer #  6  matrix conductivity =  1.206634212000000E-04
Highest matrix conductivity =  8.262565416000001  in layer  2
...
kept matrix layer # =  2
```

<u>This result meets Pass/Fail Criterion No. 1.</u>

The equivalent print statement from *v2_tpa.out* for Realization 15 is:

```
layer #  1  is type  2
layer #  2  is type  1
layer #  3  is type  2
layer #  4  is type  2
layer #  5  is type  2
layer #  6  is type  2
layer #  7  is type  2
Layer #  1  matrix conductivity =  8.268961680000000E-05
Layer #  3  matrix conductivity =  1.885834717200000E-03
Layer #  4  matrix conductivity =  5.794654005000000E-03
Layer #  5  matrix conductivity =  1.081521189000000E-03
Layer #  6  matrix conductivity =  1.206634212000000E-04
Highest matrix conductivity =  5.794654005000000E-03  in layer  4
...
kept matrix layer # = 4
```

Note that because there is no CHnv (layer #2) in v*2_tpa.inp*, the layer with highest matrix conductivity is the PPw (layer #4), which is kept as the matrix layer. <u>This result satisfies Pass/Fail Criterion No. 1.</u>

A bypass fraction was indicated for the water flux in every realization in *v2_tpa.out*. The calculation of the bypass fraction was checked as indicated below for some of the infiltration rates from Realization 23:

```
Layer #   4  matrix conductivity =   1.007541542700000E-02
```

Matrix Conductivity (layer #4) = 1.007542E-02					
Infiltration	Matrix Conductivity / Infiltration	Calculated Bypass Fraction*	Output from *v2_tpa.out*	Infiltration	Bypass Fraction
1.41E-02	0.7154	0.284603	infil	1.41E-02	0.284603
2.22E-02	0.4537	0.546314	infil	2.22E-02	0.546314
3.08E-02	0.3272	0.672837	infil	3.08E-02	0.672837
4.40E-02	0.2291	0.770869	infil	4.40E-02	0.770869
4.92E-02	0.2048	0.795191	infil	4.92E-02	0.795191
5.04E-02	0.2001	0.799897	infil	5.04E-02	0.799897
5.22E-02	0.1931	0.806949	infil	5.22E-02	0.806949
6.69E-02	0.1507	0.849349	infil	6.69E-02	0.849349
7.32E-02	0.1377	0.862292	infil	7.32E-02	0.862292

*Bypass fraction calculation = 1.0 - (matrix conductivity / infiltration)

All calculations agree with data in the output file. This result satisfies Pass/Fail Criterion No. 2.

To check that UZFT correctly changes the thickness of the kept matrix layer if travel time through that layer would otherwise be less than 20 years, the parameters in *v2_tpa.inp* were reset in *v3_tpa.inp* as follows:

Parameter as set in *v2_tpa.inp*	Changes in *v3_tpa.inp*	Remarks

`iconstant`
`StartAtRealization`
`15`
	`iconstant`
	`StartAtRealization`
	`23`	

`iconstant`
`StopAtRealization`
`24`
	`iconstant`
	`StopAtRealization`
	`23`	

`constant`
`PPw_Thickness_6SubArea[m]`
`47.7`
	`constant`
	`PPw_Thickness_6SubArea[m]`
	`0.05`
		Make the 'kept matrix layer' so thin that travel time through it is less than 20 years.

The following print statement was obtained in *v3_tpa.out*:

```
kept matrix layer # =   4
travel time =   4.999999999999999
reset leg length =   0.2002000000000000
```

With a specified thickness of 0.05 m for the PPw (layer #4) in *v3_tpa.inp*, the calculated average groundwater travel time through the layer is only 4.999 years, so UZFT resets the leg length to obtain the target minimum travel time (20 years):

$$0.05 \times 20 / 4.999 = 0.200$$

The adjusted leg length of 0.200 m ensures that the matrix layer is kept for transport calculations. Note that, in the current reference case *tpa.inp* file does not include such thin layers (e.g., distributions for CHnv are user supplied discrete distributions that include zero thickness but no values between zero and 2.5 m).

This result meets Pass/Fail Criterion No. 3.

Test 12-1: Status (PASS/FAIL): PASS.

Test 12-2: Colloid Filtration Factors

Test 12-2 Description: The transport of radionuclides that are irreversibly attached (J-species) to colloids depends on the transport fate of the colloids themselves. The model assumes that due to size restrictions, a fraction of the colloids are filtered out by flow through the rock matrix in the unsaturated zone. The validation test is designed to verify that (i) only the layers with non-zero thickness are used in determining which layer has the highest colloid filtration factor, and (ii) the colloid filtration factor used in the calculations is the one with the highest value among the existing (non-zero thickness) layers [Note that higher values filtration factor values result in less removal: e.g., 1 = no removal; 0.0 = total removal]. Where flux splitting occurs because no matrix layer can handle all of the flow, the test is designed to verify that (iii) the colloid filtration factor for the CHnv layer is applied to the "bypass fraction" of the flux.

Test 12-2 Objectives: In Test 12-2, Run 1, the objective is to confirm that colloid filtration is appropriately applied based on the hydrostratigraphic layer, of those present (i.e., non-zero thickness) in the subarea, that has the highest colloid filtration factor value. In Test 12-2, Run 2, the objective is to confirm that the colloid filtration factor for the CHnv layer is applied to the bypass fraction of flow if there is flux splitting at a particular timestep.

Test 12-2 Output files to compare or examine: Screen print (*tpa.out*), *ebscld.out, nefiiuz.src*

Test 12-2 Run 1: **Select and apply colloid filtration factor based on layers present.**
The purpose of this run is to make sure that the highest value for the colloid filtration factor is selected from all UZ layers with non-zero thickness.

Test 12-2 Run 1: Step-by-step test procedure:

1. Change *tpa.inp* to run only subarea 1 by setting the following values

```
iconstant
StartAtSubarea
1
**
iconstant
StopAtSubarea
1
```

2. Set initial defective fraction to 1.0 to ensure there would be some releases.

```
constant
DefectiveFractionOfWPs/cell
1.0
```

3. Set thickness of Calico Hills vitric unit for subarea 1 to constant of 10 m to make sure a zero thickness did not get sampled. Also changed BFw and UFZ thicknesses from zero to 10 m so that all layers would have a non-zero thickness.

```
constant
CHnvThickness_1SubArea[m]
10
**
constant
```

```
CH_Total_Thickness_1SubArea[m]
108.0
**
**
constant
PPw_Thickness_1SubArea[m]
43.1
**
constant
UCF_Thickness_1SubArea[m]
44.8
**
constant
BFw_Thickness_1SubArea[m]
10.0
**
constant
UFZ_Thickness_1SubArea[m]
10.0
```

4. Set filtration factors for each layer to values that are significantly different from eachother to facilitate being able to tell which value was used by looking at plots of colloids released from the EBS versus colloids that leave the UZ.

```
constant
PermanentLossColloidFilterFactor_TSw_[]
0.1
**
constant
PermanentLossColloidFilterFactor_CHnv[]
0.2
**
constant
PermanentLossColloidFilterFactor_CHnz[]
0.3
**
constant
PermanentLossColloidFilterFactor_PPw_[]
0.4
**
constant
PermanentLossColloidFilterFactor_UCF_[]
0.5
**
constant
PermanentLossColloidFilterFactor_BFw_[]
0.6
**
constant
PermanentLossColloidFilterFactor_UFZ_[]
0.7
```

5. Set output mode to Append All Files.

```
iconstant
OutputMode(0=None,1=All,2=UserDefined)
1
```

6. Run the code with the above parameter changes. Determine how much colloid filtration occurred by taking the ratio of filtered colloid releases to the colloids released from the EBS. The filtered colloid releases can be obtained by examining the releases specified for J-Species in the *nefiiuz.src* file. The colloids released from the EBS can be obtained from the *ebscld.out* file.

7. Output data described in step 6 will be imported into a spreadsheet named *P12_Test2_Run1.xls*, and the filtration factor will be calculated for all J-species that had releases from the EBS during the simulation period. .

8. As an additional test, after obtaining results for step 7, step through the layer thicknesses listed in step 3, setting them to zero one by one, beginning by setting the UFZ layer and moving up the list, and rerunning the code after each layer is set to zero. There is no need for a spreadsheet on this test; just spot check the J-species colloid concentrations in the *nefiiuz.src* and *ebscld.out* files. With the above parameters, the result should be that the filtration ratio should be 0.6 when UFZ layer is set to zero, 0.5 when the BFw layer is also zero; 0.4 when the UCF layer is also set to zero; 0.3 when the PPw layer is also set to zero; 0.2 when the CHnz layer is also set to zero; and 0.1 when the CHv layer is also set to zero.

Test 12-2 Run 1: Pass/Fail Criteria
Based on the input values specified above, the calculated filtration factor should be 0.7 for all J-species.
Test 12-2 Run 1: Results
A calculated colloid filtration factor of 0.7 was obtained for all J-species. This result conforms to the parameter values specified in *tpa.inp*. Relevant input and output files for step 7 are archived in a folder called *P12_Test 2_Run1* of the storage media disk described on the cover sheet of this report. This folder also contains a spreadsheet called *P12_Test2_Run1.xls* that shows the filtration factors for each J-Species calculated in step 7.

Test 12-2 Run 1: Status (PASS/FAIL): PASS.

Test 12-2 Run 2: Apply colloid filtration factor to flux splitting.
The purpose of this test is to make sure that the colloid filtration factor for the CHnv layer is applied to the "bypass fraction" for subarea realizations in which no matrix layer can handle all of the flow. The following steps were applied for this test.

1. Beginning with the *tpa.inp* file changes described for the preceding Run 1, set the matrix permeability values for all layers to very low values such that effectively all flow will be sent to the bypass fraction.

```
constant
MatrixPermeability_TSw_[m2]
1e-19
**
constant
MatrixPermeability_CHnv[m2]
```

```
1e-19
**
constant
MatrixPermeability_CHnz[m2]
1e-19
**
constant
MatrixPermeability_PPw_[m2]
1e-19
**
constant
MatrixPermeability_UCF_[m2]
1e-19
**
constant
MatrixPermeability_BFw_[m2]
1e-19
**
constant
MatrixPermeability_UFZ_[m2]
1e-19
**
```

2. Run TPA code and capture screen print in *tpa.out*. The screen print can be used to ensure nearly all source release is bypassing the UZ by comparing “Highest Release Rate from Sub Area 1" and “Highest Release Rate from UZ” and to make sure release rates [Ci/yr] for the non-colloids species released from the UZ are at least 99 percent of the Subarea release, and also making sure the times of peak releases are identical to four significant figures.

The following excerpt from *tpa.out* output was obtained, demonstrating that this was achieved.

```
                 Highest release rates from Sub Area 1
             Am241   2.0528E-01 [Ci/yr/SA] at  1.723E+03 yr
             Tc99    1.3680E-01 [Ci/yr/SA] at  2.094E+03 yr
             Am243   4.8989E-02 [Ci/yr/SA] at  5.564E+03 yr
             Ni59    1.0607E-02 [Ci/yr/SA] at  3.635E+03 yr
             Cs135   3.1049E-03 [Ci/yr/SA] at  3.076E+03 yr
             Ja241   1.8928E-03 [Ci/yr/SA] at  1.723E+03 yr
exec: calling uzft
                     Highest release rates from UZ
             Am241   2.0323E-01 [Ci/yr/SA] at  1.723E+03 yr
             Tc99    1.3556E-01 [Ci/yr/SA] at  2.602E+03 yr
             Am243   4.8615E-02 [Ci/yr/SA] at  5.564E+03 yr
             Ni59    1.0522E-02 [Ci/yr/SA] at  3.635E+03 yr
             Cs135   3.0790E-03 [Ci/yr/SA] at  3.076E+03 yr
             Ja241   1.4991E-03 [Ci/yr/SA] at  1.723E+03 yr
```

From the above numbers, the ratio of UZ releases to EBS (Sub Area 1) releases for non-colloids such as Tc99 and Cs135 is 0.991. Because Cs135 would have been retarded to some extent by sorption if there had been significant transport through the matrix, the similarility in releases from the EBS and the UZ indicates that more than 99 percent of the radionuclides bypassed the unsaturated zone. The results from *tpa.out* above also show that the peak release times are identical (no retardation).

3. Compare the colloid release rates reported in the *nefiisz.src* (output from the UZ is the source for the SZ) and *ebscld.out* files to calculate the colloid filtration factor that was applied. The change implemented in SCR 685 was that the colloid filtration factor for the CHnv layer should be applied to the bypass fraction. Based on the values used in *tpa.inp* for this test, 20 percent of the colloids that were bypassed should be removed from filtration. For simplification purposes, it is assumed, based on the information developed from step 2, that the bypass fraction is 0.991. The filtration factor for the bypass fraction was calculated in a spreadsheet named *P12_Test2_Run2.xls*. The filtration factor was calculated as 1-(UZ Release)/(EBS Release*0.991).

Test 12-2 Run 2: Pass/Fail Criteria
Based on the input data provided, the colloid filtration factor applied to the UZ bypass fraction should be very close to 0.2. This number may not be exact because the fraction of bypass changes slightly during the simulation as the infiltration rate increases and because the UZ release at later times may include a small fraction of mass that was transported through the matrix in the unsaturated zone. Values between 0.195 and 0.205 would generally indicate that the appropriate filtration is being applied to the bypass fraction.

Test 12-2 Run 2: Results
Briefly, the results obtained were as described in the above PASS/FAIL Criteria. The results contained in the spreadsheet *P12_Test 2_Run2.xls* indicate that all of the calculated filtration fractions were between 0.199 and 0.201, conforming to the expectation that 20 percent of colloids were being removed from the bypass fraction in the unsaturated zone.

Relevant input and output files for this test are archived in a folder called *P12_Test2_Run2* of the storage media disk described on the cover sheet of this report. This folder also contains a spreadsheet called *P12_Test2_Run2.xls* that shows the filtration factors for each J-Species calculated in step 3 of this test.

Test 12-2 Run 2: Status (PASS/FAIL): PASS.

Test 12-3:Sorption Coefficients and Retardation Factors

Test 12-3 Description: In each realization, matrix sorption coefficients (K_D) are calculated for the actinides Am, Np, Pu, Th, U, and Cm, from the relationship

$$K_D = (K_A * 3 * MatrixPorosity) / \{MatrixGrainDensity * (1 - MatrixPorosity) * MatrixPoreRadius\}$$

where K_A is determined from the expression

$$Log\, K_A = a + b\, pH + c\, pH^2 + d\, pH^3 + e\, pH^4 + f\, pH^5$$

and the coefficients *a–f* are listed, for specific values of PCO_2 and pH, in the file *coefkdeq.dat* for each actinide. Also in each realization, matrix retardation factors are calculated for all radionuclides, including the actinides, from the expression

$$R_D = 1 + \{MatrixGrainDensity * (1 - MatrixPorosity) * K_D\} / MatrixPorosity$$

Retardation factors are further adjusted to account for reversible colloid transport by

$$R_D^{eff} = \{R_D + (C_C\, F\, K_D\, R_C)\} / (1 + C_C\, F\, K_D)$$

where

R_D^{eff}	--	Effective retardation factor for a particular radionuclide in the presence of colloids (reversible sorption)
R_D	--	Retardation factor for a particular radionuclide in the absence of colloids
C_C	--	Colloid concentration (MatrixColloidConcentration)
F	--	SurfaceAreaFactor
R_C	--	Retardation factor specifically associated with colloid transport, MatrixColloidRetardationFactor

Retardation factors for sorption in fractures are calculated, based on an assumed constant-aperture fracture, as

$$R_D = 1 + \left(\frac{2K_A}{b}\right) f$$

where

R_D	—	Retardation factor for a specified radionuclide in the absence of groundwater colloids [unitless]
K_A	—	Surface area normalized distribution coefficient [m^3/m^2]
b	—	Fracture aperture [m]
f	—	Fracture force factor, as specified by the *tpa.inp* parameter UZFractureForceFactorForKdToRd [unitless]

The purpose of this test is to verify, by hand calculation, that the sorption coefficients and retardation factors are calculated correctly and that they are reported correctly in *uz_kdrd.out* and *uz_revers.out*.

Test 12-3 Objective: The objective is to confirm the following results:

1. Calculated sorption coefficients and retardation factors for the actinides Am, Np, Pu, Th, U, and Cm are correctly reported in *uz_kdrd.out*.
2. Retardation factors are correctly adjusted to account for reversible colloid transport and are correctly reported in *uz_revers.out*.
3. Different actinide release rates from the unsaturated zone are calculated for otherwise-identical cases that involve (i) matrix sorption and reversible colloid transport, and (ii) matrix sorption without reversible colloid transport.

Test 12-3 Output files to compare or examine: Screen print (*tpa.out*), *uz_kdrd.out*, *uz_revers.out*.

Test 12-3 Step-by-step test procedure to be used:

1. Execute a realization that includes a matrix layer and a fracture layer, adjusting layer thicknesses or permeabilities in *tpa.inp* if necessary until the desired result is obtained.
2. After Step 1 is successfully executed, prepare a new *tpa.inp* file using the *tpameans.out* file that was generated by Step 1. (This ensures that all parameter values in the later test cases will be shown as constants in *tpa.inp*. As a result, no parameters in the subsequently modified test cases will have different sampled values except where explicitly changed by the user.)
3. In the *tpa.inp* file for this realization, change the parameter PermanentLossColloidFilterFactor to a value of 1.0 for all layers. (This will filter out all irreversible (J-species) colloids so that none are released from the unsaturated zone, so that only the effect of reversibly sorbed species is examined in the test.)
4. In the *tpa_include.inp* file, change the parameter distribution type to "constant" for LogCO2PartialPressure_AllUZ_SZLayers[atm] and change the value to -2.5. Change the parameter distribution type to "constant" for pH_AllUZ_SZLayers[StandardUnits] and change the value to 7.85 (the median pH value).
5. Execute the realization, using the modified data files from Steps 2 and 3. This is Test Case A.
6. Hand-check the calculations for K_D and R_D and compare them with the reported values in *uz_kdrd.out*.
7. Hand-check the calculations for R_D^{eff} and compare them with reported values in *uz_revers.out*.
8. Using a copy of the Test Case A *tpa.inp* file, change the parameter MatrixColloidConcentration to a value of 0.0 for all layers. This removes the effect of colloid transport from the calculations, so there is no retardation of radionuclides reversibly attached to colloids.
9. Execute the realization, using the modified data file from Step 7. This is Test Case B.
10. Compare actinide releases from *tpa.out* for Test Case A and Test Case B.
11. Using a copy of the Test Case A tpa.inp file, set UZFractureForceFactorForKdToRd to a value of 1.0 to allow sorption in fractures. As a result of this change, retardation factors (RD) other than 1.0 will be calculated for the actinides and are reported in uz_kdrd.out.

Effective retardation factors, RDeff, are calculated and reported in uz_revers.out for any layers used in the NEFTRAN II calculations. This is Test Case C.

Test 12-3 Pass/Fail criteria:

1. For Test Case A, compare the hand-calculated values for K_D and R_D with the reported values in *uz_kdrd.out*. The hand-calculated values should be the same as those in the output file.
2. For Test Cases A and C, compare the hand-calculated values for R_D^{eff} with the reported values in *uz_revers.out*. The hand-calculated values should be the same as those in the output file.
3. The format of *uz_kdrd.out* should include K_D values for matrix conditions for Cm, Am, Np, Pu, Th, and U for all seven hydrostratigraphic layers in the unsaturated zone, and it should include K_D and R_D values for fracture conditions for all seven layers.
4. The format of *uz_revers.out* for Test Case A should include R_D^{eff} for matrix conditions and for fracture conditions for the layers used in NEFTRAN II transport calculations.
5. Test Case A and Test Case B should have different actinide release rates.

Test 12-3 Execution and Results of Test

Steps 1 through 3 in the modified test procedure were carried out using the reference case *tpa.inp* to generate a *tpameans.out* file in which all parameters have constant (mean) values. The input file for Test Case A differed from the reference case *tpameans.out* as follows:

Parameter in reference case	Changes in *tpa_12-3A.inp*

`iconstant`
`StartAtSubarea`
`1`
	`iconstant`
	`StartAtSubarea`
	`9`

`iconstant`
`StopAtSubarea`
`0`
	`iconstant`
	`StopAtSubarea`
	`9`

`iconstant`
`StartAtRealization`
`1`
	`iconstant`
	`StartAtRealization`
	`25`

`iconstant`
`StopAtRealization`
`1`
	`iconstant`
	`StopAtRealization`
	`25`

`iconstant`
`OutputMode(0=None,1=All,2=UserDefined`
`)`
`0`
	`iconstant`
	`OutputMode(0=None,1=All,2=UserDefined`
	`)`
	`1`

`iconstant`
`SelectAppendFiles`
`0`
	`iconstant`
	`SelectAppendFiles`
	`8`

Parameter in reference case	Changes in *tpa_12-3A.inp*
constant uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr] 1.0	constant uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr] 5.832666628567075
constant uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum 1.0	constant uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum 2.050000000000000
loguniform DefectiveFractionOfWPs/cell 1.0e-4, 1.0e	constant DefectiveFractionOfWPs/cell 0.5
constant LogCO2PartialPressureAllUZSZLayers[atm] -2.553930000000000	constant LogCO2PartialPressureAllUZSZLayers[atm] -2.5
constant pH_AllUZ_SZLayers[StandardUnits] 7.851680000000001	constant pH_AllUZ_SZLayers[StandardUnits] 7.85
constant PermanentLossColloidFilterFactor_TSw_[] 0.65	constant PermanentLossColloidFilterFactor_TSw_[] 1.0
constant PermanentLossColloidFilterFactor_CHnv[] 0.57	constant PermanentLossColloidFilterFactor_CHnv[] 1.0
constant PermanentLossColloidFilterFactor_CHnz[] 0.75	constant PermanentLossColloidFilterFactor_CHnz[] 1.0
constant PermanentLossColloidFilterFactor_PPw_[] 0.41	constant PermanentLossColloidFilterFactor_PPw_[] 1.0
constant PermanentLossColloidFilterFactor_UCF_[] 0.51	constant PermanentLossColloidFilterFactor_UCF_[] 1.0
constant PermanentLossColloidFilterFactor_BFw_[] 0.66	constant PermanentLossColloidFilterFactor_BFw_[] 1.0

Parameter in reference case	Changes in *tpa_12-3A.inp*

`constant`
`PermanentLossColloidFilterFactor_UFZ_`
`[]`
`0.0`
	`constant`
	`PermanentLossColloidFilterFactor_UFZ_`
	`[]`
	`1.0`

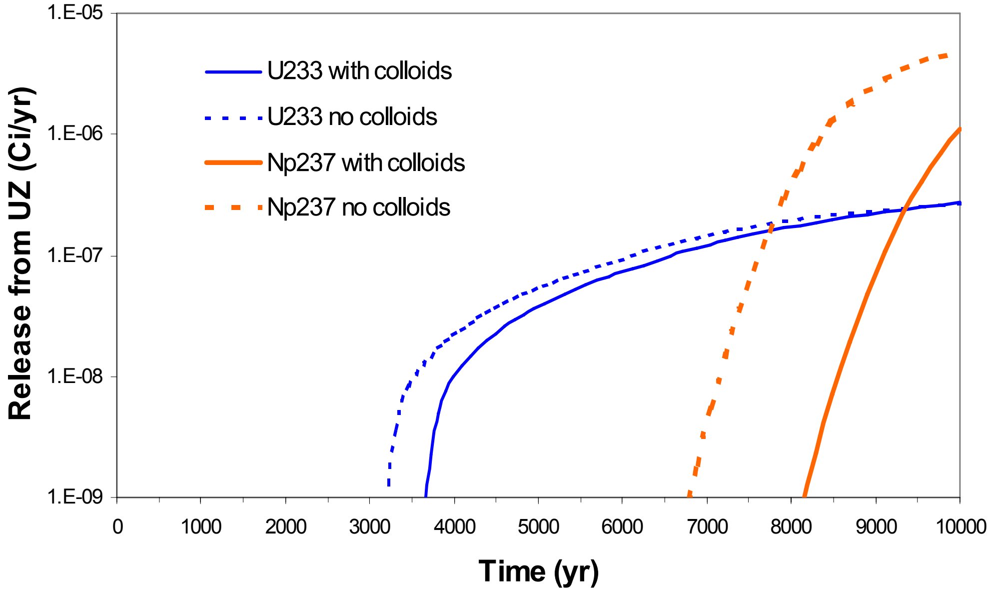
`constant`
`CHnvThickness_9SubArea[m]`
`20.00000000000000`
	`constant`
	`CHnvThickness_9SubArea[m]`
	`4.0`

The results of Test Case A (see Step 5) and Test Case C (see Step 11) were used to complete Steps 6 and 7 in the test procedure. The results of hand calculations for K_D, R_D, and R_D^{eff} and a comparison with the test case output files *uz_kdrd.out* and *uz_revers.out* files are located in the spreadsheet *P12-3 validation checksheet.xls*, which is archived in the folder called *P12Testing\SVT_P12\test3*. The results of all comparisons indicate that the K_D, R_D, and R_D^{eff} values were calculated correctly by UZFT. <u>These results satisfy Pass/Fail Criteria No. 1 and 2</u>.

The *uz_kdrd.out* file lists calculated actinide K_D and R_D values for all seven hydrostratigraphic layers. Although matrix R_D values are not listed explicitly in *uz_kdrd.out*, UZFT calculates the R_D values for the layers that are used in NEFTRAN II transport calculations and uses these values in subsequent R_D^{eff} calculations. The results of the R_D^{eff} calculations are reported by UZFT, in *uz_revers.out*, for retardation (i) in the matrix if matrix flow conditions are assigned to the layer and (ii) in the fractures if fracture flow conditions are assigned to the layer (providing sorption in fractures also has been enabled by setting the parameter UZFractureForceFactorForKdToRd to a value of 1.0). If the actinide R_D is calculated incorrectly by UZFT, then the actinide R_D^{eff} would also be in error. Because the results of all comparisons using Test Cases A and C indicate that the R_D^{eff} values for actinides were calculated correctly by UZFT, it can be inferred that the R_D values are calculated correctly.

Depending on conditions, colloid-associated transport can either enhance or retard the release of radionuclides. <u>These results satisfy Pass/Fail Criteria No. 3 and 4</u>.

Test Case B (*tpa_12-3B.inp*) was identical to Test Case A *(tpa_12-3A.inp*) except that the concentration of colloids in the matrix of all layers was set to zero in *tpa_12-3B.inp*, so the effects of reversible colloid-associated transport are removed from the simulation. A comparison of release rates for two actinides–U233 and Np237–is shown in the figure below, based on a comparison of releases to the saturated zone in *uzft.rlt* for Test Case A (with colloids) and Test Case B (no colloids).



Reversible attachment of U233 and Np237 to colloids delayed their transport through the unsaturated zone compared to transport with no colloids present. <u>These results satisfy Pass/Fail Criterion No. 5</u>.

Test 12-3: Status (PASS/FAIL): PASS.

<u>Test 12-4: NEFTRAN Input File Changes</u>

Test 12-4 Description: The first kept hydrostratigraphic layer in the NEFTRAN II input file, *nefiiuz.inp*, is divided into a repository leg (leg 1) with a specified length and an adjusted kept layer length (leg 2). This test confirms that appropriate adjustments are made to *nefiiuz.inp* as follows:

- The velocity of the first kept layer (either average or time-dependent value) is used for the repository leg velocity.
- The length of the first kept layer from *tpa.inp* is equal to the sum of the repository layer length and the adjusted length of the kept layer.
- The dispersivities of the repository leg and the adjusted first kept layer are consistent with their lengths.

Test 12-4 Objectives: The objectives are to confirm that (i) UZFT supplies either average or time-dependent velocities to NEFTRAN depending on how the UZVelocity parameter is set in *tpa.inp* and (ii) the repository leg properties (length and dispersivity) in NEFTRAN are correctly calculated, based on the properties of the first kept hydrostratigraphic layer (leg) that was selected for use in the transport calculations and based on how the UZVelocity parameter is set in *tpa.inp*.

Test 12-4 Output files to compare or examine: *nefiiuz.inp*, *nefiiuz.out*

Test 12-4 Step-by-step test procedure to be used:

1. Using the reference *tpa.inp* file, execute one realization of the test code in which the CHnv layer is assigned matrix flow properties, as indicated by *nefiiuz.inp*. This input file is <u>Case A-1</u>.
2. Change the value of UZVelocity(0=average,1=time-dependent) in Case A-1 to zero (i.e., use average velocities instead of time-dependent velocities), and execute the code again. This is <u>Case A-2</u>.
3. Examine the layer properties in *nefiiuz.inp* and *nefiiuz.out* obtained from execution of the input files for Case A-1 and Case A-2.
4. Amend Case A-1 by setting the thickness of the CHnv layer to zero in *tpa.inp* to force selection of another UZ layer for matrix flow properties. This is <u>Case B-1</u>.
5. Amend Case B-1 by setting the value of UZVelocity(0=average,1=time-dependent) in *tpa.inp* to zero (i.e., use average velocities instead of time-dependent velocities). This is <u>Case B-2</u>.
6. Examine the layer properties in *nefiiuz.inp* and *nefiiuz.out* obtained from execution of the input files for Case B-1 and Case B-2.

Test 12-4 Pass/Fail criteria:

1. When the tpa.inp parameter UZVelocity(0=average,1=time-dependent) is set to 0, the NEFTRAN input file for UZ calculations will use an average velocity value. When the parameter is set to 1, the NEFTRAN input file will select a time-dependent velocity field.
2. The length of the first kept layer from *tpa.inp* is equal to the sum of the repository layer length and the adjusted length of the kept layer, and the dispersivities of the repository leg and the adjusted first kept layer are consistent with their lengths. When time-dependent field velocities are used, the dispersivity of each leg should be calculated using

its specified leg length, such that *Dispersivity=MatrixLongitudinalDispersivity* x *leg length*. However, when an average velocity is used, the dispersivity of the repository leg (leg 1) should be calculated using the entire thickness of the first kept layer, and leg 2 should use the adjusted length of the layer.

Test 12-4 Execution and Results of Test:
The test procedure was executed as follows:

<u>Case A-1</u> (uses time-dependent velocities, so flag for UZVelocity = 1)

The reference case input file *tpa.inp* was amended to run only one subarea:

```
iconstant
StartAtSubarea
9

iconstant
StopAtSubarea
9

iconstant
StartAtRealization
25
**
iconstant
StopAtRealization
25
```

Subarea 9 was selected because it has non-zero thicknesses for all hydrostratigraphic layers except UFZ, the hypothetical fault zone (Table P12-4.1). The UFZ layer is a special case that was not considered in this validation test.

Table P12-4.1 Hydrostratigraphic Layer Thicknesses in Subarea 9

Parameter Name	*tpa.inp* Reference Value	Amended (Case A)	Amended (Case B)
TSw_Thickness_9SubArea[m]	constant 140.4		
CHnvThickness_9SubArea[m]	usersupplieddiscrete 4 4, 0.6 20, 0.1 50, 0.1 70, 0.2	constant 4.0	constant 0.0
CH_Total_Thickness_9SubArea[m]	constant 104.0		
PPw_Thickness_9SubArea[m]	constant 46.2		
UCF_Thickness_9SubArea[m]	constant 33.0		
BFw_Thickness_9SubArea[m]	constant 5.0		

Parameter Name	*tpa.inp* Reference Value	Amended (Case A)	Amended (Case B)
`UFZ_Thickness_9SubArea[m]`	`constant` `0.0`		

The Calico Hills nonwelded vitric (CHnv) layer was assigned a constant thickness of 4.0 m in Case A to (i) facilitate identification of this layer in *nefiiuz.inp* and (ii) keep the sampling of all other parameters unchanged when the CHnv layer thickness was changed to zero for Case B.

The number of defective waste packages was set in *tpa.inp* to a constant value large enough to ensure enough releases from EBS so that UZFT would be called:

```
constant
DefectiveFractionOfWPs/cell
0.5
```

The parameter UZVelocity(0=average,1=time-dependent) was left at the reference case value of 1 for Case A-1, so time-dependent velocities were supplied to NEFTRAN.

<u>Case A-2</u> was identical to Case A-1, except it sends average velocities to NEFTRAN instead of time-dependent velocities by setting:

```
iflag
UZVelocity(0=average,1=time-dependent)
0
```

The pertinent results of Case A-1 are as follows:

From *nefiiuz.inp*:

```
                    NETWORK LEG PROPERTIES ARRAY
LEG   INLET  OUTLET     LENGTH     AREA     HYDRAULIC    BRINE
 #     JCT     JCT        (M)      (M**2)    K   (M/YR)    CONC.
 1       1       2        1.0        0.0        0.0        0.0
 2       2       3      139.4        0.0        0.0        0.0
 3       3       4        4.0        0.0        0.0        0.0
                                MIGRATION PATH PROPERTIES ARRAY
LEG    DISPERS.     SPA. STEP  DIFFUS   MOBILE   IMMOB    MASS  XFER    VELOCITY
 #       (M)         (M)      N/Y=0/1   POROS.   POROS.   COEF(1/Y)       (M/YR)
  1 0.6000E-01      0.0        0     0.300E-01   0.000E+00   0.000E+00    0.575E+01
  2 0.8364E+01      0.0        0     0.300E-01   0.000E+00   0.000E+00    0.575E+01
  3 0.2400E+00      0.0        0     0.320E+00   0.000E+00   0.000E+00    0.759E-01
```

From *nefiiuz.out*:

```
                        TIME-DEPENDENT VELOCITIES
  Field    Time  (y)     Leg      Velocity     Saturation
  Index                 Index      (m/y)        Fraction

    1          0.0        1      2.14172E+00    1.000E+00
                          2      2.14172E+00    1.000E+00
                          3      2.31676E-02    1.000E+00

    2        500.0        1      3.20094E+00    1.000E+00
                          2      3.20094E+00    1.000E+00
                          3      3.81930E-02    1.000E+00

    3       1000.0        1      4.37746E+00    1.000E+00
```

		2	4.37746E+00	1.000E+00
		3	5.66051E-02	1.000E+00
4	2500.0	1	5.67228E+00	1.000E+00
		2	5.67228E+00	1.000E+00
		3	7.97665E-02	1.000E+00
5	10000.0	1	5.67228E+00	1.000E+00
		2	5.67228E+00	1.000E+00
		3	7.97665E-02	1.000E+00

The pertinent results of Case A-2 are as follows:

From *nefiiuz.inp*:

NETWORK LEG PROPERTIES ARRAY

LEG #	INLET JCT	OUTLET JCT	LENGTH (M)	AREA (M**2)	HYDRAULIC K (M/YR)	BRINE CONC.
1	1	2	1.0	0.0	0.0	0.0
2	2	3	139.4	0.0	0.0	0.0
3	3	4	4.0	0.0	0.0	0.0

MIGRATION PATH PROPERTIES ARRAY

LEG #	DISPERS. (M)	SPA. STEP (M)	DIFFUS N/Y=0/1	MOBILE POROS.	IMMOB POROS.	MASS XFER COEF(1/Y)	VELOCITY (M/YR)
1	0.8424E+01	0.0	0	0.300E-01	0.000E+00	0.000E+00	0.575E+01
2	0.8364E+01	0.0	0	0.300E-01	0.000E+00	0.000E+00	0.575E+01
3	0.2400E+00	0.0	0	0.320E+00	0.000E+00	0.000E+00	0.759E-01

From *nefiiuz.out*:

FOR STEADY-STATE FLOW

LEG NO.	PORE VELOCITY m/y
1	5.7500E+00
2	5.7500E+00
3	7.5900E-02

The leg lengths (layer thicknesses) reported in *nefiiuz.inp* for both cases (A-1 and A-2) indicate that in these examples, two hydrostratigraphic layers are used in the NEFTRAN transport model: TSw ("140.4 m") and CHnv ("4.0 m"). In both cases, the repository leg length in *nefiiuz.inp* is correctly set to 1.0 m, and the thickness of the first hydrostratigraphic layer (TSw) is reduced accordingly to 140.4 m - 1.0 m = 139.4 m in leg 2. The average groundwater travel time through the unsaturated zone in Subarea 9 (from *gwttuzsz.res*) in the Case A simulations is 97.2 years.

Where time-dependent velocities are specified for UZFT (e.g., Case A-1), dispersivity in each layer is calculated as

$$\text{Dispersivity} = \text{MatrixLongitudinalDispersivity} * \text{leg length}$$

In *tpa.inp*, the reference value for MatrixLongitudinalDispersivity[FractionOfLayer] = 0.06 for all layers. Accordingly, hand calculations indicate that the dispersivities in Case A-1 for the legs selected in *nefiiuz.inp* should be:

Leg:	Length (m)	*	MLD	=	Expected Dispersivity for Case A-1
1	1.0	*	0.06	=	0.060
2	139.4	*	0.06	=	8.364
3	4.0	*	0.06	=	0.240

Where average velocities are specified instead of time-dependent velocities (e.g., Case A-2), the dispersivity for the repository leg ("Leg 1") is calculated using the entire thickness of the first hydrostratigraphic layer. For Realization #25, this means that for the repository leg

Dispersivity = MatrixLongitudinalDispersivity * TSw_Thickness_9SubArea[m]

and the dispersivities in Case A-2 should be:

Leg:	Length (m)	*	MLD	=	Expected Dispersivity for Case A-2
1	1.0	*	0.06	=	8.424
2	139.4	*	0.06	=	8.364
3	4.0	*	0.06	=	0.240

These calculated dispersivities agree with the Case A-1 and A-2 values listed in *nefiiuz.inp*. Moreover, the *nefiiuz.out* file shows that in Case A-1, the time-dependent leg 1 (repository leg) velocities are identical to the leg 2 (TSw) velocities, and in Case A-2, the average velocity of leg 1 is identical to the average velocity of leg 2. These are the expected results.

The *tpa.inp* files for Case B-1 and Case B-2 are identical to those used for Case A-1 and Case A-2, respectively, except that in Cases B-1 and B-2 the thickness of the CHnv layer is set to zero:

```
constant
CHnvThickness_9SubArea[m]
0.0
```

For Case B-1 (= use time-dependent velocities), the pertinent results are as follows:

From *nefiiuz.inp*:

```
                    NETWORK LEG PROPERTIES ARRAY
LEG   INLET  OUTLET     LENGTH     AREA     HYDRAULIC    BRINE
 #     JCT     JCT        (M)      (M**2)    K   (M/YR)    CONC.
 1       1       2        1.0        0.0        0.0        0.0
 2       2       3       45.2        0.0        0.0        0.0
                        MIGRATION PATH PROPERTIES ARRAY
LEG    DISPERS.     SPA. STEP   DIFFUS   MOBILE   IMMOB    MASS   XFER    VELOCITY
 #       (M)          (M)      N/Y=0/1   POROS.   POROS.   COEF(1/Y)       (M/YR)
  1  0.6000E-01      0.0        0     0.250E+00   0.000E+00   0.000E+00    0.504E-01
  2  0.2712E+01      0.0        0     0.250E+00   0.000E+00   0.000E+00    0.504E-01
```

From *nefiiuz.out*:

```
                            TIME-DEPENDENT VELOCITIES
    Field     Time  (y)      Leg      Velocity      Saturation
    Index                   Index       (m/y)         Fraction

      1          0.0          1      1.58973E-02     1.000E+00
                              2      1.58973E-02     1.000E+00
```

```
    2        500.0         1      2.71595E-02    1.000E+00
                           2      2.71595E-02    1.000E+00

    3       1000.0         1      4.20236E-02    1.000E+00
                           2      4.20236E-02    1.000E+00

    4      10000.0         1      4.20236E-02    1.000E+00
                           2      4.20236E-02    1.000E+00
```

For Case B-2 (= use average velocities), the pertinent results are as follows:

From *nefiiuz.inp*:

```
          NETWORK LEG PROPERTIES ARRAY
LEG  INLET  OUTLET    LENGTH    AREA    HYDRAULIC   BRINE
 #    JCT    JCT       (M)     (M**2)   K  (M/YR)   CONC.
 1     1      2        1.0       0.0       0.0       0.0
 2     2      3       45.2       0.0       0.0       0.0
                    MIGRATION PATH PROPERTIES ARRAY
LEG  DISPERS.   SPA. STEP  DIFFUS  MOBILE   IMMOB    MASS  XFER    VELOCITY
 #     (M)        (M)     N/Y=0/1  POROS.   POROS.   COEF(1/Y)      (M/YR)
  1 0.2772E+01    0.0        0    0.250E+00  0.000E+00  0.000E+00  0.504E-01
  2 0.2712E+01    0.0        0    0.250E+00  0.000E+00  0.000E+00  0.504E-01
```

From *nefiiuz.out*:

```
          FOR STEADY-STATE FLOW
          ---------------------
          LEG NO.       PORE VELOCITY
                            m/y
             1           5.0400E-02
             2           5.0400E-02
```

In the Case B simulations, note that there are only two legs in *nefiiuz.inp* instead of three. The PPw layer, with a thickness of 46.2 m in Subarea 9 (Table P12-4.1), was identified as the matrix layer for transport calculations because the CHnv layer had zero thickness (i.e., not present). The TSw layer was not included in *nefiiuz.inp* in Case B because the PPw is generally less permeable than the CHnv, so the average groundwater travel time through the unsaturated zone in Subarea 9 (from *gwttuzsz.res*) in the Case B simulations is 959.5 years. This is almost 10 times longer than the equivalent travel time for Case A. The travel time through the TSw in Case B is less than 10 percent of the total travel time, so the TSw layer is not selected as a transport leg.

The hand-calculated dispersivities for the Case B simulations are:

Leg:	Length (m)	*	MLD	=	Expected Dispersivity for Case B-1	Expected Dispersivity for Case B-2
1	1.0	*	0.06	=	0.060	2.772
2	45.2	*	0.06	=	2.712	2.712

These dispersivity calculations agree with the values in *nefii.inp* for Case B-1 and Case B-2.

Test P12-4: Summary of Results and Pass/Fail Criteria

When the *tpa.inp* parameter UZVelocity(0=average,1=time-dependent) was set to 0, the NEFTRAN input file for UZ calculations used an average velocity value for each layer (transport leg), and when the parameter was set to 1, the NEFTRAN input file used a set of a time dependent velocity fields. <u>These results satisfy Pass/Fail Criterion No. 1</u>.

The length of the first kept layer in the NEFTRAN transport calculations was adjusted to equal the sum of the repository layer leg length (leg 1) and the adjusted first kept layer (leg 2). The dispersivity of the repository leg was calculated correctly depending on whether time-dependent velocities or average velocities were used in the transport calculations. <u>These results satisfy Pass/Fail Criterion No. 2</u>.

Test P12-4: Status (PASS/FAIL): PASS.

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 06002.01.354	
Software Name: **Total-system Performance Assessment (TPA)**		Version(s): **5.1betaB, 5.1betaY, 5.1betaX**
Test ID: **P-13**	Test Series Name: **Saturated Zone Flow and Transport**	

Test Method

- ☐ code inspection
- ■ output inspection
- ■ hand calculation
- ■ spreadsheet
- ■ graphical
- ☐ comparison with external code results

Test Objective: See Attachment A.

Test Environment Setup

Hardware (platform, peripherals): Desktop PC

Software (OS, compiler, libraries, auxiliary codes or scripts): Windows 2000; no auxiliary codes or scripts were used other than a spreadsheet for calculations for comparison to code results;

Input Data (files, data base, mode settings): See Attachment.

Assumptions, constraints, and/or scope of test:
Scope is limited to evaluating functionality of SZFT module and its outputs.

Test Procedure: See Attachment A.

Test Results

Location: See CD labeled "TPA Version 5.1 Validation Task P-13."

Test Criterion and Analysis of Results: See Attachment A

Test Evaluation (Pass/Fail): PASS

Notes:

Tester: James Winterle, Paul Bertetti	Date: June 8, 2007

Attachment A

Test Cases for TPA Version 5.1 Process-Level Validation Task P-13
Objectives, Assumptions, Test Procedures

OBJECTIVES

As described in the Software Validation Plan for TPA Version 5.1, Process-Level Task 13 (P-13), the objectives of the test activities described in this attachment are to verify that

1. Releases to the saturated zone for each repository subarea are assigned to the appropriate stream tube in *strmtube.dat* for use in transport calculations.
2. Repository Partition and retardation coefficients are correctly adjusted to account for reversible colloid transport and correctly reported in *sz_revers.out*.
3. Calculated partition and retardation coefficients for actinides are correctly reported in *sz_kdrd.out*.

ASSUMPTIONS

For the purposes of this validation test, it is assumed:

- The input parameters and their distributions supplied by tpa.inp are consistent with the abstractions of the modeled processes.
- Previous validation testing of this module and testing of subsequent SCRs affecting this module have been properly performed and may be cited as evidence of module performance.

TEST CASES:

Three test cases were developed to evaluated the objectives described above. The following sections for Test 1, Test 2, and Test 3 describe the test evaluation criteria, procedures, and results for these three tests.

Test 1: Appropriate Stream Tube Selection and Assignment of Flow Properties for NEFTRAN Transport Calculations

Test 1 Criteria

- Based on repository subarea and streamtube coordinates, SZFT transport calculations for Subareas 1, 6, 7, 8, and 9 should be assigned the Central streamtube; Subareas 2, 3, 4, and 5 should be assigned to the Northernmost streamtube; Subarea 10 should be assigned to the Southernmost streamtube.

- Appropriate porosities should be assigned to each of the three saturated zone transport leg, as follows: (i) inlet below repository leg (leg 1) should be assigned porosity of lowermost nonzero-thickness layer specified for UZFT; (ii) volcanic tuff leg (leg 2) should be assigned the value specified for FracturePorosity_STFF; the alluvium leg (leg 3) should be assigned the value specified for AlluviumTotalPorosity_SAV.

- Groundwater velocity assigned to each transport leg should be correctly calculated.

- Groundwater velocity should be appropriately scaled based on the assigned value of StreamTubeWidthMultiplier[] in *tpa.inp*.

Test 1 Description and Results

TPA Version 5.1betaB was used to verify that the appropriate stream tube for saturated zone flow and transport is properly selected for each subarea. Note that several code modifications have been made since these tests were conducted using TPA Version 5.1betaB, however, as of TPA Version 5.1betaZ, it was verified that no changes have been made to the algorithm that selects saturated zone stream tubes, and no changes have been made to the repository subarea boundaries. Therefore, the test remains valid.

A set of 10 single-realization, single-subarea test runs was conducted—one for each subarea. Prior to running these test runs, the *strmtube.dat* file in the */data* folder and the tuff and alluvium porosities in the *tpa.inp* file was modified so that each of the three stream tubes will produce different but known groundwater travel times in the saturated zone. After each run, the *gwttuzsz.res* file will be reviewed to determine the saturated zone travel time for each subarea depending on the reported groundwater travel time.

The *tpa.inp* file was modified so that the FracturePorosity_STFF, AlluviumMatrixPorosity, and AlluviumTotalPorosity_SAV were set to constant, with a assigned value of 0.1. Other specifications include setting both the Seismic Disruptive Scenario Flag and Drift Degradation Scenario Flag to zero. Additionally, the Distance To Tuff Alluvium Interface was set to 13.0 km.

In order to determine that the velocity of each transport leg is properly scaled based on the value of StreamTubeWidthMultiplier[], the TPA code was run three times for each subarea using specified streamtube width multipliers, 1, 0.5, and 2, respectively (see data folders labeled *SZ-Flow-Test-#a*, *Z-Flow-Test-#b* and *Z-Flow-Test-#c*, where # denotes subarea number). For all transport legs in all subareas, the streamtube input flux was specified at 100m^3/yr/m and streamtube width at 100m. The velocity, as generated in the *nefii.inp* file, was compared with the velocity that was calculated as follows:

Groundwater Velocity = [(streamtube input flux) ÷ [porosity × (streamtube width) × (streamtube width multiplier)]

Based on the calculated velocity, the travel time was then determined using the following equation:

Travel Time Transport Leg = (distance traveled)/(velocity)

The total travel time for each subarea was determined by adding together all the travel times for each leg. Once calculated, the travel time was compared with that determined by the TPA code, as generated in the *gwttuzsz.res* file. Results are displayed in Tables 1–10.

Based on the assigned flux and travel distance values in the modified *strmtube.dat* file, total groundwater travel time for the combined tuff and alluvium legs, with the streamtube width multiplier set to 1, should be approximately 1800 years for the Southern stream tube, 2700 years for the Central streamtube, and 3600 years for the Northern streamtube. Note, however, that the total transport distance and travel time will be longer because SZFT adds a distance for leg 1 equal to the length of a line passing from one side of a subarea to the other, through the centroid, in the direction of the streamtube. SZFT also adds length to transport leg 2 equal to the distance from the downstream end of the leg 1 line to the downstream end of the repository. Based on visual inspection of the repository subarea boundaries and the streamtube geometry definitions, it was determined that the distances computed for leg 1 and leg 2 in tables 1–10 are correctly calculated.

Based on anticipated transport distances discussed in the preceding paragraph and the calculated transport distances in Tables 1–10, it can be seen that, as expected, Subareas 1, 6, 7, 8, and 9 were assigned the Central streamtube; Subareas 2, 3, 4, and 5 should be assigned to the Northernmost streamtube; Subarea 10 should be assigned to the Southernmost streamtube.

Tables 1–10 also show that velocities and groundwater travel times are correctly calculated and correctly scaled in proportion to the assigned value of the streamtube width multiplier. It is noted that the calculated travel time values in *gwttuzsz.res* do not include the travel distance for leg 1, even though this distance is considered in the radionuclide transport calculations.

The TPA code was also run to determine the unsaturated layer in which the mobile porosity of leg 1 was assigned to in a particular subarea, which is reported in the *nefii.inp* file. By comparing the mobile porosity value with the last non-zero thickness for a particular subarea, it can be determined whether the porosity for leg 1 is assigned correctly. Subareas 3 and 10, representing the northernmost and southernmost subareas, respectively, were selected for this test (see data folders labeled *SZ-Flow-Test-3d* and *SZ-Flow-Test-10d*). For subarea 3, it is revealed in the *tpa.inp* file that the last non-zero thickness value is specified in the PPw_Thickness_3SubArea[m], which was assigned a porosity value 0.04. For subarea 10, the FracturePorosity_BFw was the last layer to possess a non-zero value, which is assigned a porosity value of 0.06. Table 11 summarizes the porosity values assigned for specified unsaturated layers for both subareas 3 and 10 in the tpa.inp file. The nefii.inp file confirms that the porosity value for leg in is 0.04 and 0.06 for subareas 3 and 10, respectively (Table 12).

Test 1 Evaluation (Pass/Fail): PASS

Table 1. Subarea 1. See files: SZ-Flow-Test-1a, SZ-Flow-Test-1b, and SZ-Flow-Test-1c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Cum. Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
1	2 - Central	1	0	1	0.1	0.000256	10	3900	235.7	23.57
		2	19500			0.1		10	20713.8	2071.38
		3	27000			0.1		10	7500	750
	Total Travel Time:									2844.95
	sa1sz (in gwttuzsz.res):									2821.40
1	2 - Central	1	0	0.5	0.1	0.000256	20	3900	235.7	11.79
		2	19500			0.1		20	20713.8	1035.69
		3	27000			0.1		20	7500	375
	Total Travel Time:									1422.48
	sa1sz (in gwttuzsz.res):									1410.70
1	2 - Central	1	0	2	0.1	0.000256	5	3900	235.7	47.14
		2	19500			0.1		5	20713.8	4142.76
		3	27000			0.1		5	7500	1500
	Total Travel Time:									5689.9
	sa1sz (in gwttuzsz.res):									5642.80

Table 2. Subarea 2. See files: SZ-Flow-Test-2a, SZ-Flow-Test-2b, and SZ-Flow-Test-2c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
2	1 - Northernmost	1	0	1	0.1	0.000256	10	3900	399.1	39.91
		2	26000			0.1		10	26851	2685.10
		3	36000			0.1		10	10000	1000
	Total Travel Time:									3725.01
	sa2sz (in gwttuzsz.res):									3685.1
2	1 - Northernmost	1	0	0.5	0.1	0.000256	20	3900	399.1	19.96
		2	26000			0.1		20	26851	1342.55
		3	36000			0.1		20	10000	500
	Total Travel Time:									1862.51
	sa2sz (in gwttuzsz.res):									1842.60
2	1 - Northernmost	1	0	2	0.1	0.000256	5	3900	399.1	79.82
		2	26000			0.1		5	26851	5370.20
		3	36000			0.1		5	10000	2000
	Total Travel Time:									7450.02
	sa2sz (in gwttuzsz.res):									7370.20

Table 3. Subarea 3. See files: SZ-Flow-Test-3a, SZ-Flow-Test-3b, and SZ-Flow-Test-3c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
3	1 - Northernmost	1	0	1	0.1	0.000353	10	2830	832.5	83.25
		2	26000			0.1		10	26361	2636.10
		3	36000			0.1		10	10000	1000
									Total Travel Time:	3719.35
									sa3sz (in gwttuzsz.res):	3636.10
3	1 - Northernmost	1	0	0.5	0.1	0.000353	20	2830	832.5	41.63
		2	26000			0.1		20	26361	1318.05
		3	36000			0.1		20	10000	500
									Total Travel Time:	1859.68
									sa3sz (in gwttuzsz.res):	1818.10
3	1 - Northernmost	1	0	2	0.1	0.000353	5	2830	832.5	166.50
		2	26000			0.1		5	26361	5272.20
		3	36000			0.1		5	10000	2000
									Total Travel Time:	7438.70
									sa3sz (in gwttuzsz.res):	7272.20

Table 4. Subarea 4. See files: SZ-Flow-Test-4a, SZ-Flow-Test-4b, and SZ-Flow-Test-4c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
4	1 - Northernmost	1	0	1	0.1	0.000353	10	2830	983.2	98.32
		2	26000			0.1		10	26191.6	2619.16
		3	36000			0.1		10	10000	1000
	Total Travel Time:									3717.48
	sa4sz (in gwttuzsz.res):									3619.20
4	1 - Northernmost	1	0	0.5	0.1	0.000353	20	2830	983.2	49.16
		2	26000			0.1		20	26191.6	1309.58
		3	36000			0.1		20	10000	500
	Total Travel Time:									1858.74
	sa4sz (in gwttuzsz.res):									1809.60
4	1 - Northernmost	1	0	2	0.1	0.000353	5	2830	983.2	196.64
		2	26000			0.1		5	26191.6	5238.32
		3	36000			0.1		5	10000	2000
	Total Travel Time:									7434.96
	sa4sz (in gwttuzsz.res):									7238.3

Table 5. Subarea 5. See files: SZ-Flow-Test-5a, SZ-Flow-Test-5b, and SZ-Flow-Test-5c

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
5	1 - Northernmost	1	0	1	0.1	0.000353	10	2830	624.8	62.48
		2	26000			0.1		10	26000	2600
		3	36000			0.1		10	10000	1000
									Total Travel Time:	3662.48
									sa5sz (in gwttuzsz.res):	3600
5	1 - Northernmost	1	0	0.5	0.1	0.000353	20	2830	624.8	31.24
		2	26000			0.1		20	26000	1300
		3	36000			0.1		20	10000	500
									Total Travel Time:	1831.24
									sa5sz (in gwttuzsz.res):	1800
5	1 - Northernmost	1	0	2	0.1	0.000353	5	2830	624.8	124.96
		2	26000			0.1		5	26000	5200
		3	36000			0.1		5	10000	2000
									Total Travel Time:	7324.96
									sa5sz (in gwttuzsz.res):	7200

Table 6. Subarea 6. See files: SZ-Flow-Test-6a, SZ-Flow-Test-6b, and SZ-Flow-Test-6c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
6	2 - Central	1	0	1	0.1	0.00182	10	551	263.5	26.35
		2	19500			0.1		10	20371.8	2037.18
		3	27000			0.1		10	7500	750
	Total Travel Time:									2813.53
	sa6sz (in gwttuzsz.res):									2787.20
6	2 - Central	1	0	0.5	0.1	0.00182	20	551	263.5	13.18
		2	19500			0.1		20	20371.8	1018.59
		3	27000			0.1		20	7500	375
	Total Travel Time:									1406.77
	sa6sz (in gwttuzsz.res):									1393.60
6	2 - Central	1	0	2	0.1	0.00182	5	551	263.5	52.70
		2	19500			0.1		5	20371.8	4074.36
		3	27000			0.1		5	7500	1500
	Total Travel Time:									5627.06
	sa6sz (in gwttuzsz.res):									5574.40

Table 7. Subarea 7. See files: SZ-Flow-Test-7a, SZ-Flow-Test-7b, and SZ-Flow-Test-7c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
7	2 - Central	1	0	1	0.1	0.00182	10	551	548.3	54.83
		2	19500			0.1		10	19849.9	1984.99
		3	27000			0.1		10	7500	750
	Total Travel Time:									2789.82
	sa7sz (in gwttuzsz.res):									2735
7	2 - Central	1	0	0.5	0.1	0.00182	20	551	263.5	27.42
		2	19500			0.1		20	20371.8	992.50
		3	27000			0.1		20	7500	375
	Total Travel Time:									1394.91
	sa7sz (in gwttuzsz.res):									1367.50
7	2 - Central	1	0	2	0.1	0.00182	5	551	548.3	109.66
		2	19500			0.1		5	19849.9	3969.98
		3	27000			0.1		5	7500	1500
	Total Travel Time:									5579.64
	sa7sz (in gwttuzsz.res):									5470

Table 8. Subarea 8. See files: SZ-Flow-Test-8a, SZ-Flow-Test-8b, and SZ-Flow-Test-8c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
8	2 - Central	1	0	1	0.1	0.000256	10	3900	725.6	72.56
		2	19500			0.1		10	19500	1950
		3	27000			0.1		10	7500	750
	Total Travel Time:									2772.56
	sa8sz (in gwttuzsz.res):									2700
8	2 - Central	1	0	0.5	0.1	0.000256	20	3900	725.6	36.28
		2	19500			0.1		20	19500	975
		3	27000			0.1		20	7500	375
	Total Travel Time:									1386.28
	sa8sz (in gwttuzsz.res):									1350
8	2 - Central	1	0	2	0.1	0.000256	5	3900	725.6	145.12
		2	19500			0.1		5	19500	3900
		3	27000			0.1		5	7500	1500
	Total Travel Time:									5545.12
	sa8sz (in gwttuzsz.res):									5400

Table 9. Subarea 9. See files: SZ-Flow-Test-9a, SZ-Flow-Test-9b, and SZ-Flow-Test-9c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
9	2 - Central	1	0	1	0.1	0.00182	10	551	504	50.40
		2	19500			0.1		10	19668.9	1966.89
		3	27000			0.1		10	7500	750
	Total Travel Time:									2767.29
	sa9sz (in gwttuzsz.res):									2716.90
9	2 - Central	1	0	0.5	0.1	0.00182	20	551	504	25.2
		2	19500			0.1		20	19668.9	983.45
		3	27000			0.1		20	7500	375
	Total Travel Time:									1383.65
	sa9sz (in gwttuzsz.res):									1358.40
9	2 - Central	1	0	2	0.1	0.00182	5	551	504	100.80
		2	19500			0.1		5	19668.9	3933.78
		3	27000			0.1		5	7500	1500
	Total Travel Time:									5534.58
	sa9sz (in gwttuzsz.res):									5433.80

Table 10. Subarea 10. See files: SZ-Flow-Test-10a, SZ-Flow-Test-10b, and SZ-Flow-Test-10c.

Subarea	Nearest Streamtube	Transport Leg (Tube Point)	Tube Length (m)	Streamtube Width Multiplier	Assigned Porosity (in tpa.inp)	Mobile Porosity (in nefii.inp)	Calculated Velocity (m/yr)	Velocity (m/yr) (in nefii.inp)	Distance Traveled (m)	Travel Time (yr)
10	3 - Southernmost	1	0	1	0.1	0.00182	10	551	816.4	81.64
		2	13000			0.1		10	13000	1300
		3	18000			0.1		10	5000	500
	Total Travel Time:									1881.64
	sa10sz (in gwttuzsz.res):									1800
10	3 - Southernmost	1	0	0.5	0.1	0.00182	20	551	816.4	40.82
		2	13000			0.1		20	13000	650
		3	18000			0.1		20	5000	250
	Total Travel Time:									940.82
	sa10sz (in gwttuzsz.res):									900
10	3 - Southernmost	1	0	2	0.1	0.00182	5	551	816.4	163.28
		2	13000			0.1		5	13000	2600
		3	18000			0.1		5	5000	1000
	Total Travel Time:									3763.28
	sa10sz (in gwttuzsz.res):									3600

Table 11. Assigned porosity values for specified unsaturated layers. See files: SZ-Flow-Test-3d and SZ-Flow-Test-10d.

Layer (in tpa.inp)	Porosity (in tpa.inp)
FracturePorosity_TSw_	0.01
FracturePorosity_CHnv	0.02
FracturePorosity_CHnz	0.03
FracturePorosity_PPw_	0.04
FracturePorosity_UCF_	0.05
FracturePorosity_BFw_	0.06
FracturePorosity_UFZ_	0.07

Table 12. Last non-zero unsaturated thickness and mobile porosity for leg 1 in each subarea. See files: SZ-Flow-Test-3d and SZ-Flow-Test-10d.

Subarea	Last Non-Zero Unsaturated Layer Thickness (in tpa.inp)	Leg 1 Mobil Porosity (in neffii.inp)
3	PPw_Thickness_3SubArea	0.04
10	BFw_Thickness_10SubArea	0.06

Test 2: Partition coefficients and retardation coefficients are correctly adjusted to account for effects of reversible colloids

Test 2 Criterion

- Retardation factors for tuff and alluvium are correctly adjusted to account for effects of reversible colloids.

Test 2 Description and Results

The reversible colloids algorithm alters the input to the NEFMKS module, as contained in the file *nefiisz.inp*, which is created by SZFT. For the alluvium leg, the retardation factor is altered by the presence of colloids. For the fractured tuff leg, the fracture retardation factor and the dimensionless distribution coefficient in the matrix are altered. In addition, a new parameter that modifies the mass transfer between matrix and fracture is introduced.

TPA Version 5.1betaY was run for a single realization and one subarea using the *tpa_means.inp* file generated by the reference data set with the following changes to parameter values to ensure radionuclide release for transport calculations and to facilitate easy hand calculations.

```
constant
DefectiveFractionOfWPs/cell
 1.0
**
constant
SurfaceAreaFactor_SAV_[]
1000.0
**
constant
SurfaceAreaFactor_STFF[]
1000.0
**
constant
FracturePorosity_STFF
 0.5
**
constant
AlluviumMatrixPorosity_SAV
 0.5
**
constant
ColloidRetardationFactor_SAV_[]
 1000.
**
constant
ColloidRetardationFactor_STFF[]
 1000.
**
constant
ColloidConcentration_SAV_[kg/m3]
 1.0
**
constant
ColloidConcentration_STFF[kg/m3]
 1.0
**
constant
AlluviumMatrixGrainDensity_SAV[kg/m3]
```

```
2000.0
**
constant
ImmobileGrainDensity_STFF[kg/m3]
2000.0
**
constant
ImmobilePorosity_STFF
0.5
**
**
constant
AlluviumTotalPorosity_SAV
 0.50
```

In addition all retardation factors specified in *tpa.inp* for all nonactinide species in mobile and immobile tuff and in alluvium were set to a value of 2.0.

After running the simulation, the values were checked to make sure retardation factor adjustments were properly calculated. The adjustment is determined in SZFT by first calculating a dimensionless colloid distribution coefficient (K_0) using the expression

$$K_0 = \frac{C_c\, F\, \phi_m \left(R_D - 1\right)}{\rho_g \left(1 - \phi\right)}$$

where

ρ_g	—	grain density of the solid phase, ImmobileGrainDensity_STFF[kg/m^3] or AlluviumMatrixGrainDensity_SAV[kg/m^3] = 2000
ϕ_m	—	porosity of the solid phase, ImmobilePorosity_STFF or AlluviumTotalPorosity_SAV [unitless] = 0.5
F	—	dimensionless factor accounting for surface area differences between solid phase and colloid, SurfaceAreaFactor_STFF[ ] or SurfaceAreaFactor_SAV[ ] = 1000
C_c	—	colloid concentration in groundwater, ColloidConcentration_STFF[kg/m^3] or ColloidConcentration_SAV_[kg/m^3] = 1.0
R_D	—	retardation factor for the radionuclide = 2.0

The assigned inputs should yield a value of 0.5 for all K_0.

K_0 is then used to adjust the R_D for each radionuclide using the expression

$$R_D^{eff} = \frac{R_D + \left(K_0\ R_c\right)}{\left(1 + K_0\right)}$$

where

R_c	—	retardation factor for colloids, ColloidRetardationFactor_STFF[ ] or ColloidRetardationFactor_SAV_[ ] [unitless] = 1000

R_D — retardation factor for the radionuclide [unitless] = 2.0

Based on the above equations and input parameter values, the calculated retardation coefficients for all non-actinide species should equal 334.66 for both saturated tuff and alluvium. Inspection of the files *sz_revers.out* and *nefiisz.inp* confirmed the correct calculation was performed for all nonactinide species (Ra, Pb, Cs, I, Tc, Ni, Se, Nb, and Cl); note, however, that the retardation factor was rounded in the *nefiisz.inp* to a value of 335 for input to NEFMKS . Note also that this adjustment is not made to leg 1 of the transport path, which represents the relatively short transport distance beneath the subarea.

The next check was to make sure the matrix diffusion coefficents were correctly adjusted to account for reversible colloid sorption. The unadjusted matrix diffusion rate coefficents should be calculated as

$$\beta = \frac{\phi_s D}{0.28\left(\frac{f}{2n}\right)^2}$$

where the following input values were assigned

D — effective matrix diffusion coefficient, DiffusionRate_STFF [m^2/yr] = 1E-3

f — ImmobilePorosityPenetrationFraction_STFF [unitless] = 1.0

ϕ_s — effective immobile (stagnant) matric porosity [unitless] = 0.5

n — number of fractures per meter, FracturesPerMeter_STFF[1/m] = 0.525

which yields β = 0.00196875

To adjust for effects of reversible colloids the rate coefficient is modified as follows

$$\beta^{eff} = \frac{\beta}{1 + K_0}$$

which is equivalent to β * 0.667. Inspection of *nefiisz.inp* reveals the values for "MASS X-FER MOD FACTOR" are indeed 0.667 for all nonactinide species

The modified matrix retardation factor is calculated from

$$R_D^{eff} = \frac{R_D}{1 + K_0} \tag{12-15}$$

which should yield a value of 1.33. Inspection of *nefiisz.inp* reveals the "IMMOBILE RD" values for the tuff leg (leg 2) are indeed 1.33 for all nonactinide species.

Test 2 Evaluation (Pass/Fail): PASS

Test 3: Calculation of Kd and Rd Values

Test 3 Criteria

- Output values of pH and pCO_2 are consistent with input distributions and correlations.
- K_A values (calculated from output K_D values) for the five actinide species Am, Np, Pu, Th, and U, are consistent with the underlying surface complexation model over the input range of pH and pCO_2 values.
- Output for saturated tuff (STFF) specific surface area is correct.
- Conversion of K_D to R_D values for actinide species are correctly computed.
- Calculated K_D values for Cm and Am are the same (i.e., an intentional simplification in the abstraction is that the calculated coefficient for Am is used also for Cm in transport calculations).

Test 3 Description and Results

TPA Version 5.1BetaX was used to run a 500-realization simulation for Subarea 1 only. TPA outputs file *sz_kdrd.out* and *sz_revers.out*. files were examined and used in spreadsheet calculations to ensure correct calculation of retardation coefficients and to conduct graphical comparisons of output to surface complexation model-predicted curves representing specific area normalized distribution coefficient (KA) values for each of the five actinides over a range of pH and at several CO2 values. The following analysis of results is presented in the order of the above-specified criteria.

<u>Check pH and Log-CO_2 Distribution and Correlation</u>
Output values of pH and Log-CO_2 are reported in the *sz_kdrd.out* file. The *tpa.inp* input files specifies that these outputs should be correlated with a correlation coefficient value of −0.95. The plot in figure 1 shows a regression of pH and Log-CO_2. The calculated correlation coefficient for these values is −0.948088, which is very close to the specified value. Additionally, the output values are within the ranges of user-specified values in the *tpa-include.inp* file.

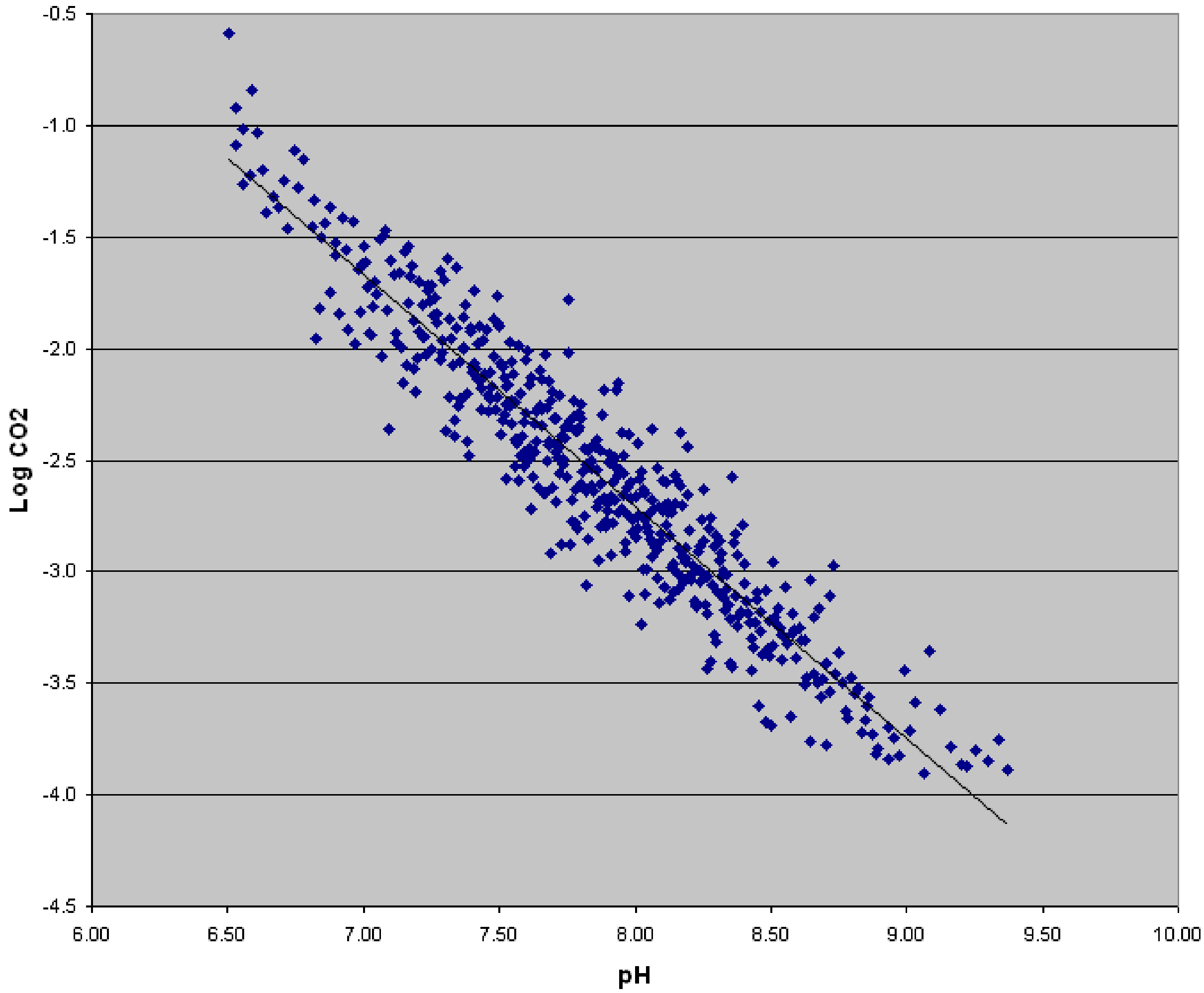


Figure 1. Correlation of pH and Log-pCO_2

<u>Check Calculated K_A Values</u>

The next step was to evaluate whether K_A values for the five actinide species Am, Np, Pu, Th, and U, are consistent with the underlying surface complexation model. This was done by first converting the output K_D values (in m^3/kg) for Am, Np, Pu, Th, and U to K_A values (in ml/m2) by dividing by specific surface area (ssarea) and a factor of 10^{-6}. These K_A values were then compared to the surface complexation model K_A curves for each of the five actinides over a range of pH and pCO_2. The surface complexation model curves are produced by the same data used to generate the information contained within the *coefkdeq.dat* auxiliary file. Generated K_A values for each of the five actinides should plot within the sorption envelope produced by the surface complexation model predicted K_A curves. Note that all K_A values should plot between below the envelope for Log pCO_2 = −4.0 and above the envelope for Log pCO_2 = −0.5. Figures 2–6 below show that the K_A values fit the desired profile and, hence, the K_D properly represent the underlying model. The spreadsheet file named *sz_kdrd_TPA51betaX.xls* contains the calculations for conversion of output data to K_A values and generation of Figures 1–6.

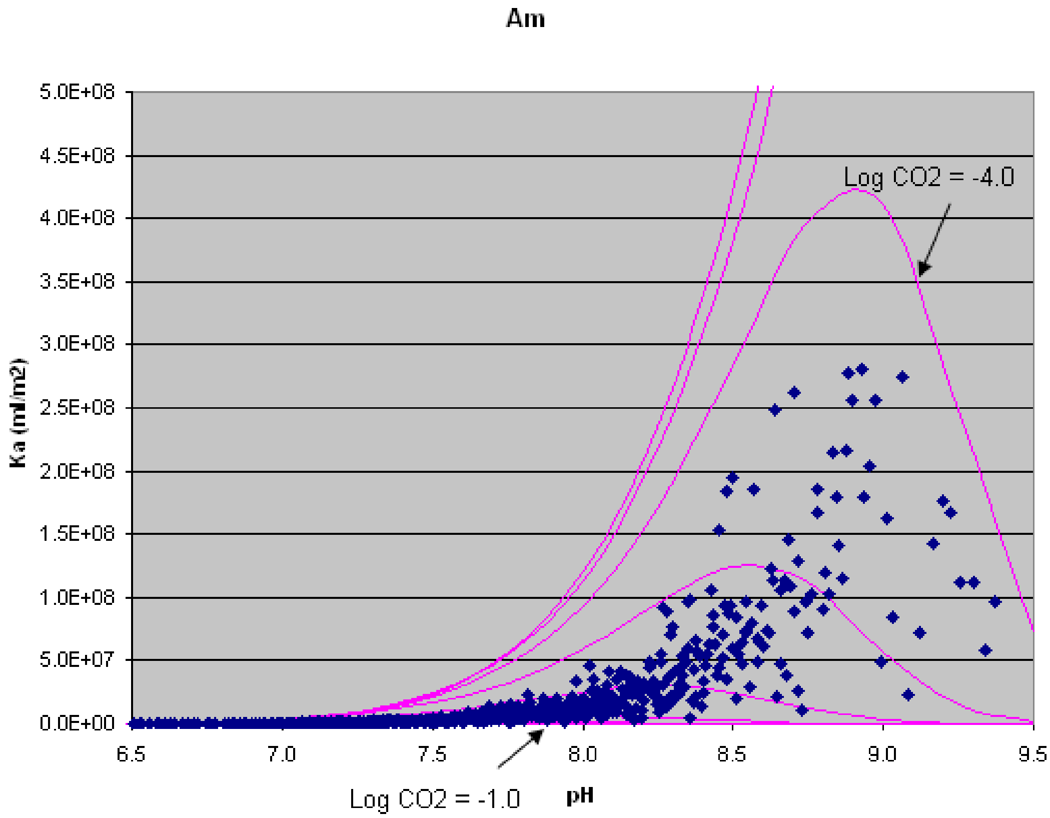


Figure 2. Plot of K_A values for Am, compared to complexation model envelopes.

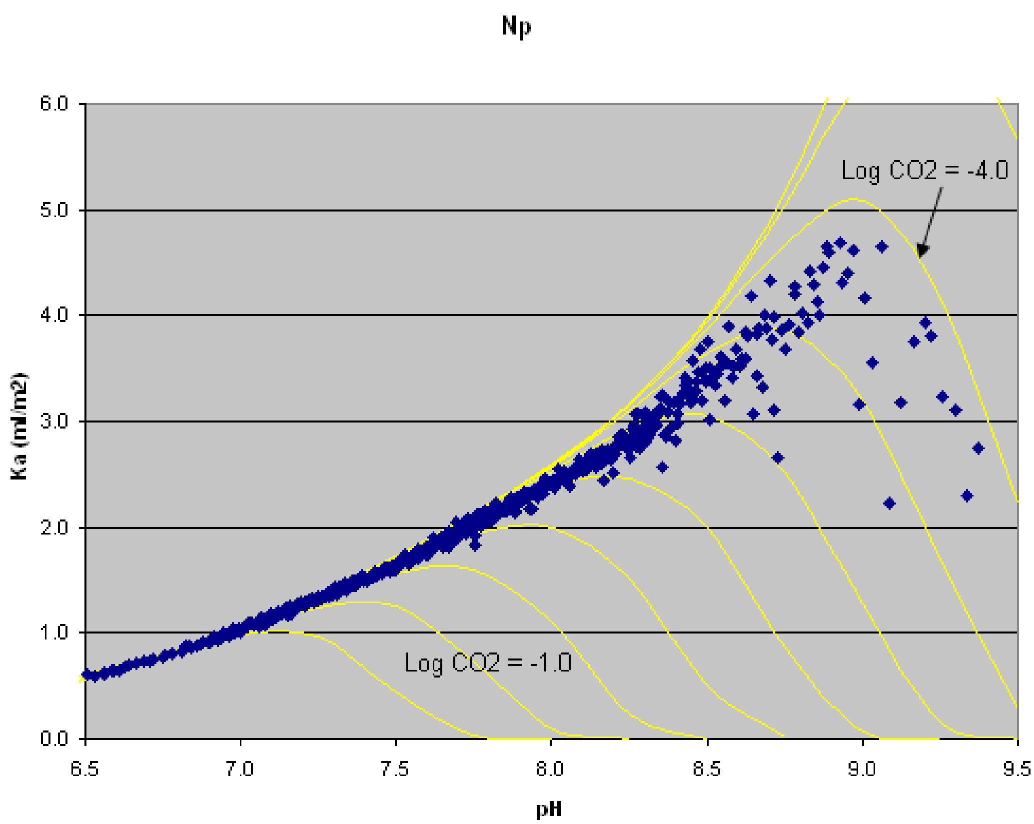


Figure 3. Plot of K_A values for Np, compared to complexation model envelopes.

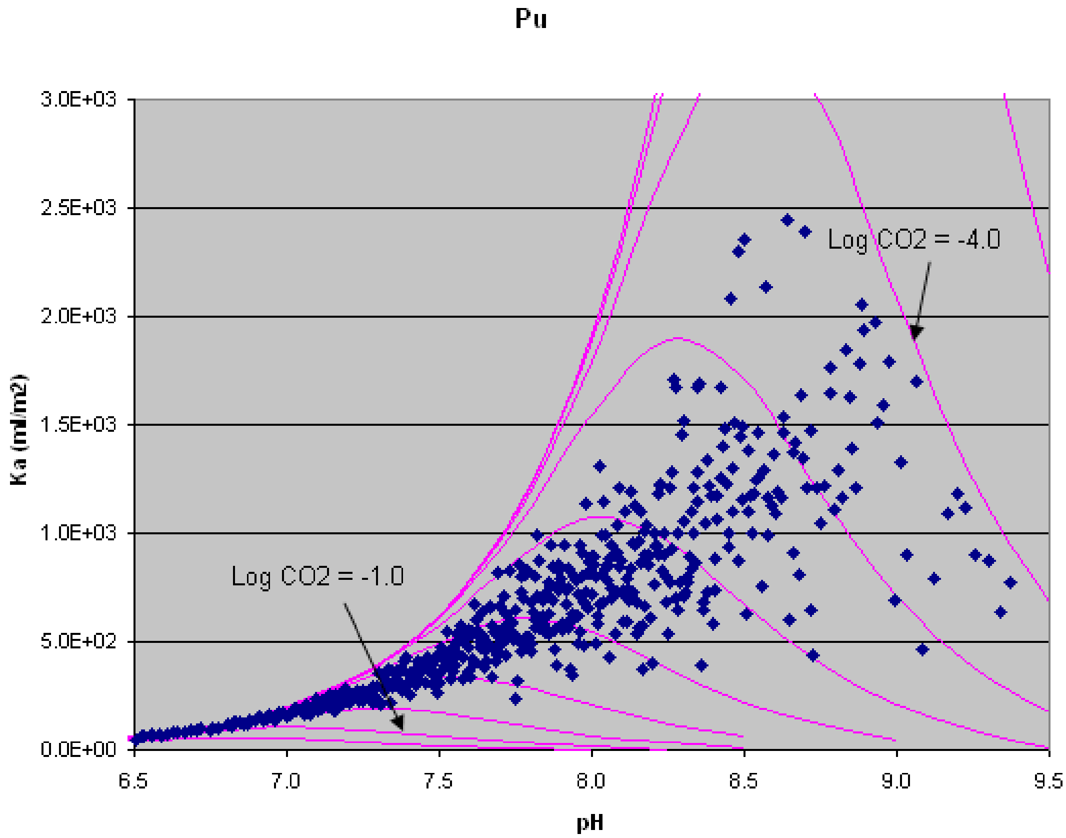


Figure 4. Plot of K_A values for Pu, compared to complexation model envelopes.

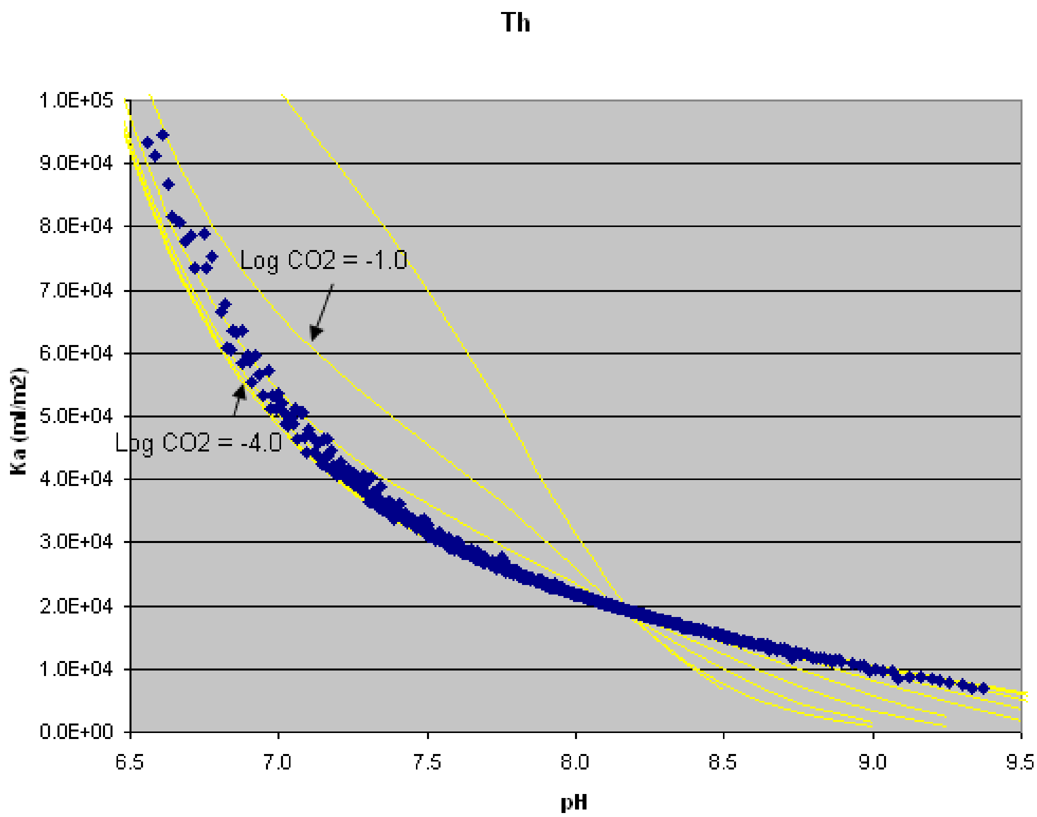


Figure 5. Plot of K_A values for Np, compared to complexation model envelopes.

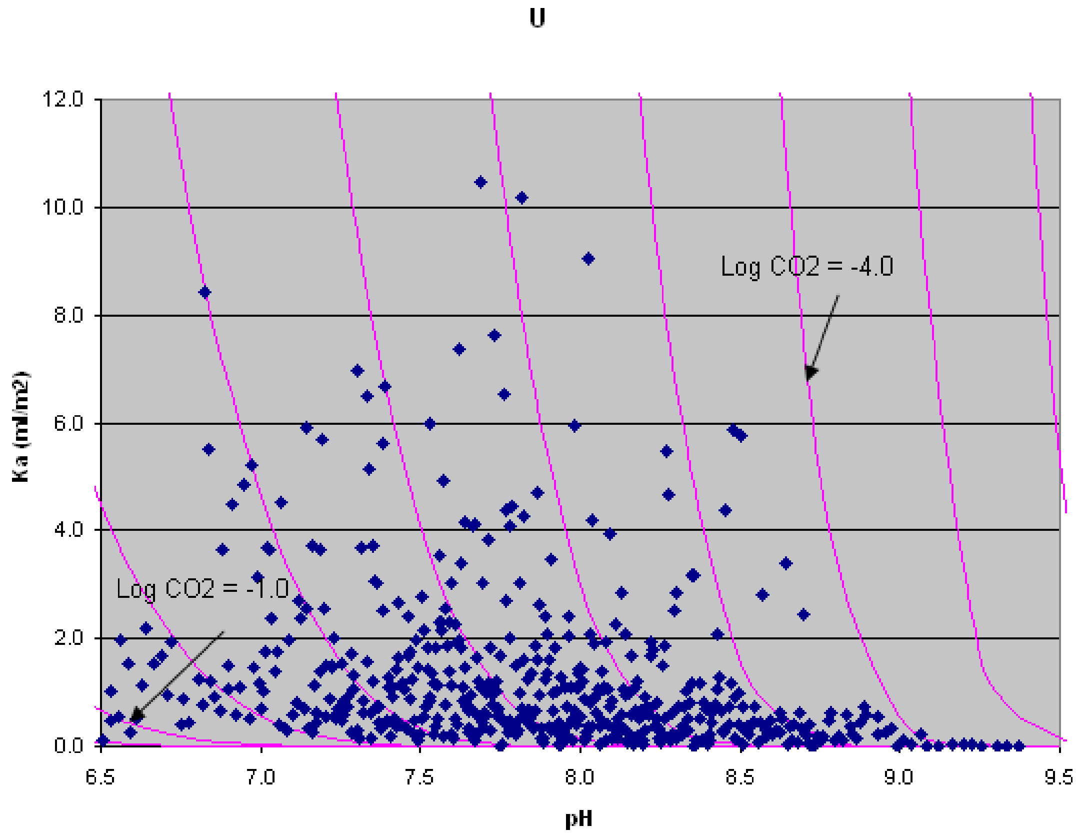


Figure 6. Plot of K_A values for U, compared to complexation model envelopes.

<u>Check Saturated Tuff Specific Surface Area</u>

Calculations to verify that output for saturated tuff (STFF) specific surface area is correct were performed using the equation:

$$SSA = \frac{3\theta}{\rho r}$$

where

SSA = specific surface area (m^2/kg)
θ = porosity (ImmobilePorosity_STFF)
ρ = grain density (kg/m^3) (ImmobileGrainDensity_STFF)
r = pore radius (m) (ImmobilePoreRadius_STFF)

ImmobilePorosity_STFF, ImmobileGrainDensity_STFF, and ImmobilePoreRadius_STFF are assigned constant values of 0.2, 2470 kg/m^3, and 5.0E-8 m, respectively, in the *tpa.inp* file. Based on the above equation, these values yield SSA = 4,858 m^2/kg, which is identical to the output value reported for the tuff transport leg in *sz_kdrd.out*.

Check Conversion of K_D to R_D Values for Actinide Species

Calculations to verify TPA correct conversion from K_D to R_D for the actinide species were performed using the equation:

$$R_D = 1 + \frac{\rho(1-\theta)}{\theta} K_D$$

where

R_D = retardation factor

K_D = distribution coefficient

ρ = grain density

θ = porosity

Using the K_D, porosity, and density values reported in the *sz_kdrd.out* file R_D was calculated by hand using the above equation and compared the reported R_D value in *sz_kdrd.out*. These hand calculations were performed only for the first two lines of *sz_kdrd.out* file, which represent tuff matrix and alluvium for the first realization of the simulation; since all realizations perform the same calculation, there was no need to repeat for other realizations. The hand calculations produced R_D values identical to those reported in *sz_kdrd.out*.

Check that K_D values for Cm and Am are the Same

The K_D and R_D values for Cm are not reported in the *sz_kdrd.out* file, but the R_D values for tuff and alluvium are written to the NEFMKS input file *nefii.inp* for use in transport calculations. Below is an excerpt from the *nefii.inp* file, which represents the NEFMKS input for the 500th realization of the simulation. In this excerpt, Element Index 1 represents Cm and Index 2 represents Am; Leg 2 is tuff and Leg 3 is alluvium. It can be seen that the highlighted R_D values below for Cm and Am are identical. These R_D values also reflect the correction to account for the effects of reversible sorption to colloids, which are reported in the output file *sz_revers.out* (See for Test 2 for discussion of the correction for colloid effects).

```
ELEM.    SOLUBILITY    LEG   MOBIL RD       IMMOBILE RD        MASS XFER
INDEX      (KG/KG)      #                                      MOD FACTOR
    1    0.000E+00      1    0.121E+02      0.100E+01          0.141E-04
                        2    0.121E+02      0.207E+04          0.141E-04
                        3    0.289E+04      0.100E+01          0.000E+00
    2    0.000E+00      1    0.108E+01      0.100E+01          0.992E+00
                        2    0.108E+01      0.167E+02          0.992E+00
                        3    0.180E+02      0.100E+01          0.000E+00
    3    0.000E+00      1    0.121E+02      0.100E+01          0.141E-04
                        2    0.121E+02      0.207E+04          0.141E-04
                        3    0.289E+04      0.100E+01          0.000E+00
```

Test 3 Evaluation (Pass/Fail): PASS

SOFTWARE VALIDATION REPORT (SVR)

SVTR#:	Project#:06002.01.354
Software Name: TPA Code	Version:5.1BetaU
Test ID: **P-14**	Test Series Name: **Volcano**

Test Method

☐ code inspection
☒ output inspection
☐ hand calculation
☐ spreadsheet
☐ graphical
☐ comparison with external code results

Test Objective:
A. To examine that the algorithm that predicts the timing of volcanic events provides results consistent with statistical probability and is not unduly biased.
B. To examine that the geometric and distribution models for computing the number of failed waste packages for any subarea is correctly implemented and number of failed waste packages is consistent with number of intersected drifts.
C. To verify that counting intersected waste packages as both a groundwater source and an ejected source does not unduly bias results.
D. To check and verify that the number of waste packages reported in the *screenprint* should agree with the number displayed in the *wpsfail.res* file.

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): WINDOWS

Input Data (files, data base, mode settings): See Attachment 1, Input Data :

Assumptions, constraints, and/or scope of test: See Attachment A, Assumptions

Test Procedure:

See Attachments A and B

Test Results

Location: See attached CD labeled “TPA Version 5.1 Validation Task P-14"

Test Criterion or Expected Results: See Attachments A and B

Test Evaluation (Pass/Fail): **PASS**

Notes:

Tester: Ron Janetzke and Debashis Basu	Date: 5/2//07

Attachment A

TPA Version 5.1 Validation Task P-14
Objectives, Assumptions, Test Descriptions

OBJECTIVES

The objectives of Software Validation Task P-14 are to verify process level calculations performed by the TPA module VOLCANO. The specific issues to be addressed by Task P-14 are the following:

A. To examine that the algorithm that predicts the timing of volcanic events provides results consistent with statistical probability and is not unduly biased.
B. To examine that the geometric and distribution models for computing the number of failed waste packages for any subarea is correctly implemented and the number of failed waste packages is consistent with the number of intersected drifts.
C. To verify that counting intersected waste packages as both a groundwater source and an ejected source does not unduly bias results.
D. To check and verify that the number of waste packages reported in the *screenprint* should agree with the number displayed in the *wpsfail.res* file.

ASSUMPTIONS

For the purposes of this validation test, it is assumed:

- The input parameters and their distributions supplied by *tpa.inp* are consistent with the abstractions of the modeled processes
- Previous validation testing of this module and testing of subsequent SCRs affecting this module have been properly performed, and may be cited as evidence of module performance.
- Most of the parametric studies will be performed for a single realization. The assumption is that the transfer of stochastic parameters is correct when running multiple realizations if the test is successful for a single realization of a multiple realization simulation.
- Some of the input parameters will be held constant.

TEST

The following tests sequentially address the objectives of this SVR:

1) Execute 6 realizations (1 realization for each of 6 proposed cases) by varying the endpoint of the input parameter TimeOfNextVolcanicEventinRegionOfInterest[yr] and the sample size and keeping the start point as well as the probability value constant. This test will provide information regarding the algorithm that predicts the timing of a volcanic event (Objective A)

Cases	Parameter	Value	Sample Size	Number of Realizations
Case a	TimeOfNextVolcanicEventinRegion OfInterest[yr]	100.0, 10000.0, 1.0e-7	500	1
Case b	TimeOfNextVolcanicEventinRegion OfInterest[yr]	100.0, 100000.0, 1.0e-7	500	1
Case c	TimeOfNextVolcanicEventinRegion OfInterest[yr]	100.0, 1000000.0, 1.0e-7	500	1
Case d	TimeOfNextVolcanicEventinRegion OfInterest[yr]	100.0, 10000.0, 1.0e-7	1024	1
Case e	TimeOfNextVolcanicEventinRegion OfInterest[yr]	100.0, 100000.0, 1.0e-7	1024	1
Case f	TimeOfNextVolcanicEventinRegion OfInterest[yr]	100.0, 1000000.0, 1.0e-7	1024	1

For each realization, we will examine the occurrence of the volcanic event and how its timing is influenced by changing the endpoint in the input parameter.

2) Execute 1 realization for each of the following four scenarios :

a) Geometric Extrusive
b) Geometric Intrusive
c) Distribution Extrusive
d) Distribution Intrusive

These realizations will be used to verify that both the geometric and distribution models are correctly implemented (Objective B). The sample size will be 500 for all four cases, but the parameters VolcanoModel(1=Geometric,2=Distribution) and ExtrusiveEventFlag(extrusive=1,intrusive=0) will be varied:

Realizations	Sample Size	Parameter	Value
		VolcanoModel(1=Geometric,2=Distribution)	1
1	500	(Case a : Geometric Extrusive) ExtrusiveEventFlag(extrusive=1,intrusive=0)	1
1	500	(Case b: Geometric Intrusive) ExtrusiveEventFlag(extrusive=1,intrusive=0)	0

		VolcanoModel(1=Geometric,2=Distribution)	2
1	500	(Case c: Distribution Extrusive) ExtrusiveEventFlag(extrusive=1,intrusive=0)	1
1	500	(Case d : Distribution Intrusive) ExtrusiveEventFlag(extrusive=1,intrusive=0)	0

We will compare the number of failed waste packages determined for the two models (geometric and distribution). For each model, the number of failed waste packages should be consistent with (i) the number of waste packages in an affected drift, and (ii) the number of affected drifts. We will also check that the total number of waste packages failed in each subarea does not exceed the number of waste packages in that subarea (Objective B).

In the distribution extrusive case, we will verify that the total number of ejected waste packages varies between 1 and 150 according to the input parameter NumberOfWPsEntrainedByEjecta[ ]**.** In addition, for both the distribution and geometric extrusive cases, we will verify that the waste packages ejected are from only one subarea.

3) Execute 1 realization for the distribution extrusive model, in which the parameter NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] is set to a value of one to ensure that all the waste packages fail in all the drifts and subareas. In doing so, we can verify i) If waste packages failed extrusively (ejected source) fail again intrusively (groundwater source), and ii) if allowing waste packages failed extrusively to also fail intrusively unduly biases results (Objective C)

4) We will compare the *wpsfail.res* files to the *screenprint* to verify the results in the *wpsfail.res* files (Objective D).

Attachment B

TPA 5.1 Software Validation Task P-14 Test Results

Following are test results for the validation test cases described in Attachment A for TPA Version 5.1 code Software Validation Task P- 14. Additional details related to test procedures are also provided.

Test 1. To examine that the algorithm that predicts the timing of volcanic events provides results consistent with statistical probability

Path for run directory:

Test Case 1a : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 1b : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 1c : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 1d : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 1e : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 1f : Romeo: D:\TPARUN\tpa51betaU\run

Environment variable:

Test Case 1a : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 1b : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 1c : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 1d : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 1e : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 1f : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU

Path for the run data storage directory:

Test CASE 1a: Romeo: D:\TPARUN\tpa51betaU\geometric\extru-10000-year-500sample
Test CASE 1b: Romeo:D:\TPARUN\tpa51betaU\geometric\extru-100000-year-500sample
Test CASE 1c: Romeo:D:\TPARUN\tpa51betaU\geometric\extru-1000000-year-500sample
Test CASE 1d: Romeo:D:\TPARUN\tpa51betaU\geometric\extru-10000-year-1024sample
Test CASE 1e: Romeo:D:\TPARUN\tpa51betaU\geometric\extru-100000-year-1024sample
Test CASE 1f: Romeo:D:\TPARUN\tpa51betaU\geometric\extru-1000000-year-1024sample

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

All six test cases (1a-1f) were performed using the geometric extrusive model. Two sample sizes were considered: 500 and 1024. The test cases were carried out varying the endpoint of the input parameter TimeOfNextVolcanicEventinRegionOfInterest[yr] and keeping the start point as well as the probability value constant.

For all the cases the VolcanismDisruptiveScenarioFlag was set to 1.

```
**        ***>>>  Disruptive Scenario Flags  <<<***
**
iflag
VolcanismDisruptiveScenarioFlag(yes=1;no=0)
1
```

Specific input changes made for each specific case is described below

Cases	Sample Size	StartAt Realization	StopAt Realization	Volcano Model	TimeOfNextVolcanic EventinRegionOf Interest[yr]	Extrusive EventFlag
1a	500	1	1	1	100.0, 10000.0, 1.0e-7	1
1b	500	1	1	1	100.0, 100000.0, 1.0e-7	1
1c	500	1	1	1	100.0, 1000000.0, 1.0e-7	1
1d	1024	1	1	1	100.0, 10000.0, 1.0e-7	1
1e	1024	1	1	1	100.0, 100000.0, 1.0e-7	1
1f	1024	1	1	1	100.0, 1000000.0, 1.0e-7	1

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify that the occurrence of the igneous event varies with changing sample sizes and parameter ranges.

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *screenprint* and *wpsfail.res file*

Test Procedure:

1) Execute the TPA code six times, using the *tpa.inp* file and saving the results for examination.
2) Examine the *screenprint* and the *wpsfail.res* file

Pass/Fail criteria:

1) For test cases 1a, 1b, and 1c, the year of occurrence of the igneous event should remain the same.
2) For test cases 1d, 1e, and 1f, the year of occurrence of the igneous event should be different from 1a, 1b, and 1c, but the same for test cases 1d, 1e, and 1f.

Test results:

Test Case 1a :
The following is a section of the *screenprint* of the output for test case 1a

```
--------------------------------------------------------------------
   subarea   4 of  10
--------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      377.4  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Corrosion Breach on WP Welded Areas
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =   1430 at TPA time =   9107.2 yr
 *** failed WPs:  1430   out of  1793   ***
```

The following is a section of the *wpsfail.res* file generated for test case 1a

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.00000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.43000E+03**
1	**8**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.23000E+02**

Test Case 1b :

The following is a section of the *screenprint* of the output for test case 1b

```
------------------------------------------------------------------------
    subarea   3 of  10
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      501.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1660.0  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    103 at TPA time =   1640.9 yr
exec: failed WPs from VOLCANIC   event =    900 at TPA time =   9107.2 yr
 *** failed WPs:  1003   out of  2904  ***
```

The following is a section of the *wpsfail.res* file generated for test case 1b

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.00000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.43000E+03**
1	**8**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.23000E+02**

Test Case 1c :

The following is a section of the *screenprint* of the output for test case 1c

```
------------------------------------------------------------------------
    subarea   3 of  10
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      501.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
```

```
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1660.0  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    103 at TPA time =   1640.9 yr
exec: failed WPs from VOLCANIC   event =    900 at TPA time =   9107.2 yr
 *** failed WPs:  1003   out of  2904  ***
```

The following is a section of the *wpsfail.res* file generated for test case 1c

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.00000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.43000E+03**
1	**8**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.23000E+02**

Test Case 1d :
The following is a section of the *screenprint* of the output for test case 1d

```
-----------------------------------------------------------------------
    subarea   3 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      306.2  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1409.4  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    102 at TPA time =   1380.8 yr
exec: failed WPs from VOLCANIC   event =    903 at TPA time =   4606.8 yr
 *** failed WPs:  1005   out of  2904  ***
```

The following is section of the *wpsfail.res* file generated for test case 1d

Realization	Subarea	Number of	Number of	Number of	Number of	Number of

Number	Number	Time	Initial	Corrosion	Mechanical	Faulting	Igneous Activity
(unitless)	(unitless)	(yr)	(unitless)	(unitless)	(unitless)	(unitless)	(unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	3.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	9.46861E+02	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	6	9.96390E+02	0.00000E+00	3.43000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	9	1.18896E+03	0.00000E+00	7.23000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.28153E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	10	1.28153E+03	0.00000E+00	1.74700E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.38075E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	4	1.41539E+03	0.00000E+00	1.79300E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	4.60683E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.00000E+02
1	4	4.60683E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.43000E+03
1	**8**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.66000E+02**
1	**9**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.22000E+02**
1	**10**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.01000E+02**

Test Case 1e :
The following is a section of the *screenprint* of the output for test case 1e

```
-----------------------------------------------------------------
    subarea   3 of  10
-----------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      306.2  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1409.4  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    102 at TPA time =   1380.8 yr
exec: failed WPs from VOLCANIC   event =    903 at TPA time =   4606.8 yr
 *** failed WPs:  1005   out of  2904   ***
 *** ejected WPs:  3
```

The following is a section of the *wpsfail.res* file generated for test case 1e

Realization	Subarea		Number of	Number of	Number of	Number of	Number of
Number	Number	Time	Initial	Corrosion	Mechanical	Faulting	Igneous Activity
(unitless)	(unitless)	(yr)	(unitless)	(unitless)	(unitless)	(unitless)	(unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	3.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	9.46861E+02	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	6	9.96390E+02	0.00000E+00	3.43000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	9	1.18896E+03	0.00000E+00	7.23000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.28153E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	10	1.28153E+03	0.00000E+00	1.74700E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.38075E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	4	1.41539E+03	0.00000E+00	1.79300E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**3**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.00000E+02**
1	**4**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.43000E+03**
1	**8**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.66000E+02**
1	**9**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.22000E+02**
1	**10**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.01000E+02**

Test case 1f :

The following is a section of the *screenprint* of the output for test case 1f

```
------------------------------------------------------------------------
    subarea   3 of  10
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      306.2  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1409.4  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    102 at TPA time =   1380.8 yr
exec: failed WPs from VOLCANIC   event =    903 at TPA time =   4606.8 yr
 *** failed WPs:  1005   out of  2904   ***
 *** ejected WPs:  3
```

The following is a section of the *wpsfail.res* file generated for test case 1f

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	3.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	9.46861E+02	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	6	9.96390E+02	0.00000E+00	3.43000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	9	1.18896E+03	0.00000E+00	7.23000E+02	0.00000E+00	0.00000E+00	0.00000E+00

1	5	1.28153E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	10	1.28153E+03	0.00000E+00	1.74700E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.38075E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	4	1.41539E+03	0.00000E+00	1.79300E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**3**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.00000E+02**
1	**4**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.43000E+03**
1	**8**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.66000E+02**
1	**9**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.22000E+02**
1	**10**	**4.60683E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.01000E+02**

The following table provides the summary for test cases 1a-1f as reported in *screenprint*

Cases	Sample Size	Number of Realizations	TimeOfNextVolcanicEventin RegionOfInterest[yr]	Occurrence of Igneous Event
1a	500	1	100.0, 10000.0, 1.0e-7	9107.2
1b	500	1	100.0, 100000.0, 1.0e-7	9107.2
1c	500	1	100.0, 1000000.0, 1.0e-7	9107.2
1d	1024	1	100.0, 10000.0, 1.0e-7	4606.8
1e	1024	1	100.0, 100000.0, 1.0e-7	4606.8
1f	1024	1	100.0, 1000000.0, 1.0e-7	4606.8

***Observations*:** On changing the sample size from 500 to 1024, the time at which the volcanic event occurred changed from 9107.2 years to 4606.8 years. The result was same irrespective of the end points (10,000, 100,000 or 1,000,000).

Test 1 results (PASS/FAIL): **PASS**

Test 2. **To examine that the geometric and distribution models for computing the number of failed waste packages for any subarea is correctly implemented and number of failed waste packages is consistent with number of intersected drifts.**

Path for run directory:

Test Case 2a : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 2b : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 2c : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 2d : Romeo: D:\TPARUN\tpa51betaU\run

Environment variable:

Test Case 2a : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 2b : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 2c : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 2d : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU

Path for the run data storage directory:

Test Case 2a :Romeo:D:\TPARUN\tpa51betaU\geometric\extrusive
Test Case 2b :Romeo:D:\TPARUN\tpa51betaU\geometric\intrusive
Test Case 2c :Romeo:D:\TPARUN\tpa51betaU\distribution\extrusive
Test Case 2d :Romeo:D:\TPARUN\tpa51betaU\distribution\intrusive

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

The four test cases (2a - 2d) were performed using both the geometric and distribution models and involve both extrusive and intrusive failure scenarios as described in Attachment A. All the test cases were carried out for only one realization, and one sample size was considered (500). The test cases were carried out by keeping the start point, the end point, and the probability values of the TimeOfNextVolcanicEventinRegionOfInterest[yr] constant.

For all the cases the VolcanismDisruptiveScenarioFlag was set to 1.

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

** for both models
**
```

finiteexponential
TimeOfNextVolcanicEventinRegionOfInterest[yr]
100.0, 10000.0, 1.0e-7
**

Specific input changes made for each specific case is described below

Cases	Sample Size	Start at Realization	Stop at Realization	Parameter	Value
				VolcanoModel(1=Geometric, 2=Distribution)	1
2a	500	1	1	(Geometric Extrusive) ExtrusiveEventFlag(extrusive=1, intrusive=0)	1
2b	500	1	1	(Geometric Intrusive) ExtrusiveEventFlag(extrusive=1, intrusive=0)	0
				VolcanoModel(1=Geometric, 2=Distribution)	2
2c	500	1	1	(Distribution Extrusive) ExtrusiveEventFlag(extrusive=1, intrusive=0)	1
2d	500	1	1	(Distribution Intrusive) ExtrusiveEventFlag(extrusive=1, intrusive=0)	0

Additional input parameters for the distribution model

beta
NumberOfWPsEntrainedByEjecta[]
1.0, 150.0, 1.0, 2.0
**
usersuppliedpwisecdf
NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[]
19
0.   0.000
8.941e-6 0.084
.01788 0.094
.05364 0.117
.08941 0.141
.1252 0.175
.1609 0.213
.1886 0.257

.1887	0.475
.2527	0.562
.2813	0.588
.2814	0.712
.4470	0.781
.5633	0.813
.6974	0.843
.8156	0.881
.8157	0.967
.8444	0.969
.8445	1.000

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Verify that both the geometric and distribution models are correctly implemented and the number of failed waste packages is consistent with the total number of waste packageas in each drift and the affected drifts.

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *screenprint* and *wpsfail.res*

Test Procedure:

1) Execute the TPA code four times, using the *tpa.inp* file (with the specific changes in the input file depending on the specific case) and saving the results for examination.
2) Examine the *screenprint* and the *wpsfail.res* file

Pass/Fail criteria:

1. The number of failed waste packages determined for the two models will be compared. For each model, the number of failed waste packages should be consistent with
   i) the number of waste packages in an affected drift
   ii) the number of affected drifts
   iii) the total number of waste packages failed in each subarea

2. In the distribution extrusive case, we will verify that the total number of ejected waste packages varies between 1 and 150 according to the input parameter NumberOfWPsEntrainedByEjecta[ ]**.** In addition, for both the distribution and geometric extrusive cases, we will verify that the waste packages ejected are from only one subarea.

Test results:

Test Case 2a :
The following is a section of the *screenprint* of the output for test case 2a (geometric-extrusive scenario)

```
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
   #      [m^2]     [MTU]
   1    224091.0    3025.5          526
   2    448476.0    6108.4         1062
   3   1241313.5   16703.3         2904
   4    775953.1   10313.0         1793
   5    605892.0    8351.7         1452
   6    152357.0    1972.9          343
   7    318122.0    4003.3          696
   8    439350.0    5355.0          931
   9    305880.0    4158.6          723
  10    747165.5   10048.4         1747
-----------------------------------------------------------------------
    subarea   3 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      501.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1660.0  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    103 at TPA time =   1640.9 yr
exec: failed WPs from VOLCANIC   event =    900 at TPA time =   9107.2 yr
 *** failed WPs:  1003   out of  2904   ***

-----------------------------------------------------------------------
    subarea   4 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      377.4  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =   1430 at TPA time =   9107.2 yr
 *** failed WPs:  1430   out of  1793   ***

-----------------------------------------------------------------------
    subarea   7 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
```

```
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      296.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =        9 at TPA time =   9107.2 yr
 *** failed WPs:  9    out of  696   ***
 *** ejected WPs:  9

-----------------------------------------------------------------------
    subarea   8 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      388.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     923 at TPA time =   9107.2 yr
 *** failed WPs:  923   out of  931   ***
```

The following is a section of the *wpsfail.res* file generated for test case 2a (geometric-extrusive scenario)

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.00000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.43000E+03**
1	**8**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.23000E+02**

The following table provides the failure summary for test case 2a as reported in *screenprint* and *wpsfail.res* file.

Subarea #	Total # of WPs	Time of Igneous Event (Year)	Number of Intrusive Failures	Number of Extrusive Failures
1	526	----	0	0
2	1062	-----	0	0
3	2904	9107.2	900	0
4	1793	9107.2	1430	0
5	1462	-------	0	0
6	343	------	0	0
7	696	9107.2	0	9
8	981	9107.2	923	0
9	723	---------	0	0
10	1747	--------	0	0

***Observations*:** The number of waste package failures in the respective subareas for the geometric extrusive scenario is consistent with the number of waste packages in an affected drift. The extrusive event takes place in subarea 7; 9 waste packages are ejected. It is evident from the *screenprint* and the *wpsfail.res* file that no intrusive failures take place in subarea 7, indicating that the conduit and dike affect different subareas. Subareas 3, 4, and 8 have intrusive failures, and the number of failed waste packages in those subareas are also consistent with the total number waste packages in each subarea. Thus, irrespective of the extrusive event, intrusive failure will take place.

Test Case 2b :

The following is a section of the *screenprint* of the output for test case 2b (geometric-intrusive scenario)

```
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]       [MTU]
   1    224091.0     3025.5          526
   2    448476.0     6108.4         1062
   3   1241313.5    16703.3         2904
   4    775953.1    10313.0         1793
   5    605892.0     8351.7         1452
   6    152357.0     1972.9          343
   7    318122.0     4003.3          696
   8    439350.0     5355.0          931
   9    305880.0     4158.6          723
  10    747165.5    10048.4         1747
```

```
----------------------------------------------------------------------
    subarea   3 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      501.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1660.0  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    103 at TPA time =   1640.9 yr
exec: failed WPs from VOLCANIC   event =    900 at TPA time =   9107.2 yr
 *** failed WPs:  1003   out of  2904  ***

----------------------------------------------------------------------
    subarea   4 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      377.4  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =   1430 at TPA time =   9107.2 yr
 *** failed WPs:  1430   out of  1793  ***

----------------------------------------------------------------------
    subarea   8 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      388.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    923 at TPA time =   9107.2 yr
 *** failed WPs:  923   out of  931  ***
```

The following is a section of the *wpsfail.res* file generated for test case 2b (geometric-intrusive scenario)

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.00000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.43000E+03**
1	**8**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.23000E+02**

The following table provides the failure summary for test case 2b as reported in *screenprint* and *wpsfail.res* file.

Subarea #	Total # of WPs	Time of Igneous Event (Year)	Number of Intrusive Failures	Number of Extrusive Failures
1	526	----	0	0
2	1062	-----	0	0
3	2904	9107.2	900	0
4	1793	9107.2	1430	0
5	1462	-------	0	0
6	343	------	0	0
7	696	--------	0	0
8	981	9107.2	923	0
9	723	---------	0	0
10	1747	--------	0	0

Observations : The number of waste packages failed intrusively in subareas 3, 4, and 8 is consistent with the total number of waste packages in the respective subareas, i.e., the total number of waste packages failed in each of these subareas does not exceed the number of waste packages in that subarea. Also, the number of failed waste packages reported in the *screenprint* match the number reported in the *wpsfail.res* for intrusive failures.

Test case 2c :

The following is a section of the *screenprint* of the output for test case 2c (distribution-extrusive scenario)

```
REPOSITORY DESIGN INFORMATION
Subarea   Area       Waste   Number of WP
   #      [m^2]      [MTU]
   1    224091.0     3025.5          526
   2    448476.0     6108.4         1062
   3   1241313.5    16703.3         2904
   4    775953.1    10313.0         1793
   5    605892.0     8351.7         1452
   6    152357.0     1972.9          343
   7    318122.0     4003.3          696
   8    439350.0     5355.0          931
   9    305880.0     4158.6          723
  10    747165.5    10048.4         1747

----------------------------------------------------------------------
    subarea    1 of   10
----------------------------------------------------------------------
exec: calling uzflow
        Mean Annual Infiltration at Start(AAI0):    6.9049E+00
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
dataFile= dsfailt.dat
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      435.7  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1167.8  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: calling volcano
exec: failed WPs from LOC CORR   event =     22 at TPA time =   1159.5 yr
exec: failed WPs from VOLCANIC   event =     99 at TPA time =   9107.2 yr
 *** failed WPs:  121   out of   526   ***

----------------------------------------------------------------------
    subarea    2 of   10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      306.2  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    200 at TPA time =   9107.2 yr
 *** failed WPs:  200   out of   1062   ***
----------------------------------------------------------------------
    subarea    3 of   10
----------------------------------------------------------------------
exec: calling uzflow
```

```
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      501.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1660.0  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    121 at TPA time =   1640.9 yr
exec: failed WPs from VOLCANIC   event =    547 at TPA time =   9107.2 yr
 *** failed WPs:  668   out of  2904   ***

-----------------------------------------------------------------------
    subarea   4 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      377.4  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    338 at TPA time =   9107.2 yr
 *** failed WPs:  338   out of  1793   ***

-----------------------------------------------------------------------
    subarea   5 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      399.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1511.6  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     60 at TPA time =   1487.1 yr
exec: failed WPs from VOLCANIC   event =    274 at TPA time =   9107.2 yr
 *** failed WPs:  334   out of  1452   ***
-----------------------------------------------------------------------
    subarea   6 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      623.3  yr
     *** No Drip Shield Failure by General Corrosion ***
```

```
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =      65 at TPA time =   9107.2 yr
 *** failed WPs:  65   out of  343   ***

----------------------------------------------------------------------
    subarea   7 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      296.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     253 at TPA time =   9107.2 yr
 *** failed WPs:  253   out of  696   ***
 *** ejected WPs:  122

----------------------------------------------------------------------
    subarea   8 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      388.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     175 at TPA time =   9107.2 yr
 *** failed WPs:  175   out of  931   ***
----------------------------------------------------------------------
    subarea   9 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      559.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     136 at TPA time =   9107.2 yr
```

```
 *** failed WPs:  136   out of  723  ***

------------------------------------------------------------------------
    subarea  10 of  10
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      461.1  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     329 at TPA time =   9107.2 yr
 *** failed WPs:  329   out of  1747   ***
```

The following is a section of the *wpsfail.res* file generated for test case 2c (distribution-extrusive-scenario)

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**1**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.90000E+01**
1	**2**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**2.00000E+02**
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**5.47000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**3.38000E+02**
1	**5**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**2.74000E+02**
1	**6**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**6.50000E+01**
1	**7**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.31000E+02**
1	**8**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.75000E+02**
1	**9**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.36000E+02**
1	**10**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**3.29000E+02**

The following table provides the failure summary for test case 2c as reported in *screenprint* and *wpsfail.res* file.

Subarea #	Total # of WPs	Time of igneous event (year)	Number of Intrusive Failures	No. of Extrusive Failures
1	526	9107.2	121	--------
2	1062	9107.2	200	---------
3	2904	9107.2	668	---------
4	1793	9107.2	338	--------
5	1452	9107.2	334	--------
6	343	9107.2	65	---------
7	696	9107.2	131	122
8	981	9107.2	175	----------
9	723	9107.2	136	----------
10	1747	9107.2	329	----------

Observations: The total number of failed waste packages in each subarea is consistent with the number of waste packages in that subarea. Intrusive failures occur in every subarea, and extrusive failures occur only in subarea 7. The total number of ejected waste packages (122) in subarea 7 varies between 1 and 150 according to the input parameter NumberOfWPsEntrainedByEjecta[ ]**.**

Test Case 2d :
The following is a section of the *screenprint* of the output for test case 2d (distribution-intrusive scenario)

```
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste    Number of WP
   #      [m^2]       [MTU]
   1     224091.0     3025.5          526
   2     448476.0     6108.4         1062
   3    1241313.5    16703.3         2904
   4     775953.1    10313.0         1793
   5     605892.0     8351.7         1452
   6     152357.0     1972.9          343
   7     318122.0     4003.3          696
   8     439350.0     5355.0          931
   9     305880.0     4158.6          723
  10     747165.5    10048.4         1747
-----------------------------------------------------------------------
    subarea    1 of   10
-----------------------------------------------------------------------
exec: calling uzflow
        Mean Annual Infiltration at Start(AAI0):    6.9049E+00
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
dataFile= dsfailt.dat
```

```
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      435.7  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1167.8  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: calling volcano
exec: failed WPs from LOC CORR   event =     22 at TPA time =   1159.5 yr
exec: failed WPs from VOLCANIC   event =     99 at TPA time =   9107.2 yr
 *** failed WPs:  121   out of  526  ***

-----------------------------------------------------------------------
    subarea   2 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      306.2  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    200 at TPA time =   9107.2 yr
 *** failed WPs:  200   out of  1062  ***

-----------------------------------------------------------------------
    subarea   3 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      501.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1660.0  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =    121 at TPA time =   1640.9 yr
exec: failed WPs from VOLCANIC   event =    547 at TPA time =   9107.2 yr
 *** failed WPs:  668   out of  2904  ***
-----------------------------------------------------------------------
    subarea   4 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      377.4  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
```

```
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC    event =     338 at TPA time =   9107.2 yr
 *** failed WPs:  338   out of  1793  ***

-----------------------------------------------------------------------
    subarea   5 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      399.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1511.6  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR    event =      60 at TPA time =   1487.1 yr
exec: failed WPs from VOLCANIC    event =     274 at TPA time =   9107.2 yr
 *** failed WPs:  334   out of  1452  ***

-----------------------------------------------------------------------
    subarea   6 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      623.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC    event =      65 at TPA time =   9107.2 yr
 *** failed WPs:  65   out of  343  ***

-----------------------------------------------------------------------
    subarea   7 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      296.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC    event =     131 at TPA time =   9107.2 yr
 *** failed WPs:  131   out of  696  ***
```

```
-----------------------------------------------------------------------
    subarea   8 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      388.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC    event =     175 at TPA time =   9107.2 yr
 *** failed WPs:  175   out of  931  ***

-----------------------------------------------------------------------
    subarea   9 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      559.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC    event =     136 at TPA time =   9107.2 yr
 *** failed WPs:  136   out of  723  ***

-----------------------------------------------------------------------
    subarea  10 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      461.1  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC    event =     329 at TPA time =   9107.2 yr
 *** failed WPs:  329   out of  1747  ***
```

The following is a section of the *wpsfail.res* file generated for test case 2d (distribution-intrusive scenario)

Realization Number	Subarea Number	Time	Number of Initial	Number of Corrosion	Number of Mechanical	Number of Faulting	Number of Igneous Activity
(unitless)	(unitless)	(yr)	(unitless)	(unitless)	(unitless)	(unitless)	(unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**1**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.90000E+01**
1	**2**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**2.00000E+02**
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**5.47000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**3.38000E+02**
1	**5**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**2.74000E+02**
1	**6**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**6.50000E+01**
1	**7**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.31000E+02**
1	**8**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.75000E+02**
1	**9**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.36000E+02**
1	**10**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**3.29000E+02**

The following table provides the failure summary for test case 2d as reported in *screenprint* and *wpsfail.res* file.

Subarea #	Total # of WPs	Time of Igneous Event	Number of Intrusive Failures	Number of Extrusive Failures
1	526	9107.2	121	0
2	1062	9107.2	200	0
3	2904	9107.2	668	0
4	1793	9107.2	338	0
5	1452	9107.2	334	0
6	343	9107.2	65	0
7	696	9107.2	131	0
8	981	9107.2	175	0
9	723	9107.2	136	0
10	1747	9107.2	329	0

Observations: In the distribution intrusive test case, the total number of failed waste packages in each subarea is consistent with the number of waste packages in an affected drift and the number of affected drifts.

Test 2 results (PASS/FAIL): **PASS**

Test 3. To verify that counting intersected waste packages as both a groundwater

source and an ejected source does not unduly bias results.

Path for run directory:

Test case 3x : Romeo: D:\TPARUN\tpa51betaU\run

Environment variable:

Test case 3 : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU

Path for the run data storage directory:

Test case 3 : Romeo:D:\TPARUN\tpa51betaU\distribution\extrusive-all-fail

Special input files or modifications to input files required :

In the input file, the user suppliedpwisecdf for NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[] was set to 1.

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

The test case was performed with the distribution extrusive model. A sample size of 500 was considered.

The VolcanismDisruptiveScenarioFlag was set to 1.

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

** for both models
**
finiteexponential
TimeOfNextVolcanicEventinRegionOfInterest[yr]
100.0, 10000.0, 1.0e-7
**
```

Specific input changes made for each specific case is described below

Case	Sample Size	StartAt Realization	StopAt Realization	Parameter	Value
3	500	1	1	NormalizedMagmaInducedMechanicalFailuresRemainingInDrift[]	1
				VolcanoModel (1=Geometric,2=Distribution)	2
				ExtrusiveEventFlag (extrusive=1,intrusive=0)	1

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: To verify that counting intersected waste packages as both a groundwater source and an ejected source does not unduly bias results.

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *screenprint and wpsfail.res file*

Test Procedure:

1) Execute the TPA code, using the *tpa.inp* file (with the specified change in the input file) and saving the results for examination.
2) Examine the *screenprint* and the *wpsfail.res* file

Pass/Fail criteria:

1) The number of failed waste packages reported in the *wpsfail.res* file should be those that are failed intrusively.
2) The number of ejected waste packages should not be reported in the *wpsfail.res* file and initial failures should be accounted for in subareas with extrusive and intrusive failures.
3) The number of ejected waste packages should range between 1 and 150 compared to the thousands of waste packages failed intrusively.

Test results:

Test Case 3 :
The following is a section of the *screenprint* of the output for test case 3 (distribution-extrusive scenario where all the waste packages fail).

```
REPOSITORY DESIGN INFORMATION
Subarea   Area       Waste   Number of WP
   #     [m^2]       [MTU]
   1    224091.0     3025.5          526
   2    448476.0     6108.4         1062
   3   1241313.5    16703.3         2904
   4    775953.1    10313.0         1793
   5    605892.0     8351.7         1452
   6    152357.0     1972.9          343
   7    318122.0     4003.3          696
   8    439350.0     5355.0          931
   9    305880.0     4158.6          723
  10    747165.5    10048.4         1747

----------------------------------------------------------------------
    subarea   1 of  10
----------------------------------------------------------------------
exec: calling uzflow
        Mean Annual Infiltration at Start(AAI0):    1.9953E+01
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
dataFile= dsfailt.dat
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      435.7  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: calling volcano
exec: failed WPs from VOLCANIC   event =     526 at TPA time =   6407.3 yr
 *** failed WPs: all WPs failed ( 526 ) ***

----------------------------------------------------------------------
    subarea   2 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      559.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    1061 at TPA time =   6407.3 yr
 *** failed WPs:  1061   out of  1062   ***
----------------------------------------------------------------------
    subarea   3 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      245.6  yr
```

```
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =   2902 at TPA time =   6407.3 yr
 *** failed WPs:  2902   out of  2904  ***
 *** ejected WPs:  3

----------------------------------------------------------------------
    subarea   4 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      606.8  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =   1792 at TPA time =   6407.3 yr
 *** failed WPs:  1792   out of  1793  ***
----------------------------------------------------------------------
    subarea   5 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      325.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =   1451 at TPA time =   6407.3 yr
 *** failed WPs:  1451   out of  1452  ***
----------------------------------------------------------------------
    subarea   6 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      335.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    343 at TPA time =   6407.3 yr
```

```
 *** failed WPs: all WPs failed ( 343 ) ***

-----------------------------------------------------------------------
    subarea   7 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      279.0  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     696 at TPA time =   6407.3 yr
 *** failed WPs: all WPs failed ( 696 ) ***

-----------------------------------------------------------------------
    subarea   8 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      515.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     930 at TPA time =   6407.3 yr
 *** failed WPs:   930   out of  931   ***

-----------------------------------------------------------------------
    subarea   9 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      399.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     723 at TPA time =   6407.3 yr
 *** failed WPs: all WPs failed ( 723 ) ***
-----------------------------------------------------------------------
    subarea  10 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
```

```
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      315.6  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =   1746 at TPA time =   6407.3 yr
 *** failed WPs:  1746   out of  1747   ***
```

The following is a section of the *wpsfail.res* file generated for test case 3 (distribution-all fail)

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	**1**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**5.26000E+02**
1	**2**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.06100E+03**
1	**3**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**2.89900E+03**
1	**4**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.79200E+03**
1	**5**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.45100E+03**
1	**6**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**3.43000E+02**
1	**7**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**6.96000E+02**
1	**8**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.30000E+02**
1	**9**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**7.23000E+02**
1	**10**	**6.40726E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.74600E+03**

The following table provides the failure summary for test case 3 as reported in *screenprint* and *wpsfail.res* file.

Subarea #	Total # of WPs	Time of Igneous Event	Number of Intrusive Failures	Number of Extrusive Failures
1	526	6407.3	526	0
2	1062	6407.3	1061	0
3	2904	6407.3	2899	3
4	1793	6407.3	1792	0
5	1452	6407.3	1451	0
6	343	6407.3	343	0
7	696	6407.3	696	0
8	981	6407.3	930	0
9	723	6407.3	723	0
10	1747	6407.3	1746	0

Observations : The number of waste packages reported in the *wpsfail.res* file include only those failed intrusively. The extrusive event takes place in subarea 3, and 3 waste packages are ejected. The total number of waste packages in subarea 3 is 2904, with 2 initial failures, thus, 2902 waste packages are available to fail by disruptive events. Out of the 2902 waste packages, 3 fail extrusively and are ejected. The remaining 2899 fail intrusively and are reported in the *wpsfail.res* file.

Test 3 results (PASS/FAIL): **PASS**

Test 4. To check and verify that the number of waste packages reported in the *screenprint* should agree with the number displayed in the *wpsfail.res* file

Results from the test cases 2b and 2d were used.

Path for run directory:

Test Case 2b : Romeo: D:\TPARUN\tpa51betaU\run
Test Case 2d : Romeo: D:\TPARUN\tpa51betaU\run

Environment variable:

Test Case 2b : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU
Test Case 2d : TPA_TEST=D:\TPA\tpa51betaU
TPA_DATA=D:\TPA\tpa51betaU

Path for the run data storage directory:

Test Case 2b : Romeo:D:\TPARUN\tpa51betaU\geometric\intrusive
Test Case 2d : Romeo:D:\TPARUN\tpa51betaU\distribution\intrusive

Special input files or modifications to input files required : None

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.):

The two tests were performed using the geometric intrusive model and the distribution intrusive models. Both the tests were carried out for only one realization with a total sample size of 500.

The VolcanismDisruptiveScenarioFlag was set to 1.

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

** for both models
**
finiteexponential
TimeOfNextVolcanicEventinRegionOfInterest[yr]
100.0, 10000.0, 1.0e-7
**
```

Specific input changes made for each specific case is described below

Cases	Sample Size	Start at Realization	Stop at Realization	Parameter	Value
				VolcanoModel(1=Geometric, 2=Distribution)	1
2b	500	1	1	(Geometric Intrusive) ExtrusiveEventFlag (extrusive=1, intrusive=0)	0
				VolcanoModel (1=Geometric, 2=Distribution)	2
2d	500	1	1	(Distribution Intrusive) ExtrusiveEventFlag (extrusive=1, intrusive=0)	0

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: To check and verify that the number of waste packages failed by igneous intrusive processes reported in the *screenprint* agrees with the number displayed in the *wpsfail.res* file. The *wpsfail.res* file only displays intrusive failures, thus an extrusive scenario was not applicable to this objective.

Assumptions: None, other than those made within the TPA code.

Constraints: None

Output files to compare or examine: *screenprint* and *wpsfail.res file*

Test Procedure:

1) Execute the TPA code two times, using the *tpa.inp* file (with the specific changes in the input file depending on the specific case) and saving the results for examination.
2) Examine the *screenprint* and the *wpsfail.res* file

Pass/Fail criteria:

1) The number of failed waste packages reported in the *wpsfail.res* file should be same as the number that is reported in the *screenprint*.

Test results:

Test Case 4a (2b):
The following is a section of the *screenprint* of the output for test case 2b (geometric-intrusive scenario).

```
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste   Number of WP
   #      [m^2]       [MTU]
   1    224091.0     3025.5          526
   2    448476.0     6108.4         1062
   3   1241313.5    16703.3         2904
   4    775953.1    10313.0         1793
   5    605892.0     8351.7         1452
   6    152357.0     1972.9          343
   7    318122.0     4003.3          696
   8    439350.0     5355.0          931
   9    305880.0     4158.6          723
  10    747165.5    10048.4         1747

This shows the number of waste packages in each subarea.

-----------------------------------------------------------------------
    subarea   3 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      501.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1660.0  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR    event =    103 at TPA time =   1640.9 yr
exec: failed WPs from VOLCANIC    event =    900 at TPA time =   9107.2 yr
 *** failed WPs:  1003   out of  2904   ***

-----------------------------------------------------------------------
    subarea   4 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      377.4  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC    event =   1430 at TPA time =   9107.2 yr
 *** failed WPs:  1430   out of  1793   ***
```

```
------------------------------------------------------------------------
    subarea    8 of   10
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      388.5   yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC    event =      923 at TPA time =    9107.2 yr
 *** failed WPs:   923    out of   931   ***
```

The following is a section of the *wpsfail.res* file generated for test case 2b (geometric-intrusive scenario)

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.00000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**1.43000E+03**
1	**8**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.23000E+02**

The following table provides the failure summary for test case 4a (2b) as reported in *screenprint* and *wpsfail.res* file.

Subarea #	Total # of WPs	Time of Igneous Event (Year)	Number of Intrusive Failures (screenprint)	Number of Extrusive Failures (wpsfail.res)
1	526	----	0	0
2	1062	-----	0	0
3	2904	9107.2	900	0
4	1793	9107.2	1430	0
5	1462	-------	0	0

6	343	------	0	0
7	696	--------	0	0
8	981	9107.2	923	0
9	723	---------	0	0
10	1747	--------	0	0

<u>Observations:</u> The number of waste package failures in subareas 3, 4 and 8 for the geometric intrusive scenario as displayed in the *wpsfail.res* file is exactly the same as that reported in the *screenprint* (900, 1430 and 923).

Test Case 4b (2d):
The following is a section of the *screenprint* of the output for test case 2d (distribution-intrusive scenario).

```
REPOSITORY DESIGN INFORMATION
Subarea    Area       Waste   Number of WP
   #      [m^2]       [MTU]
   1    224091.0     3025.5         526
   2    448476.0     6108.4        1062
   3   1241313.5    16703.3        2904
   4    775953.1    10313.0        1793
   5    605892.0     8351.7        1452
   6    152357.0     1972.9         343
   7    318122.0     4003.3         696
   8    439350.0     5355.0         931
   9    305880.0     4158.6         723
  10    747165.5    10048.4        1747

-----------------------------------------------------------------------
    subarea    1 of   10
-----------------------------------------------------------------------
exec: calling uzflow
        Mean Annual Infiltration at Start(AAI0):    6.9049E+00
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
dataFile= dsfailt.dat
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      435.7  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1167.8  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: calling volcano
exec: failed WPs from LOC CORR    event =     22 at TPA time =   1159.5 yr
exec: failed WPs from VOLCANIC    event =     99 at TPA time =   9107.2 yr
 *** failed WPs:  121   out of  526  ***
-----------------------------------------------------------------------
    subarea    2 of   10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
```

```
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      306.2  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     200 at TPA time =   9107.2 yr
 *** failed WPs:  200   out of  1062  ***

-----------------------------------------------------------------------
    subarea   3 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      501.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1660.0  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     121 at TPA time =   1640.9 yr
exec: failed WPs from VOLCANIC   event =     547 at TPA time =   9107.2 yr
 *** failed WPs:  668   out of  2904  ***

-----------------------------------------------------------------------
    subarea   4 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      377.4  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     338 at TPA time =   9107.2 yr
 *** failed WPs:  338   out of  1793  ***
-----------------------------------------------------------------------
    subarea   5 of  10
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      399.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1511.6  yr
```

```
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     60 at TPA time =   1487.1 yr
exec: failed WPs from VOLCANIC   event =    274 at TPA time =   9107.2 yr
 *** failed WPs:  334   out of  1452  ***

----------------------------------------------------------------------
    subarea   6 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      623.3  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =     65 at TPA time =   9107.2 yr
 *** failed WPs:  65   out of  343  ***

----------------------------------------------------------------------
    subarea   7 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      296.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    131 at TPA time =   9107.2 yr
 *** failed WPs:  131   out of  696  ***

----------------------------------------------------------------------
    subarea   8 of  10
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      388.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    175 at TPA time =   9107.2 yr
 *** failed WPs:  175   out of  931  ***
```

```
------------------------------------------------------------------------
    subarea   9 of  10
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      559.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    136 at TPA time =   9107.2 yr
 *** failed WPs:  136   out of  723  ***

------------------------------------------------------------------------
    subarea  10 of  10
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      461.1  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from VOLCANIC   event =    329 at TPA time =   9107.2 yr
 *** failed WPs:  329   out of  1747   ***
```

The following is a section of the *wpsfail.res* file generated for test case 2d (distribution-intrusive-scenario)

Realization Number (unitless)	Subarea Number (unitless)	Time (yr)	Number of Initial (unitless)	Number of Corrosion (unitless)	Number of Mechanical (unitless)	Number of Faulting (unitless)	Number of Igneous Activity (unitless)
1	1	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	2	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	3	0.00000E+00	4.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	4	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	5	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	7	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	8	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	9	0.00000E+00	1.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	10	0.00000E+00	2.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1	1	1.15950E+03	0.00000E+00	5.26000E+02	0.00000E+00	0.00000E+00	0.00000E+00
1	5	1.48711E+03	0.00000E+00	1.45200E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	3	1.64091E+03	0.00000E+00	2.90400E+03	0.00000E+00	0.00000E+00	0.00000E+00
1	**1**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**9.90000E+01**
1	**2**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**2.00000E+02**
1	**3**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**5.47000E+02**
1	**4**	**9.10716E+03**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**0.00000E+00**	**3.38000E+02**

1	5	9.10716E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.74000E+02
1	6	9.10716E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	6.50000E+01
1	7	9.10716E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.31000E+02
1	8	9.10716E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.75000E+02
1	9	9.10716E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.36000E+02
1	10	9.10716E+03	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.29000E+02

The following table provides the failure summary for test case 2d as reported in *screenprint* and *wpsfail.res* file.

Subarea #	Total # of WPs	Time of Igneous Event (Year)	Number of Intrusive Failures (screenprint)	Number of Extrusive Failures (wpsfail.res)
1	526	9107.2	121	0
2	1062	9107.2	200	0
3	2904	9107.2	668	0
4	1793	9107.2	338	0
5	1452	9107.2	334	0
6	343	9107.2	65	0
7	696	9107.2	131	0
8	981	9107.2	175	0
9	723	9107.2	136	0
10	1747	9107.2	329	0

Observations : The number of waste packages reported in the *screenprint* agrees with the number displayed in the *wpsfail.res* file.

Test 4 results (PASS/FAIL): **PASS**

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 06002.01.354
Software Name: TPA Code	Versions: 5.1BetaT (Tests 1&2), 5.1BetaV (Tests 3&4)
Test ID: P-15	Test Series Name: Volcanic Ash Remobilization

Test Method

- ☐ code inspection
- ■ output inspection
- ☐ hand calculation
- ■ spreadsheet
- ■ graphical
- ☐ comparison with external code results

Test Objectives:

1. Outdoor and indoor contributions to the total inhalation dose function as intended.
2. Waste concentration factor functions properly and produces the intended effect on the resulting doses for realizations with an initial tephra deposit at the receptor location.
3. Fluvial contributions work as intended (e.g., compare test cases with 100 percent fluvial contribution and evaluate how long Fortymile Wash yields remobilized tephra).
4. Eolian contributions work as intended (e.g., compare test cases with 100 percent eolian contribution and evaluate the magnitude of the eolian dilution factor).

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): Windows XP

Input Data (files, data base, mode settings): See Attachment A

Assumptions, constraints, and/or scope of test: See Attachment A

Test Procedure: See Attachment A

Test Results

Location: See attached CD labeled "TPA 5.1 Validation Task P-15"

Test Criterion and Analysis of Results: See Attachment A for test procedure setup and test criteria. Additional information on specific input settings can be obtained from the *tpa.inp* file for each test simulation. Attachment B includes a summary of the result analysis and an evaluation for each test criterion. Additional information on test results can be obtained from the spreadsheet, *ashremob.out*, *totdose.res*, and *tpa.out* files.

Overall Test Evaluation (Pass/Fail): **PASS**

Notes:

Testers: R. Benke and A. Simpkins	Date: April 27, 1007

Attachment A

TPA Version 5.1 Validation
Task P-15 Test Description

This attachment describes the four individual tests. All validation tests were performed with the following flag settings: VolcanismDisruptiveScenarioFlag(yes=1,no=0) set to 1, DirectReleaseOnlyFlag(yes=1,no=0) set to 1, and AshEvolutionMode[0=no_ashremob,1=ashremob] set to 1.
Refer to the individual tests for additional information on input settings.

TEST 1 (Initial deposit at receptor location contribution only)

Assumptions, constraints, and/or scope of test.
Use only those realizations with initial deposit exceeding 1-cm thickness (i.e. initial mass per unit area exceeding 1.2E+04 g/m^2 that relates to a thickness of 1.2E+04g/m2 * 1E-04 m2/cm2 / 1.2 g/cm3 = 1.0 cm)

Examine remob_lut.data file results in using the following values for AshPlumeRealizationIndex[]: 74, 193, 258, 476, 489, 582, 610, 705, 855, 916, 999.

Include a case without an initial deposit at the receptor location AshPlumeRealizationIndex[]=1
Perform tests at two different event times: 100 yr and 500,000 yr

Input data (files, data base, mode settings) modified from default.
DurationOfCompliancePeriod[yr]=1E+04 for 100 yr volcano and 1E+06 for 500,000 yr volcano
MaximumTime[yr]=1E+04 for 100 yr volcano and 1E+06 for 500,000 yr volcano
NumberOfRealizations=1
TimeOfNextVolcanicEventinRegionOfInterest=100 yr or 500,000 yr
AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]=5.5E-03
AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]=5.5E-04
AirborneMassLoadInsideHeavyDisturbance[g/m3]=5.3E-04
AirborneMassLoadInsideLightDisturbance[g/m3]=5.3E-05
AshPlumeRealizationIndex[]= One of {74, 193, 258, 476, 489, 582, 610, 705, 855, 916, 999}
WeightingFactorInitialDeposit[]=1.0
WeightingFactorFluvial[]=0.0
WeightingFactorEolian[]=0.0

Include 500,000-year-event simulation (HINT: To use finer timesteps for 500,000-year-event explore alternative values for RatioOfLastToFirstTimeStepInCompliancePeriod and RatioOfLastToFirstTimeStepAfterCompliancePeriod)

Test Criteria
Check the time dependence of H_RMEI_outdoor & H_RMEI
-Verify highest values are for the time of the event and decrease with time following the event
-Verify that values level off at 100 years following the event
-Verify that values decrease when the ash deposit thickness decreases to less than the

resuspendible layer thickness (0.3 cm)

Check the time dependence of H_RMEI_indoor
-Verify constant value until ash deposit thickness decreases to less than the resuspendible layer thickness (0.3 cm)

Check and verify that H_RMEI_offsite is zero.

Check the time dependence of ashmassheavy and ashmasslight
-Verify highest values are for the time of the event and decrease with time following the event.
-Verify that values level off at 100 years following the event

For the time of the event, plot realization inhalation dose with its HLW concentration factor value
-Verify that the higher HLW concentration factors result in higher realization inhalation doses

For the case without an initial deposit at the receptor location, verify zero values of H_RMEI_outdoor, H_RMEI_indoor, H_RMEI & H_RMEI_offsite.

TEST 2 (Fluvial contribution only)

<u>Assumptions, constraints, and/or scope of test</u>
Constrain code 100% contribution from the fluvial source region
Perform test for realizations with small and large tephra masses in Fortymile Wash
Perform tests at two different event times: 100 yr and 500,000 yr

<u>Input data (files, data base, mode settings) modified from default</u>
DurationOfCompliancePeriod[yr]=1E+04 for 100 yr volcano and 1E+06 for 500,000 yr volcano
MaximumTime[yr]=1E+04 for 100 yr volcano and 1E+06 for 500,000 yr volcano
NumberOfRealizations=1
TimeOfNextVolcanicEventinRegionOfInterest=100 yr and 500,000 yr
AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]=5.5E-03
AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]=5.5E-04
AirborneMassLoadInsideHeavyDisturbance[g/m3]=5.3E-04
AirborneMassLoadInsideLightDisturbance[g/m3]=5.3E-05
WeightingFactorInitialDeposit[]=0.0
WeightingFactorFluvial[]=1.0
WeightingFactorEolian[]=0.0
Set AmbientSedimentYieldVolumePerBasinAreaPerEvent[m/event] to a constant at 3.0E-05
Set PostEruptionFluvialAshYieldVolumePerAreaPerEvent[m/event] to a constant at 6.0E-05

Comment out sediment and ash yield correlations; see following lines:
correlateinputs
AmbientSedimentYieldVolumePerBasinAreaPerEvent[m/event]
PostEruptionFluvialAshYieldVolumePerAreaPerEvent[m/event]
0.99

Assign zero values for HLW mass in the initial deposit column of the lookup table

Perform test for realizations with small and large tephra masses in Fortymile Wash by setting AshplumeRealizationIndex equal to 826 or 397 for a low or high fluvial mass deposited.

Include 500,000-year-event simulation (HINT: To use finer timesteps for 500,000-year-event explore alternative values for RatioOfLastToFirstTimeStepInCompliancePeriod and RatioOfLastToFirstTimeStepAfterCompliancePeriod)

Test Criteria
Check the time dependence of fluvial airborne mass load, H_RMEI_outdoor, H_RMEI_indoor, and H_RMEI
-Verify constant value following the eruption and zero value after t_duration

Check and verify that H_RMEI_offsite is zero

Infer t_duration values (time that Fortymile Wash yields contaminated sediment) from the dose results and compare to offline calculations of t_duration
-Verify that t_duration values match to within 5 percent (maximum time may need to be increased to determine t_duration for a large fluvial deposit)

TEST 3 (Eolian contribution only)

Assumptions, constraints, and/or scope of test
Constrain code 100% contribution from the eolian source region
Perform test for realizations with small and large tephra masses in eolian source region
Perform tests at two different event times: 100 yr and 500,000 yr

Input data (files, data base, mode settings) modified from default
DurationOfCompliancePeriod[yr]=1E+04 for 100 yr volcano and 1E+06 for 500,000 yr volcano
MaximumTime[yr]=1E+04 for 100 yr volcano and 1E+06 for 500,000 yr volcano
NumberOfRealizations=1
TimeOfNextVolcanicEventinRegionOfInterest=100 yr and 500,000 yr
AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]=5.5E-03
AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]=5.5E-04
AirborneMassLoadInsideHeavyDisturbance[g/m3]=5.3E-04
AirborneMassLoadInsideLightDisturbance[g/m3]=5.3E-05
WeightingFactorInitialDeposit[]=0.0
WeightingFactorFluvial[]=0.0
WeightingFactorEolian[]=1.0
Assign zero values for HLW mass in the initial deposit column of the lookup table
Perform test for realizations with small and large tephra masses in eolian source region
Include 500,000-year-event simulation

Test Criteria
Check the time dependence of H_RMEI_outdoor & H_RMEI

-Verify highest values are for the time of the event and decrease with time following the event
-Verify that values level off at 100 years following the event
[Ash deposit thickness is used differently in the eolian source region, and its comparison to the resuspendible layer thickness over time, as was done for the initial tephra deposit case in Test 1, is not necessary. An offline calculation of the dilution factor, which is dependent on the ash deposit and resuspendible layer thicknesses, is included for the eolian source region below.]

Check the time dependence of H_RMEI_indoor
-Verify short-term values decrease to a constant value at about 100 years following the event

Check and verify that H_RMEI_offsite is zero

Obtain *ashremob.out* intermediate results for the eolian source region: (i) time-dependent airborne concentration of HLW, H_e, and (ii) time-dependent airborne mass load. Use these intermediate results and values for other inputs to infer a time history of the eolian dilution factor (d_e).
-Verify that 0 ≤dilution factor ≤ 1 and the dilution factor is constant in time after the eruption.

Calculate the dilution factor offline using only input parameter and lookup table parameters. Compare the dilution factors from TPA code inputs and intermediate results (above) with the values calculated offline
-Verify differences in the dilution factors are less than 10 percent

Compare the values for the dilution factor for the two realizations with small and large tephra masses in the eolian source region.
-Check and verify that dilution factor(small tephra mass case) < dilution factor(large tephra mass case)

TEST 4 (Default weights for initial deposit, fluvial, and eolian contributions)

Assumptions, constraints, and/or scope of test
Full stochastic run with 1024 realizations
Assimilate output into average values over all realizations

Input data (files, data base, mode settings) modified from default
DurationOfCompliancePeriod[yr]=1E+04 for 100-yr volcano and 1E+06 for 500,000-yr volcano
MaximumTime[yr]=1E+04 for 100-yr volcano and 1E+06 for 500,000-yr volcano
NumberOfTimeStepsInCompliancePeriod=51 for 100-yr volcano
NumberOfRealizations=1024
StopAtRealization=1024
TimeOfNextVolcanicEventinRegionOfInterest=100 and 500,000 yr
AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]=5.5E-03
AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]=5.5E-04
AirborneMassLoadInsideHeavyDisturbance[g/m3]=5.3E-04
AirborneMassLoadInsideLightDisturbance[g/m3]=5.3E-05
WeightingFactorInitialDeposit[]=0.3334 (Default)

WeightingFactorFluvial[]=0.3333 (Default)
WeightingFactorEolian[]=0.3333 (Default)

Include 500,000-year-event simulation
NumberOfTimeStepsInCompliancePeriod=5001 for 500,000-yr volcano
RatioOfLastToFirstTimeStepInCompliancePeriod=1.0
NumberOfTimeStepsAfterCompliancePeriod=0

Remember to refresh lookup table to unmodified version

<u>Test Criteria</u>
Check the time dependence of H_RMEI_outdoor & H_RMEI
-Verify highest values are for the time of the event
-Verify that short-term spike immediately following the eruption (within 100 years) transitions to a longer-term values at later times
-Verify overall that values decrease with increasing time

Check the time dependence of H_RMEI_indoor
-Verify higher values near the time of the eruption with an overall decrease over time in the first 5,000 years following eruption

Check and verify that H_RMEI_offsite is zero

Check the time dependence of ashmassheavy and ashmasslight
-Verify highest values are for the time of the event and decrease with time following the event
-Verify that values level off at 100 years following the event

Attachment B

Task P-15 Test Results

This attachment presents the results for the four individual tests. Test results and evaluations are presented for each test criterion. The test criteria from Attachment A are included in italic font. The overall evaluation for all tests of Task P-15 is PASSED.

TEST 1 (Initial deposit at receptor location contribution only)

Check the time dependence of H_RMEI_outdoor & H_RMEI
-Verify highest values are for the time of the event and decrease with time following the event
Passed

-Verify that values level off at [time periods of about] 100 years [or more] following the event
Passed

-Verify that values decrease when the ash deposit thickness decreases to less than the resuspendible layer thickness (0.3 cm)
Passed

Check the time dependence of H_RMEI_indoor
-Verify constant value until ash deposit thickness decreases to less than the resuspendible layer thickness (0.3 cm)
Passed

Check and verify that H_RMEI_offsite is zero
Passed

Check the time dependence of ashmassheavy and ashmasslight
-Verify highest values are for the time of the event and decrease with time following the event.
Passed

-Verify that values level off at 100 years following the event
Passed

For the time of the event, plot realization inhalation dose with its HLW concentration factor value
-Verify that the higher HLW concentration factors result in higher realization inhalation doses
Passed

For the case without an initial deposit at the receptor location, verify zero values of H_RMEI_outdoor, H_RMEI_indoor, H_RMEI & H_RMEI_offsite.
Passed

<u>Result Summary</u>
Results for the 100-yr and 500,000-yr event simulations are contained in the spreadsheets named Test1,100yrEruption.xls and Test1,500,000yrEruption.xls, respectively. Both spreadsheets are located in the \P15 Test 1\ folder.

Figure 1-1 shows the results for a 100-yr event simulation using Realization Index #74 of the ASHREMOB lookup table. The time dependence of H_RMEI_outdoor and H_RMEI, met the test criteria above. Ash deposit thickness becomes less than the resuspendible layer thickness of 0.3 cm somewhere near 6,500 years, as evidenced by Figure 1-1. In the spreadsheet named Test1,100 yr eruption.xls, hand calculations of this time period result in a time of 6,510 years, which is in agreement with the TPA code result. For the 500,000-yr event simulations, the time steps show that the leveling off occurs somewhere within 200 years following the eruption. H_RMEI_offsite is zero for all time steps as evidenced in the *ashremob.out* file. Figure 1-2 shows the ashmassheavy and ashmasslight mass loading values as a function of time. For the 500,000 yr eruptions, the time steps are such that it is apparent that they level off somewhere within 200 yrs following the eruption. Figure 1-3 plots the HLW concentration factor with dose for several realizations.

For Realization Index 1, all H_RMEI values are zero in *ashremob.out*. This was determined by direct inspection of output.

All the test criteria are passed for the other realizations, which can be found in the spreadsheets named Test1,100yrEruption.xls and Test1,500,000yrEruption.xls.

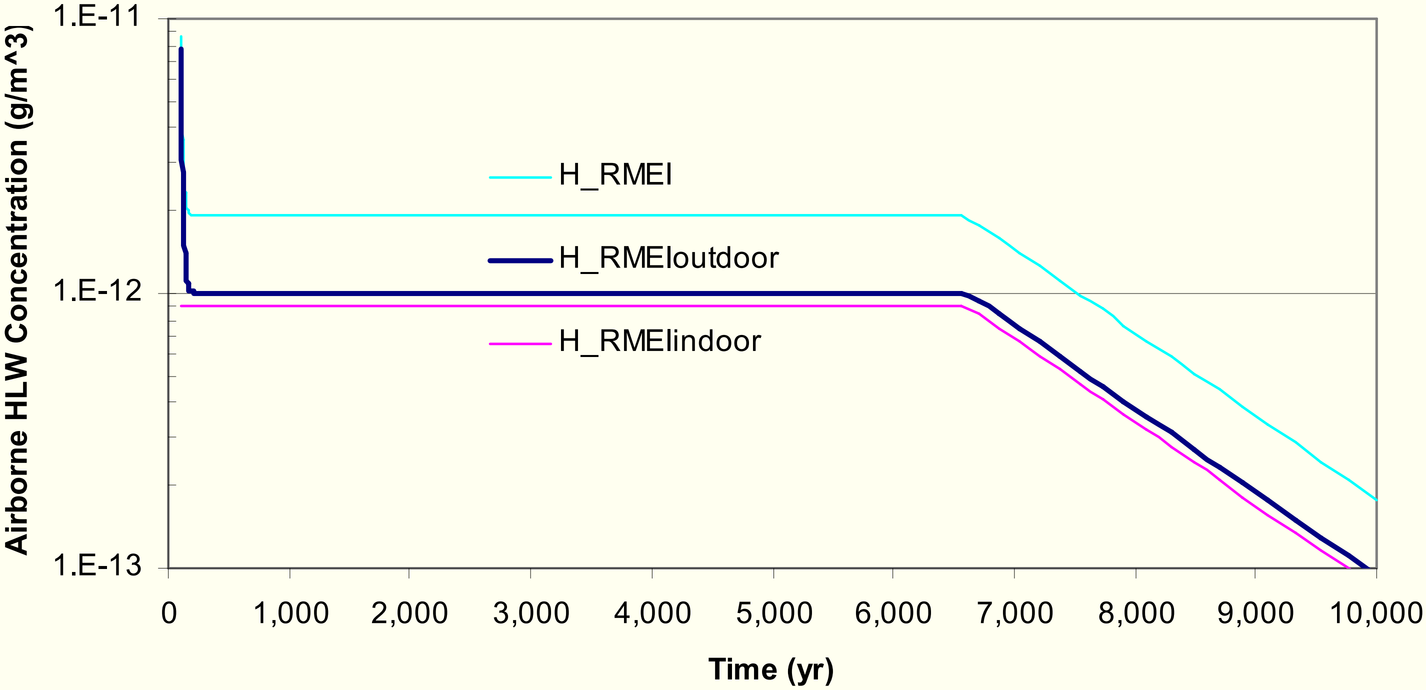


Figure 1-1. Realization index 74 results for an eruption at 100 years

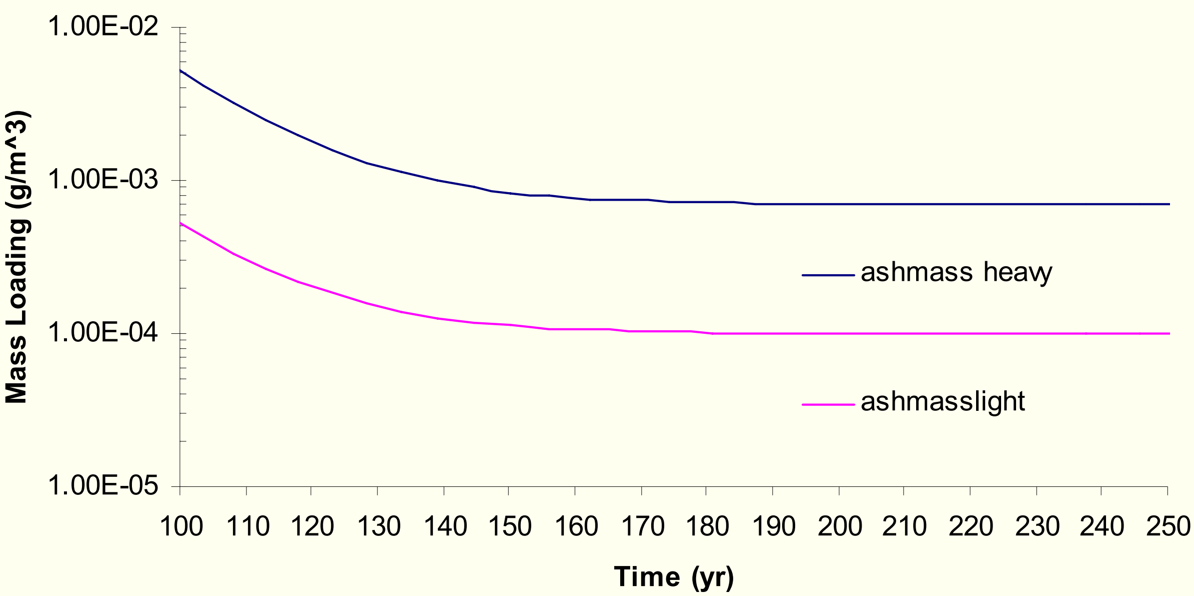


Figure 1-2. Airborne mass loading for ash following an eruption at 100 years for realization index 74

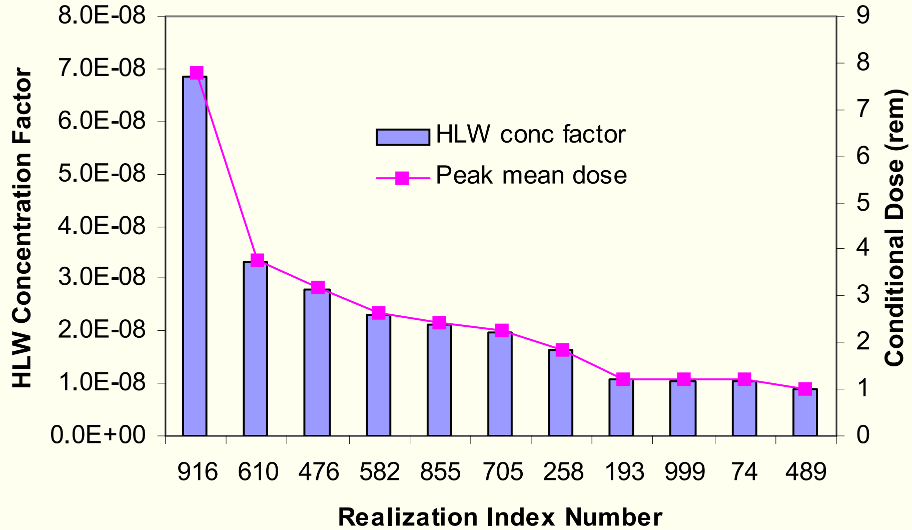


Figure 1-3. Influence of HLW Concentration Factor on Conditional Dose

TEST 2 (Fluvial contribution only)

Check the time dependence of fluvial airborne mass load, H_RMEI_outdoor, H_RMEI_indoor, and H_RMEI
-Verify constant value following the eruption and zero value after t_duration
Passed

Check and verify that H_RMEI_offsite is zero
Passed

Infer t_duration values (time that Fortymile Wash yields contaminated sediment) from the dose results and compare to offline calculations of t_duration
-Verify that t_duration values match to within 5 percent (maximum time may need to be increased to determine t_duration for a large fluvial deposit)
Passed

Result Summary

Results are contained in the spreadsheet named *Test2.xls*, which is located in the \P15 Test 2\ folder. Figure 2 and *ashremob.out* show that the fluvial deposit is gone at a time of around 200 yrs or 100 yrs posteruption. This agrees with spreadsheet calculations of 103 yr, shown in the t_duration workbook within the *Test2.xls* spreadsheet. H_RMEI, H_RMEI outdoor, and H_RMEI indoor are constant and nonzero during the 100 years posteruption and drop to zero afterwards to represent complete depletion of contaminated tephra from Fortymile Wash. Realization indexes 397 and 826 did not require modification of the lookup table for testing purposes. Other results are in agreement as well.

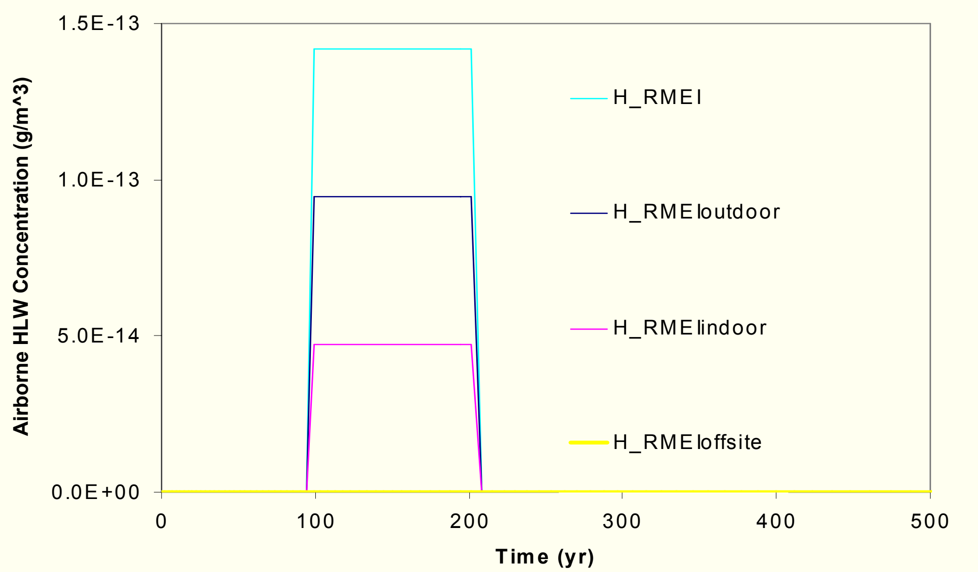


Figure 2. Fluvial contribution from realization index 826 for an eruption at 100 years

100-yr Eruption Time

Looking at the *totdos.res* file for realization index 826 with the 100-yr eruption time, the first dose was reported at 98.89 years and the last was reported at 200.98 yrs, which corresponds to a t_duration of 102.1 yrs. This is in agreement with the 103 yr duration, calculated in the *Test2.xls* file. The 5-percent criterion was met for the 100-yr event simulation.

For realization index 397 with the 100-yr eruption time, the 10,000-yr eruption doses continue over the entire simulation period, which does allow for a t_duration comparison. To reconcile this situation, an additional simulation was performed with an increased simulation time and number of time steps, so that t_duration could be assessed from *totdos.res* with an accuracy sufficient for the 5-percent test criterion. The files for this additional simulation are named *tpa397,100,longsim.inp*, *tpa397,100,longsim.out*, *ashremob397,100,longsim.out*, and *totdos397,100,longsim.res*. From *totdos397,5 100,longsim.res*, the first and last doses were reported at 100 years and 41,440 years and correspond to a t_duration value of 41,340 yrs, which is within 5 percent of the 41,300-yr value calculated in *Test2.xls*.

500,000-yr Eruption Time

For realization index 826 with the 500,000-yr eruption, only dose shown in the *totdose397,500000.res* file is at 4.9451E+05 yrs. The next time is 5.0632E+05 yrs, which indicates the time step after the eruption is too large to apply the 5-percent criterion. To reconcile this situation, an additional simulation was performed with a reduced simulation time of 500,000 yrs, a maximum number of time steps of 5,001, and the eruption time moved to 400,000 yrs. The files for this additional simulation are named *tpa826,400000,5001timesteps.inp*, *tpa826,400000,5001timesteps.out*, *ashremob826,400000,5001timesteps.out*, and *totdos826,400000,5001timesteps.res*. From *totdos826,400000,5001timesteps.res*, the first and last doses were reported at 400,000 years and 400,100 years and correspond to a t_duration value of 100 yrs, which is within 5 percent of the 103-yr value calculated in *Test2.xls*.

Doses for realization index 397 with a 500,000-yr eruption are shown in *totdose397,500000.res* for a time period corresponding to 36,360 yrs, which differs from the 41,300 yrs calculated in the spreadsheet. Due to the large time steps of about 12,000 years, the 5 percent criterion could not be applied for this simulation. To reconcile this situation, an additional simulation was performed with an increased number of time steps (i.e., `NumberOfTimeStepsInCompliancePeriod` was set to 2001 and `RatioOfLastToFirstTimeStepInCompliancePeriod` was set to 1.0), so that t_duration could be assessed from *totdos.res* with an accuracy that is sufficient for the 5-percent test criterion. The files for this additional simulation are named *tpa397,500000,2001timesteps.inp*, *tpa397,500000,2001timesteps.out*, *ashremob397,500000,2001timesteps.out*, and *totdos397,500000,2001timesteps.res*. From *totdos397,500000,2001timesteps.res*, the first and last doses were reported at 500,000 years and 541,000 years and correspond to a t_duration value of 41,000 yrs, which is within 5 percent of the 41,300-yr value calculated in the spreadsheet.

The criteria were passed for the other tests (see *Test2.xls* for results). Results from the additional simulations, described on this page, are contained in the previously mentioned files; the *Test2.xls* spreadsheet does not contain the results for the additional simulations.

TEST 3 (Eolian contribution only)

Check the time dependence of H_RMEI_outdoor & H_RMEI
-Verify highest values are for the time of the event and decrease with time following the event
PASSED

-Verify that values level off at 100 years following the event
PASSED

Check the time dependence of H_RMEI_indoor
-Verify short-term values decrease to a constant value at about 100 years following the event
PASSED

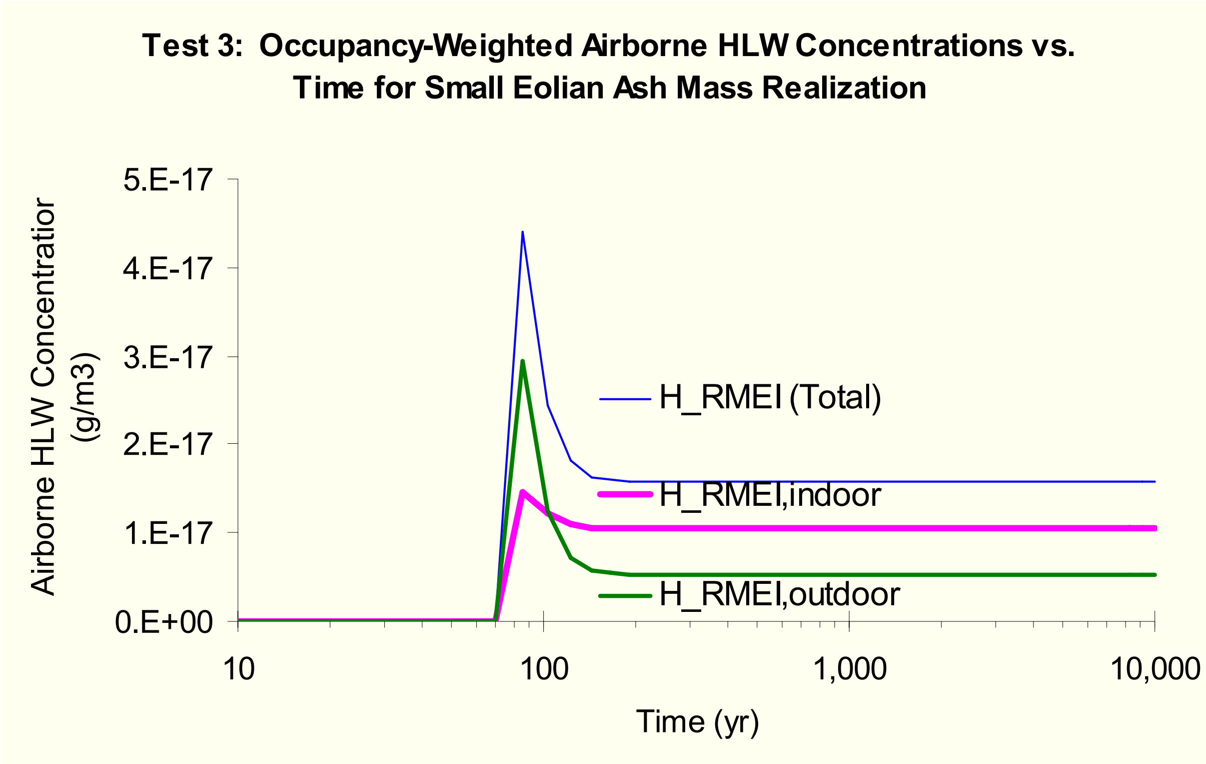
Check and verify that H_RMEI_offsite is zero
PASSED

Obtain ashremob.out intermediate results for the eolian source region: (i) time-dependent airborne concentration of HLW, H_e (9th column), and (ii) time-dependent airborne mass load [for ash with light disturbance (5th column)]. Use these intermediate results and values for other inputs to infer a time history of the eolian dilution factor (d_e).
-Verify that 0 ≤dilution factor ≤ 1 and the dilution factor is constant in time after the eruption.
PASSED

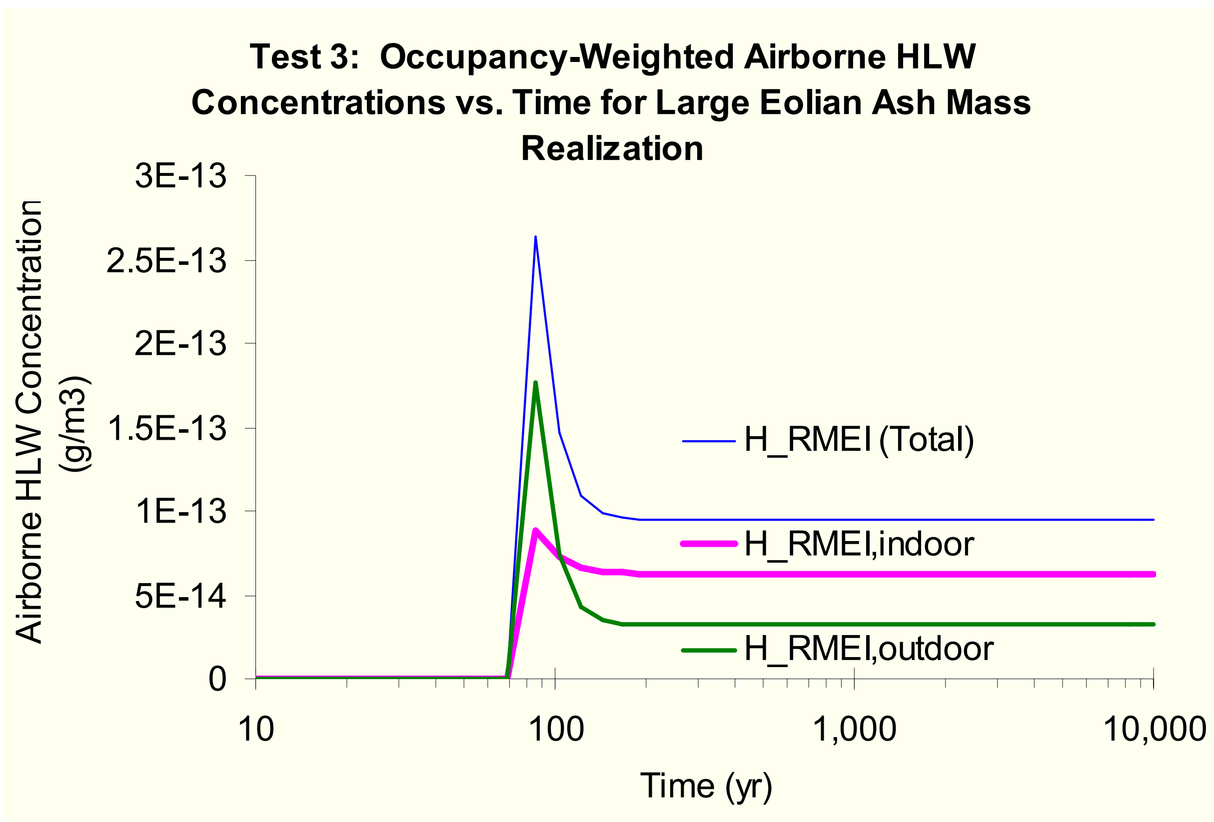
Calculate the dilution factor offline using only input parameter and lookup table parameters. Compare the dilution factors from TPA code inputs and intermediate results (above) with the values calculated offline
-Verify differences in the dilution factors are less than 10 percent
PASSED

Compare the values for the dilution factor for the two realizations with small and large tephra masses in the eolian source region.
-Check and verify that dilution factor(small tephra mass case) < dilution factor(large tephra mass case)
PASSED

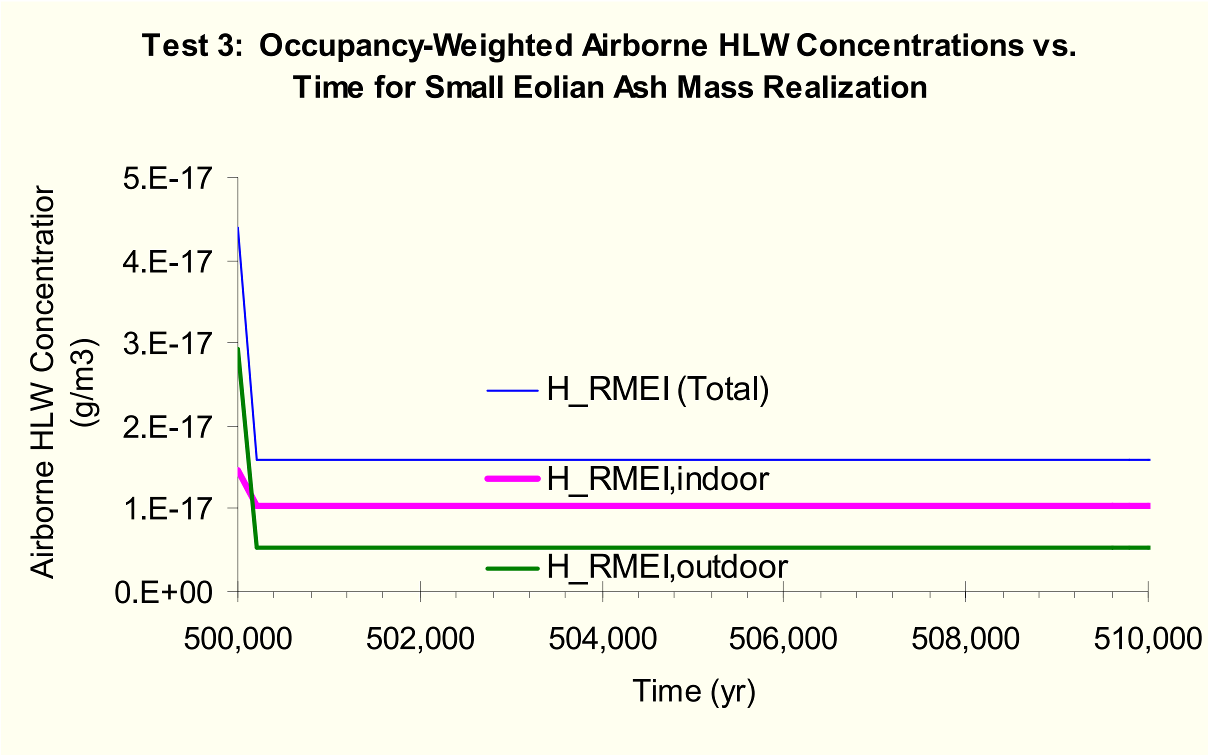
Result Summary
Results and offline dilution factor calculations for the 100-yr and 500,000-yr event simulations are contained in the spreadsheets named Test3_100yr.xls and Test3_500ka.xls, respectively. Both spreadsheets are located in the \P15 Test 3\ folder. Additional supporting files are contained in the subfolders named SmallMash-e_100yr, LargeMash-e_100yr, SmallMash-e_500ka, and LargeMash-e_500ka. Realization indexes of 64 and 189 were used for the small and large eolian ash mass cases, respectively, and did not require modification of the lookup table for testing purposes. Figures of Test 3 results are presented next for the two eruption times of 100 and 500,000 years.

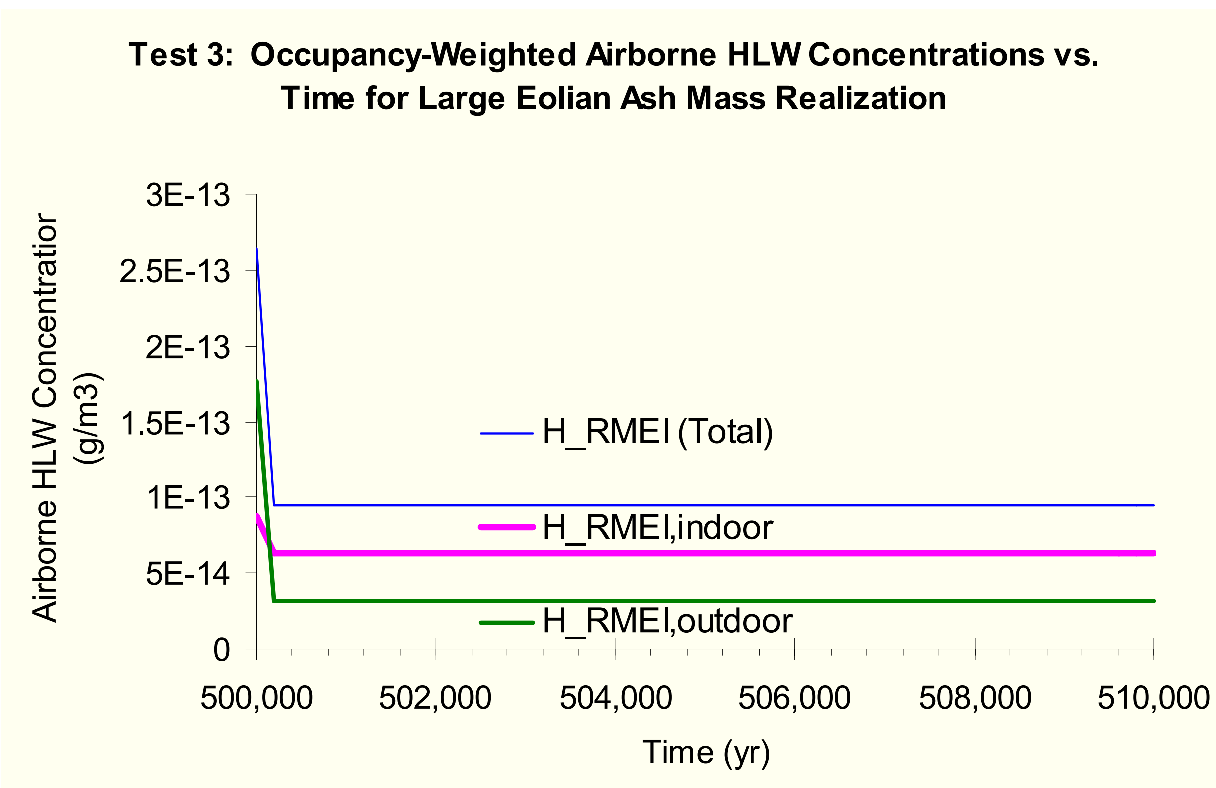


Test 3: Occupancy-Weighted Airborne HLW Concentrations vs. Time for Small Eolian Ash Mass Realization
Airborne HLW Concentratior (g/m3)
5.E-17
4.E-17
3.E-17
2.E-17
1.E-17
0.E+00
10
100
1,000
10,000
Time (yr)
H_RMEI (Total)
H_RMEI,indoor
H_RMEI,outdoor



Test 3: Occupancy-Weighted Airborne HLW Concentrations vs. Time for Large Eolian Ash Mass Realization
Airborne HLW Concentration (g/m3)
3E-13
2.5E-13
2E-13
1.5E-13
1E-13
5E-14
0
10
100
1,000
10,000
Time (yr)
H_RMEI (Total)
H_RMEI,indoor
H_RMEI,outdoor


Test 3: Occupancy-Weighted Airborne HLW Concentrations vs. Time for Small Eolian Ash Mass Realization
Airborne HLW Concentratior (g/m3)
5.E-17
4.E-17
3.E-17
2.E-17
1.E-17
0.E+00
500,000
502,000
504,000
506,000
508,000
510,000
Time (yr)
H_RMEI (Total)
H_RMEI,indoor
H_RMEI,outdoor


Test 3: Occupancy-Weighted Airborne HLW Concentrations vs. Time for Large Eolian Ash Mass Realization
Airborne HLW Concentratior (g/m3)
3E-13
2.5E-13
2E-13
1.5E-13
1E-13
5E-14
0
500,000
502,000
504,000
506,000
508,000
510,000
Time (yr)
H_RMEI (Total)
H_RMEI,indoor
H_RMEI,outdoor

TEST 4 (Default weights for initial deposit, fluvial, and eolian contributions)

Check the time dependence of H_RMEI_outdoor & H_RMEI
-Verify highest values are for the time of the event
PASSED
-Verify that short-term spike immediately following the eruption (within 100 years) transitions to a longer-term values at later times
PASSED
-Verify overall that values decrease with increasing time [after the event]
PASSED

Check the time dependence of H_RMEI_indoor
-Verify higher values near the time of the eruption with an overall decrease over time in the first 5,000 years following eruption
PASSED

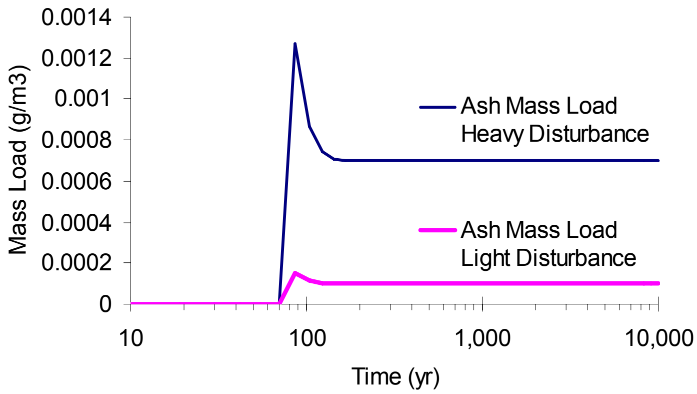
Check and verify that H_RMEI_offsite is zero
PASSED

Check the time dependence of ashmassheavy and ashmasslight [2nd & 3rd columns of ashremob.out]
-Verify highest values are for the time of the event and decrease with time following the event
PASSED
-Verify that values level off at 100 years following the event
PASSED

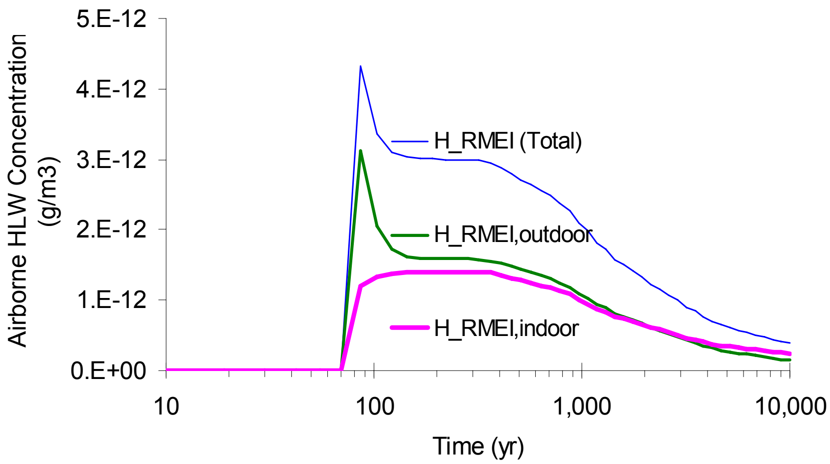
Result Summary

Results for the 100-yr and 500,000-yr event simulations are contained in the spreadsheets named Test4_100yr.xls and Test4_500ka.xls, respectively. Both spreadsheets are located in the \P15 Test 4\ folder. Additional supporting files are contained in the subfolders named 100yrEruption and 500kaEruption. Figures of Test 4 results are presented next for the two eruption times of 100 and 500,000 years.

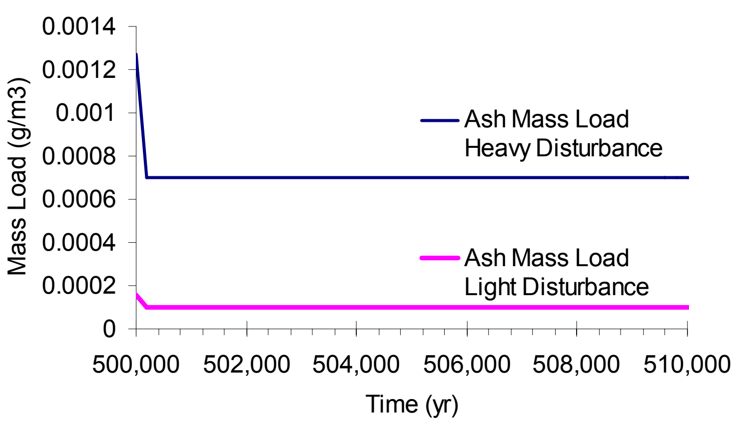
Test 4: Time Dependence of Ash Mass Loads for Any Initial Deposit at Receptor Location (Average of 1024 Realizations)

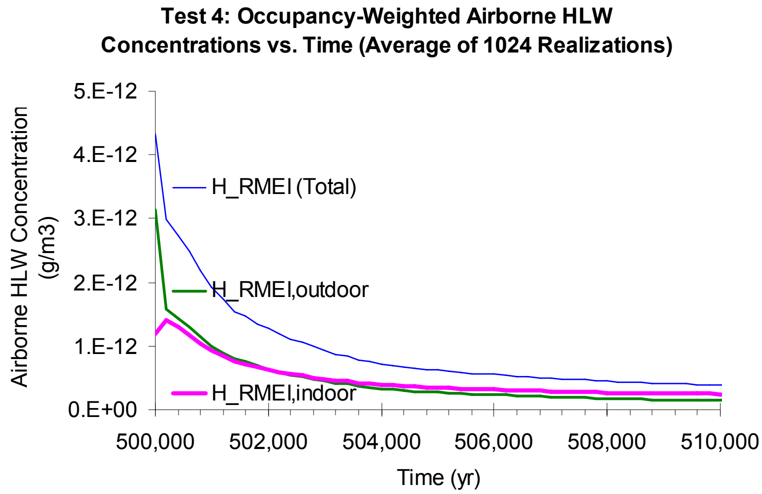


Test 4: Occupancy-Weighted Airborne HLW Concentrations vs. Time (Average of 1024 Realizations)



Test 4: Time Dependence of Ash Mass Loads for Any Initial Deposit at Receptor Location (Average of 1024 Realizations)




Test 4: Occupancy-Weighted Airborne HLW Concentrations vs. Time (Average of 1024 Realizations)
Airborne HLW Concentration (g/m3)
5.E-12
4.E-12
3.E-12
2.E-12
1.E-12
0.E+00
H_RMEI (Total)
H_RMEI,outdoor
H_RMEI,indoor
500,000
502,000
504,000
506,000
508,000
510,000
Time (yr)

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 06002.01.354	
Software Name: TPA Code		Version: 5.1BetaV, 5.1 BetaW
Test ID: **P-16**	Test Series Name: Inhalation Pathway Dose from Ground Surface (DCAGS and ASHREMOB)	

Test Method

- ☐ code inspection
- ■ output inspection
- ■ hand calculation
- ■ spreadsheet
- ☐ graphical
- ☐ comparison with external code results

Test Objectives: See Attachment A

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): Windows XP

Input Data (files, data base, mode settings): See Attachment A

Assumptions, constraints, and/or scope of test: See Attachment A

Test Procedure: See Attachment A

Test Results

Location: See Attached CD labeled “TPA Version 5.1 Validation Task P-16"

Test Criterion and Analysis of Results: See Attachment A for test criteria

Test Evaluation (Pass/Fail): PASS

Notes:

Testers: P. LaPlante, R. Benke (contributor)	Date: 5/06/07

Attachment A

(Test Cases for Tasks P-16, inhalation dose tests only)

TEST 1

Verification of Inhalation Dose Calculations in DCAGS

Modifications to input files:

Data file *gnewdf.dat* is edited so all ICRP72 ingestion dose coefficients for an adult receptor are set to zero. Similarly *ggrdf.dat* file is edited so all FGR12 external dose coefficients for ground surface are zero. (these changes will produce dose output from a DCAGS run that is only for inhalation pathway).

Test uses TPA run of an otherwise unmodified base case *tpa.inp,* with changed input parameters as follows:

OutputMode(0=None,1=All,2=UserDefined) set to 1 (all),
VolcanismDisruptiveScenarioFlag (yes=1,no=0) set to 1 (yes)
AshEvolutionMode[0=no_ashremob,1=ashremob] set to 0
NumberOfRealizations set to 20
StopAtRealization set to 20
SelectAppendFiles set to 1
TimeOfNextVolcanicEventinRegionOfInterest[yr] set to constant, 100

A second run is done similar to the first, however, the mass loading and occupancy fractions input parameters are arbitrarily modified to values different from the default values to verify that these inputs are functioning as expected. These modifications include the following additional changes to input parameters:

constant
AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]
3.0e-2
****
constant
AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]
7.5e-4
****
constant
AirborneMassLoadOutsideHeavyDisturbance[g/m3]
2.0e-3
****
constant
AirborneMassLoadOutsideLightDisturbance[g/m3]
8.0e-4
****
constant
AirborneMassLoadInsideHeavyDisturbance[g/m3]
2.00e-4
****
constant

AirborneMassLoadInsideLightDisturbance[g/m3]
1.20e-5
****
constant
AirborneMassLoadOffsite[g/m3]
0.0
****
constant
OccupancyFractionOutsideHeavyDisturbance[]
0.225
****
constant
OccupancyFractionOutsideLightDisturbance[]
0.104
****
constant
OccupancyFractionInsideHeavyDisturbance[]
0.084
****
constant
OccupancyFractionInsideLightDisturbance[]
0.483
****
constant
OccupancyFractionOffsite[]
0.104

Utility codes needed in the analysis of the test data:
Microsoft Excel2002

Test description:

Objective:
Verification of Inhalation Dose Calculations in DCAGS including:

A. Verification of calculations in DCAGS that convert ground surface radionuclide concentrations provided by ASHRMOVO module to radionuclide specific inhalation doses written to TPA output file *airpkds_c.res* using input parameters from *tpa.inp* and dose coefficients from *gnewdf.dat* file.

B. Verification that data files *tpa.inp*, *gnewdf.dat*, and output from ASHRMOVO module are being read correctly by the TPA code for the calculation of inhalation dose from ground surface deposition of radionuclides resulting from an igneous event.

C. Verification that TPA inhalation dose output for ground surface from the DCAGS module is written correctly to file *airpkds_c.res.*

D. Verification that new DCAGS inhalation dose input parameters for mass loads and occupancy fractions are functioning in the calculations as expected.

Assumptions:
This test verifies TPA calculations of inhalation dose in DCAGS for a 20 realization run which is assumed to represent stochastic code operations. A second run with changed mass loads and occupancy

fractions verifies that results change as expected when these inputs are changed. Previously validated portions of the calculations are assumed to be working as intended. This test is designed to check parts of the calculations that were changed since TPA version 5.0.

Constraints:
Test is limited to verifying calculations in a 20 realization run using constants for mass load to allow efficient verification calculations on a spreadsheet.

Output files to compare or examine:
From TPA Run:
ashrmovo.rlt, ashout.res, airpkds_c.res

Step-by-step test procedure:

Set environment variables to point to directory where current version of TPA code resides:

set TPA_TEST=c:\TPA51betaV\
set TPA_DATA=c:\TPA51betaV\

Create alias in Windows XP that will allow running the TPA code from its original directory using the *tpa.inp* file in a unique test directory by typing the execution command ..\tpa.exe >tpa.out at the command prompt from the unique test directory.

Run an unmodified reference case *tpa.inp* file with the input parameter changes previously described.

Copy output from TPA files to appropriate cells of the spreadsheet (the same approach applies to both runs). From *ashrmovo.rlt* copy the ground surface deposition values (Ci/m^2) for each radionuclide (Am-241, Pu-238, Pu-239, Pu-240) and realization. These radionuclides have been shown in prior analyses to be important contributors to the igneous release inhalation dose calculation (NRC, 2005). From *ashout.res* copy the areal ash density (g/cm^2), ash thickness (cm) and clean soil dilution factor for each realization. For any rows on the spreadsheet with ash thickness less than the thickness of the resuspension layer, include the formula for the clean soil dilution factor under the clean soil dilution column (otherwise set to 1.0). From *airpkds_c.res* copy dose values by radionuclide and realization. Copy adult ICRP 72 inhalation dose coefficients for four key radionuclides from *gnewdf.dat* to the appropriate section of spreadsheet.

For the 2nd set of runs (based on modified mass loads and occupancy fraction inputs), use appropriate portions of equations 1, 2, and 3 (the inhalation dose calculation in DCAGS), to compute the average annual mass load (for input to the spreadsheet) from the modified values for the mass loads and occupancy fractions (in *tpa.inp*) used in the test run. This is done for the year of the eruption as the sum of variables C_1 and C_2 (i.e., no contribution by rate of reduction of mass loading with time, $\lambda_r t$).

In DCAGS, the inhalation dose per year (rem/yr) for the j^{th} radionuclide is calculated as

$$D_{\text{inh},j}(t) = BI_j \eta_j(t) f_R(t) U_{conv}\left[C_1 e^{-\lambda_r t} + C_2\right] \quad (1)$$

with

$$\begin{aligned} C_1 = {} & f_{\text{out-H}}\left(S_{\text{ash,out-H}} - S_{\text{out-H}}\right) + f_{\text{out-L}}\left(S_{\text{ash,out-L}} - S_{\text{out-L}}\right) \\ & + f_{\text{in-H}} S_{\text{in-H}} + f_{\text{in-L}} S_{\text{in-L}} + f_{\text{offsite}} S_{\text{offsite}} \end{aligned} \quad (2)$$

and

$$C_2 = f_{\text{out}-H} S_{\text{out}-H} + f_{\text{out}-L} S_{\text{out}-L} \tag{3}$$

where

B	—	Breathing rate [cm^3/s] as specified by the *tpa.inp* parameter InhalationRate5[cm3/s] {for *tpa.inp* parameter Age&Dosimetry[1=Inf,2=Todl,3=PTeen,4=Teen,5=Adlt,6=AdltFG11] equal to 5}
I_j	—	Inhalation dose coefficient per unit intake [Sv/Bq] for the j^{th} radionuclide provided in the auxiliary data file, *gnewdf.dat*
$\eta_j(t)$	—	Time-dependent activity of the j^{th} radionuclide per gram of ash near the receptor location [Ci/g] computed by DCAGS (Eq. 17-6)
$f_R(t)$	—	Fraction of airborne particulate mass resuspended from the contaminated volcanic ash layer [unitless] computed by DCAGS (Eq. 17-7)
λ_r	—	Rate of reduction of airborne mass load [1/yr]as specified by the *tpa.inp* parameter RateOfReductionOfMassLoadingFactor[1/yr]
f_{out-H}	—	Fraction of time receptor spends outdoors with heavy disturbance [unitless] as specified by the *tpa.inp* parameter OccupancyFractionOutsideHeavyDisturbance[]
$S_{ash,out-H}$	—	Outdoor mass load above fresh ash with heavy distrubance [g/m^3] as specified by the *tpa.inp* parameter AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3]
S_{out-H}	—	Outdoor mass load above soil with heavy disturbance [g/m^3] as specified by the *tpa.inp* parameter AirborneMassLoadOutsideHeavyDisturbance[g/m3]
f_{out-L}	—	Fraction of time receptor spends outdoors with light disturbance [unitless] as specified by the *tpa.inp* parameter OccupancyFractionOutsideLightDisturbance[]
$S_{ash,out-L}$	—	Outdoor mass load above fresh ash with light disturbance [g/m^3] as specified by the *tpa.inp* parameter AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3]
S_{out-L}	—	Outdoor mass load above soil with light disturbance [g/m^3] as specified by the *tpa.inp* parameter AirborneMassLoadoutsideLightDisturbance[g/m3]
f_{in-H}	—	Fraction of time receptor spends indoors with heavy disturbance as specified by the *tpa.inp* parameter OccupancyFractionInsideHeavyDisturbance[]
S_{in-H}	—	Indoor mass load for dust with heavy disturbance (g/m^3) as specified by the *tpa.inp* parameter AirborneMassLoadInsideHeavyDisturbance[g/m3]
f_{in-L}	—	Fraction of time receptor spends indoors with light disturbance as specified by the *tpa.inp* parameter OccupancyFractionInsideLightDisturbance[]
S_{in-L}	—	Indoor mass load for dust with light disturbance (g/m^3) as specified by the *tpa.inp* parameter AirborneMassLoadInsideLightDisturbance[g/m3]
$f_{offsite}$	—	Fraction of time receptor spends offsite as specified by the *tpa.inp* parameter OccupancyFractionOffsite[]
$S_{offsite}$	—	Offsite airborne mass load [g/m^3] as specified by the *tpa.inp* parameter AirborneMassLoadOffsite[g/m3]
U_{conv}	—	Factor used to implement unit conversions

Compare spreadsheet calculated dose results with the TPA code output copied from *airpkds_c.res* for each realization for both sets of runs.

Pass/fail criteria:
Test passes if:
–dose results reported by the TPA code (in airpkds_c.res) in both sets of test runs agree with the relevant spreadsheet calculated doses (within an error tolerance of 5%).

Test Results:

Deviation from test plan: All test code runs were executed directly from the root directory where the TPA5.1BetaV code was installed and output files were manually copied to archive directories. This change is not expected to have any impact on test results.

Results are archived in an attached CD in directory \P16\Test1
Spreadsheet that demonstrates results of test is *DCAGS-ValidationTest.xls*

All dose results compared on the spreadsheet agree with code test run results.

Overall Test Status (**PASS/FAIL**/): **PASS**

References:

NRC. NUREG-1762. "Integrated Issue Resolution Status Report". Vol2, Rev. 1. Washington DC: Nuclear Regulatory Commission. April, 2005, Appendix D, Figure 4-46.

TEST2

Verification of Age Dependent Dosimetry Functionality for DCAGS Inhalation Dose

Modifications to input files:

Dose coefficient data file *gnewdf.dat* is edited so all ICRP72 ingestion dose coefficients for receptor age groups Toddler, Adult, and Adult FG11 are set to zero. Similarly the edited *ggrdf.dat* file from TEST 1 (with all FGR12 external dose coefficients for ground surface at zero) is used for this test as well. These changes will produce dose output from a DCAGS run that is only for the inhalation pathway.

Test uses TPA runs of an otherwise unmodified base case *tpameans.out* file (copied to *tpa.inp*) with the following input changes:

OutputMode(0=None,1=All,2=UserDefined) set to 1 (all),
VolcanismDisruptiveScenarioFlag (yes=1,no=0) set to 1 (yes)
AshEvolutionMode[0=no_ashremob,1=ashremob] set to 0
NumberOfRealizations set to 1
StopAtRealization set to 1
SelectAppendFiles set to 1
TimeOfNextVolcanicEventinRegionOfInterest[yr] set to constant, 100.0
Age&Dosimetry(1=Inf,2=Todl,3=PTeen,4=Teen,5=Adlt,6=AdltFG11) set to 2, 5, 6 for consecutive sets of test runs.

Note: When Age&Dosimetry is set to a particular age group for a run, the corresponding age-dependent input parameters in the DCAGW section of tpa.inp also need to be "uncommented out" and all other non selected age group inputs need to be "commented out". These inputs include consumption rates, inhalation rate, and exposure times. Because this is an inhalation only calculation, only the InhalationExposureTime6[hr] and InhalationRate6[cm3/s] inputs are used however all for the age group will be made "active" for completeness. Tester needs to verify and ensure the values for these inputs are identical for each age group run to ensure the only difference in the computations are the dose coefficients used.

A second set of runs is done in the same manner as the first set with the exception that AshEvolutionMode[0=no_ashremob,1=ashremob] is set to 1 so ASHREMOB is run instead of ASHPLUMO, ASHRMOVO and DCAGS.

Utility codes needed in the analysis of the test data:
Microsoft Excel2002

Test description:
Objective:

To verify age dependent dosimetry functionality is implemented correctly for DCAGS and ASHREMOB inhalation dose calculations

Assumptions:

Previously validated portions of the calculations are assumed to be working as intended. This test is designed to check parts of the calculations that were changed since TPA version 5.0.

Constraints:

Test is limited to verifying calculations in a single deterministic run.

Output files to compare or examine:
From TPA Run:
rgsnr.tpa
gnewdf.dat

Step-by-step test procedure:
Set environment variables to point to directory where current version of TPA code resides:

set TPA_TEST=c:\TPA51betaV
set TPA_DATA=c:\TPA51betaV

Create alias in Windows XP that will allow running the TPA code from its original directory using the *tpa.inp* file in a unique test directory by typing the execution command

..\tpa.exe >tpa.out

at the command prompt from the unique test directory.

Run an otherwise unmodified base case *tpa.inp* and rename the file *tpameans.out* to *tpa.inp*, change input parameters as described above.

Execute a single realization mean value run (one that executes DCAGS) for each dosimetry age group tested (Toddler, Adult, Adult FG11). Execute a similar set of runs that use ASHREMOB for air transport, remobilization, and dose calculations instead of DCAGS.

For each set of runs (DCAGS-based, ASHREMOB-based), use a spreadsheet to compute the ratio of comparable age-dependent inhalation dose coefficients from one age group to another using the coefficients in the *gnewdf.dat* file used for the test runs. For example, the ratio of Adult5 coefficients to Toddler and Adult5 (ICRP72) coefficients to Adult6 (FGR11) coefficients. Import the dose output (by radionuclide and timestep) from the TPA test runs for each age group provided in the *rgsnr.tpa* files for each run into the spreadsheet and compute similar types of ratios for doses by age group as was done for the dose coefficients (e.g., ratio of Adult5 doses to Toddler etc).

Use the spreadsheet to compare the applicable dose coefficient ratios to the dose output ratios for comparable age group sets. A match for a ratio comparison verifies that selection of age-dependent dose coefficients from one age group specific run to the another correctly utilized the appropriate age dependent dose coefficients in each run and appropriately scaled the computed doses as expected (because a) dose coefficients were the only parameters that changed values among the sets of results being compared, b) dose coefficients vary by age group, and c) dose coefficients are included in the dose calculations as factors, the dose output should scale directly with changes in magnitude of dose coefficients).

Pass/fail criteria:

Test passes if all compared ratios of radionuclide specific age dependent doses for the year of the igneous event agree with ratios based on the magnitude of dose coefficient changes from one age group to another (acceptable error tolerance within 5%).

Test Results

Deviation from test plan: All test code runs were executed directly from the root directory where the TPA5.1BetaV code was installed and output files were manually copied to archive directories. A final set of tests for problem resolution was conducted with TPA5.1BetaW using a similar execution approach. This change is not expected to have any impact on test results. Also, initial plan was to test 4 age groups, however, this was limited to 3 age groups to improve efficiency of test without significantly compromising the validity of the test.

Results are archived in an attached CD in directory \P16\Test2

Spreadsheet that demonstrates results of test for ASHREMOB is *Test2.ashremob.results.xls*
Original computed ratios of dose coefficients from *gnewdf.dat* data file are in *gnewdf.dat.ratios.xls*
Spreadsheet that demonstrates results of test for DCAGS is
\P16\Test2\Tpa51betaW\nodaughter*Test2.dcags.results.xls*

Results for ASHREMOB test showed agreement for all radionuclide-specific dose output for the year of eruption for the first execution of the test. The year of eruption is the valid point of comparison because the model includes the contribution of decay and erosion of the ash blanket over time and shorter lived radionuclides will decay to essentially zero (1E-15) over a few timesteps and the ratio of computed doses will eventually converge to 1.0 while the ratio of dose coefficients remains constant. Using the time of eruption for this comparison eliminates this artifact of the test approach from interfering with results.

Results for DCAGS initial test showed agreement (passing) for many radionuclides, but some anomalous results (lack of agreement) was found for a subset (Am242m, Pb210, Th229, Cm244, U232, Sn126, Sn121m, Zr93, and Sr90). See initial results file *\P16\Test2\Test2.dcags.results.xls* Intermediate results checking investigated ratios of computed inhalation "DCF" values for Adult5 and Adult6 runs in output file gsdcf.cum (*Test2.dcags.adult56.BDCF.comp.xls*) to verify that the same set of radionuclides exhibited magnitude changes in computed results that went beyond the magnitude of dose coefficient changes from one age group to the other.

Because the inhalation DCFs reported in *gsdcf.cum* are merely the product of breathing rate and dose coefficient, and breathing rate is a constant input in tpa.inp attention was focused on the dose coefficients. Inspection of Fortran code in *dcags.f* file indicated that progeny dose coefficient values are summed into parent radionuclide dose coefficients prior to the DCF compilation in the output file. This summation was not included in the design of the spreadsheet computation for this test and therefore any differences in test results due to the daughter summation in the TPA code is just an artifact of the test design rather than an indication of a problem with the code.

To verify that the differences in test results were due to daughter summation in DCAGS, runs for the current test were re-run using a modified gnewdf.dat dose coefficient file with all progeny dose coefficients zero'd out for the aforementioned radionuclides with anomalous results (thereby removing the progeny summation effect on the computed doses). Progeny that were zero'ed out from the gnewdf.dat file include Am242, Cm242, Bi210, Po210, Ra225, Ac225, Pu244, U240, Th232, Ra228, Ac228, Th228, Ra224, Pb212, Bi212, Sb126m, Sb126, Sn121, Nb93m, Y90. This set of runs was done using the same approach as the first set, however, the TPA5.1BetaW code was used instead of TPA5.1BetaV because the more recent version was available and was also being used for another test. Note that code environment variables were setup as noted above however the paths changed to c:\TPA5.1BetaW instead of c:\ TPA51BetaV. The dose results from this revised set of runs were copied to the test spreadsheets and this caused all radionuclide code results to be in agreement (verifying that the progeny summation was contributing to the former anomalous results, see \P16\Test2\Tpa51betaW\nodaughter*Test2.dcags.results.xls).* The suspected reason why this limitation of the test did not impact all radionuclide results is that while many of the radionuclides included in the dose calculation involve daughter products, only a subset of radionuclides have daughter product dose coefficients that notably increase the magnitude of the combined dose coefficient when added to the dose coefficient for the parent radionuclide.

These results therefore, identified a limitation of the test as initially planned (it was based on an assumption that the progeny summation was not likely to significantly change results), however, the additional investigation into the anomalous results, and re-run of test with daughter summation removed, allowed the test to eventually pass because the test has verified that the age-dependent dose coefficients are being used as intended in the calculations and the Age&Dosimetry flag is working as designed in selecting the correct columns of dose coefficients based on user selections in tpa.inp.

All dose results compared on the spreadsheet (\P16\Test2\Tpa51betaW\nodaughter*Test2.dcags.results.xls*) agree with code test run results.

Overall Test Status (PASS/FAIL): **PASS**

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 06002.01.354	
Software Name: TPA Code		Version: 5.1BetaV and 5.1 BetaW
Test ID: P-17	Test Series Name: All Pathway Dose from Groundwater (DCAGW); Non-inhalation Pathway Dose from Ground Surface (DCAGS)	

Test Method

- ☐ code inspection
- ■ output inspection
- ■ hand calculation
- ■ spreadsheet
- ☐ graphical
- ☐ comparison with external code results

Test Objectives: See Attachment A

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): Windows XP

Input Data (files, data base, mode settings): See Attachment A

Assumptions, constraints, and/or scope of test: See Attachment A

Test Procedure: See Attachment A

Test Results

Location: See attached CD labeled “TPA Version 5.1 Validation Task P-17"

Test Criterion and Analysis of Results: See Attachment A

Test Evaluation (Pass/Fail): PASS

Notes:

Testers: P. LaPlante	Date: 5/25/2007

Attachment A

Test Cases for Tasks P-16 and P-17

TEST 1

Verification of Dose Conversion Factor Calculations in DCAGW and DCAGS
(DCAGS non-inhalation pathways only)

Modifications to input files:

Test uses TPA Version 5.1 run of an unmodified base case *tpa.inp* and output file *tpameans.out* is renamed to to *tpa.inp*. The *tpa.inp* is modified as follows:

OutputMode(0=None,1=All,2=UserDefined) parameter to 1 (all), and
VolcanismDisruptiveScenarioFlag (yes=1,no=0) to 1 (yes)

Utility codes needed in the analysis of the test data:
Microsoft Excel2002

Test description:

Objective:
Verification of Dose Conversion Factor Calculations in DCAGW and DCAGS including:

A. Verification of calculations in DCAGW and DCAGS that convert intakes/exposures calculated by GENTPA and GENTPAGS to radionuclide specific dose conversion factors (i.e., rem/yr per Ci/m3 in groundwater and rem/yr per Ci/m2 in soil) written to TPA Version 5.1 output files *gw_cb_ad.dat, gw_pb_ad.dat, gs_cb_ad.dat*, and *gs_pb_ad.dat*.

B. Verification that data files *tpa.inp*, *gnewdf.dat*, and *ggrdf.dat* are being read correctly by the TPA Version 5.1 code for the calculation of age-dependent dose conversion factors written to TPA Version 5.1 output files *gw_cb_ad.dat*, *gw_pb_ad.dat*, and *gs_cb_ad.dat*, and *gs_pb_ad.dat*.

C. Verification that summation of pathway-specific dose conversion factors into more general pathway categories in the TPA Version 5.1 code is being executed correctly. An example of this type of summation is that “poultry”, “eggs”, and “beef” pathway-specific dose conversion factors are summed to create the broader category “animal product ingestion”).

D. Verification that progeny dose conversion factors are summed into parent radionuclide dose conversion factors prior to writing values to output files *gw_cb_ad.dat*, *gw_pb_ad.dat*, *gs_cb_ad.dat*, *gs_pb_ad.dat*.

E. Verification that TPA Version 5.1 dose conversion factor output is written to files *gw_cb_ad.dat*, *gw_pb_ad.dat*, *gs_cb_ad.dat*, *gs_pb_ad.dat* correctly.

F. Verification that the correct age-dependent dose coefficients are used in dose conversion factor calculations when the Age&Dosimetry flag is changed.

Assumptions:
This test verifies TPA Version 5.1 calculations of dose conversion factors in DCAGW and DCAGS (except for DCAGS inhalation dose calculation which is covered under Task P-16) for a single realization mean value TPA Version 5.1 run. Stochastic operation is not tested.

Constraints:
Test is limited to verifying calculations in a single deterministic run.

Output files to compare or examine:
From TPA Version 5.1 Run:
genv.cum,
genv.out,
gw_cb_ad.dat,
gw_pb_ad.dat,
gs_cb_ad.dat,
gs_pb_ad.dat.

Step-by-step test procedure:

Set environment variables to point to directory where current version of TPA Version 5.1 code resides:

set TPA_TEST=c:\TPA51betaV\
set TPA_DATA=c:\TPA51betaV\

Create alias in Windows XP that will allow running the TPA Version 5.1 code from its original directory using the tpa.inp file in a unique test directory by typing the execution command ..\tpa.exe >tpa.out at the command prompt from the unique test directory.

Run an unmodified reference case *tpa.inp*, interrupt the job at prompt by using Ctrl-C command, and rename the file *tpameans.out* to *tpa.inp*, copy *tpa.inp* to unique run directory edit *tpa.inp* by changing inputs as follows:

OutputMode (0=None,1=All,2=UserDefined) parameter to 1 (all),
VolcanismDisruptiveScenarioFlag (yes=1,no=0) to 1 (yes)
AshEvolutionMode[0=no_ashremob,1=ashremob] to 0

and run TPA Version 5.1 with the new file by typing the aforementioned execution command.

Copy the *tpa.inp* file from the previous run into a separate directory, and edit the *tpa.inp* file to select the Adult 6 age-category by changing the *Age&Dosimetry(1=Inf,2=Todl,3=PTeen,4=Teen,5=Adlt,6=AdltFG11)* flag to 6. Further edit the *tpa.inp* file to remove comment symbols from the applicable age group 6 age-dependent input parameters in *tpa.inp* in the DCAGW and GENTPA sections.

Copy the *tpa.inp* file from the previous run into a separate directory, and edit the *tpa.inp* file to select the Toddler age-category by changing the *Age&Dosimetry(1=Inf,2=Todl,3=PTeen,4=Teen,5=Adlt,6=AdltFG11)* flag to 2. Further edit the *tpa.inp* file to remove comment symbols from the applicable age group 2 age-dependent input parameters in *tpa.inp* in the DCAGW and GENTPA sections. Values for the age dependent input parameters for group 2 that are different from the adult input parameter values are entered to verify changes to input values are propagated through calculations.

Obtain the GENTPA and GENTPAGS subroutine's output files (from *genv.cum*) for each of the age-dependent sets of TPA Version 5.1 calculations run. For each age-dependent calculation obtain the "intake" output by radionuclide and pathway for the four relevant source/biosphere/climate categories (groundwater, current biosphere; groundwater, pluvial biosphere; soil source, current biosphere; soil source, pluvial biosphere) and copy the applicable "intakes" output for each source/biosphere/climate category into the corresponding verification spreadsheet in Excel 2002. Current biosphere results for a soil source are the same as pluvial biosphere results, however, both categories are tested to ensure results in each are correct.

The "intakes" output by radionuclide and pathway from *genv.cum* is copied into the first two columns of the appropriate spreadsheets named *dcf.verify.tpa51.age5.dcagw.cb.xls*, *dcf.verify.tpa51.age5.dcagw.pb.xls*, *dcf.verify.tpa51.age5.dcags.cb.xls*, *dcf.verify.tpa51.age5.dcags.pb.xls*. (one such set for each age group run). Spreadsheet names identify the 3 age categories and 4 source/biosphere/climate categories used for TPA Version 5.1 dose conversion factor calculations selected for this test. Into the same spreadsheets, copy the applicable TPA Version 5.1 dose conversion factor output from files *gw_cb_ad.dat, gw_pb_ad.dat, gs_cb_ad.dat, gs_pb_ad.dat* under the highlighted columns heading "Copied output from TPA Version 5.1 Code DCF Output Files" that begins in column S.

Calculation spreadsheets for each age-category must contain the appropriate age-dependent internal dose coefficients from the TPA Version 5.1 *gnewdf.dat* auxiliary data file. Due to the large number of dose coefficients, to limit data entry burden, a subset of radionuclide specific dose coefficients will be hand entered and/or copied into each spreadsheet to verify calculations for a subset of radionuclides. The subset of radionuclides will include radionuclides shown in past TPA calculations to be important contributors to dose results (NRC, 2005) including: Np237, Tc99, I129, Pu239, Pu238, Am241, U234, Se79, Cl36.

The test spreadsheets were designed to reproduce TPA Version 5.1 calculations to convert the "intakes" (intermediate TPA Version 5.1 code output in *genv.cum*) to dose conversion factors using "intake to dose" conversion factors (called "dose coefficients" in the spreadsheet) from TPA 5.1 data files *gnewdf.dat* and *ggrdf.dat*. The spreadsheets also sum the doses into pathway categories consistent with the TPA Version 5.1 output files, sum progeny results into parent radionuclides, and organize the results into the format of the TPA Version 5.1 dose conversion factor output files for efficient comparison. For added transparency of calculations, a reviewer can view spreadsheets using the tools/options menu in Excel 2002 and show the formulas.

Observe test comparison results (compared spreadsheet calculated dose conversion factors with TPA 5.1 code calculated values) in the yellow highlighted area of each spreadsheet. Values of "1" indicate agreement between spreadsheet calculated values and TPA Version 5.1 output. Some zeros are possible when the dose calculations lead to results that equal zero. Any zeros in the results section should be verified that actual results from both the spreadsheet and TPA Version 5.1 were zero.

An additional comparison will assess the changes to "intakes" reported in the *genv.cum* for adult and toddler age selection to verify that input parameter changes from one age group to another in *tpa.inp* (e.g., consumption rates, etc) have been propagated to calculation results. Ratios of the intakes from one age group vs another will be computed on a spreadsheet (one each for DCAGW and DCAGS calculations).

Pass/fail criteria:
Test passes if:

Criterion 1: All radionuclide and pathway specific dose conversion factors in the TPA Version 5.1 output files (*gw_cb_ad.dat, gw_pb_ad.dat, gs_cb_ad.dat, gs_pb_ad.dat*) for each age-group tested agree with the relevant spreadsheet calculated dose conversion factors within an error tolerance of 5% for all test spreadsheets.

Criterion 2: Comparison of age-dependent intakes computed by the TPA Version 5.1 code respond to changes in input parameters in *tpa.inp*. Test is passed if calculated intakes change as expected for Toddler and Adult receptor age classifications.

Criterion 3: All "divide by zero" results are confirmed to be zero for both spreadsheet based results and TPA Version 5.1 code results (zero results for some radionuclide intakes are expected based on input parameter choices)

Test Results:

Deviation from test plan: Due to limitations in output from DCAGS (i.e., no cumulative output of "intakes"), only pluvial "intakes" are available for testing. This is because the last execution of GENTPAGS in a TPA Version 5.1 realization is for pluvial climate. A separate test spreadsheet for "current biosphere" DCAGS dose conversion output was therefore not included in test results (aforementioned *dcf.verify.tpa51.age5.dcags.cb.xls* results files *dcf.verify.tpa51.age5.dcags.cb.xls*). This artifact is part of the code design because the non-inhalation pathway biosphere computations implemented by GENTPAGS in DCAGS are not impacted by climate because the climate implementation only impacts irrigation deposition of contaminants and DCAGS computations do not include deposition of contaminants by irrigation. Because the resulting *dose conversion factors* are included in *dcfgs.cum* output, a comparison was added to verify both current and pluvial dose conversion factors from DCAGS are equal (i.e., as expected) thereby extending the applicability of verification results for pluvial dose conversion factors to current climate dose conversion factors. Comparison results are in files archived by age group (*dcfgs.cum.comp.xls, one for each age group*).

Results are archived in an attached CD in \P17\Test1 directory:

> TPA Version 5.1 run inputs and full results are provided by age group on CD \P17\Test1
> Spreadsheets for test are provided by age group on CD in \P17\Test1
> Files *dcf.verify.tpa.dcagw.cb.xls, dcf.verify.tpa.dcagw.pb.xls, dcf.verify.tpa.dcags.pb.xls* for each age group demonstrate agreement in results for Criterion 1 and 3. The additional comparisons of changes in intake results with age group (Criterion 2) are provided in *genv.cum.comp.dcags.xls* and *genv.cum.comp.dcags.xls*

Criterion 1: **PASSED**
Criterion 2: **PASSED**
Criterion 3: **PASSED**

Overall Test Status: PASS
References:

NRC. NUREG-1762. "Integrated Issue Resolution Status Report". Vol2, Rev. 1. Washington DC: Nuclear Regulatory Commission. April, 2005, Appendix D, Figure 4-46.

TEST2

Verification of Groundwater Protection Calculations in DCAGW

Modifications to input files:

Run an unmodified base case *tpa.inp* and rename the file *tpameans.out* to *tpa.inp*, change OutputMode(0=None,1=All,2=UserDefined) parameter to 1.

Utility codes needed in the analysis of the test data:
Microsoft Excel2002

Test description:
Objective:
Verification of Groundwater Protection Calculations in DCAGW:

- Groundwater concentrations at the receptor well head are calculated as intended using the saturated zone release estimates and the pumping rate specified in *tpa.inp*

- Input parameters in *tpa.inp* and information in data files *nuclides.dat* (categorization of radionuclides into groups) and *organdf.dat* (organ and whole body dose coefficients) are used as intended in concentration and dose calculations for groundwater protection

- TPA Version 5.1 output in files *dcagw.ech*, *gwppktim.res*, *gwp_ave.res* contain correct information that is verified by comparison with spreadsheet calculations

Assumptions:

The test repeats the calculations done in DCAGW to convert saturated zone (groundwater) release estimates for 20 radionuclides to concentrations and doses of the types that are required by 10 CFR Part 63 groundwater protection limits. One timestep is verified and assumed to be representative of all timesteps since the same equations are applied to each timestep. Thus, the time-stepping is not specifically tested, however, the TPA Version 5.1 output from the calculations will be reviewed to check for anomalous behavior across timesteps.

Constraints:
Test is limited to verifying calculations in a single deterministic run and a small stochastic run.

Output files to compare or examine:
From TPA Version 5.1 Run:

nuclides.dat
organdf.dat
dcagw.ech
gwp_ave.res
gwppktim.res

Step-by-step test procedure:

Set environment variables to point to directory where current version of TPA Version 5.1 code resides:

set TPA_TEST=c:\TPA51betaW
set TPA_DATA=c:\TPA51betaW

Create alias in Windows XP that will allow running the TPA Version 5.1 code from its original directory using the *tpa.inp* file in a unique test directory by typing the execution command

..\tpa.exe >tpa.out

at the command prompt from the unique test directory.

Run an unmodified base case *tpa.inp* and rename the file *tpameans.out* to *tpa.inp*, change OutputMode(0=None,1=All,2=UserDefined) parameter to 1 to allow output of *.ech files.

Open the output file *dcagw.ech* in MS Excel, reformat to a single row of columns for each realization and copy the final annual SZ release (flux) values for the 10,000 yr time step into the highlighted bottom row of the spreadsheet (filename *tpa51.validation.gwprot.xls*) labeled "Copied TPA Output from *dcagw.ech* (SZ release at 10 kyr)". Enter by hand into the spreadsheet column labeled *[ciperyrallsafromsz]* the same annual saturated zone flux values from the 10 kyr timestep for each radionuclide from *dcagw.ech*.

The spreadsheet was designed to compute the same groundwater protection calculations as TPA Version 5.1. The spreadsheet is populated with parameters and data from the TPA Version 5.1 base case run (*tpa.inp* and supporting data files *nuclides.dat*, and *organdf.dat*). The calculations in the spreadsheet are simple and expected to be understood by a competent analyst without recourse to the originator. Using the tools/options menu in Excel to reveal formulas can provide transparency of the information flow on the spreadsheet. The spreadsheet takes saturated zone release estimates in TPA Version 5.1 output (copied from *dcagw.ech* file) and:

- estimates a groundwater concentration by dividing the release rate by the pumping volume,
- estimates the human intake of radionclides from drinking the water at the estimated concentration,
- converts the human intake to organ and whole body doses using factors contained in TPA Version 5.1 input data file *organdf.dat*
- sums the concentration and dose results to categories that match TPA Version 5.1 code output in files *gwp_ave.res* and *gwppktim.res*.

Open the output file *gwp_ave.res* in MS Excel and copy the values for the 10,000 yr time step into the aforementioned spreadsheet (filename *tpa51.validation.gwprot.xls*) in the yellow highlighted areas under the relevant headings (i.e., gross alpha, radium, various organs).

Compare by visual inspection the spreadsheet calculated values with the TPA Version 5.1 output copied to the spreadsheet.

Visually inspect the output of *gwppktim.res* file and verify that results are consistent with results reported in *gwp_ave.res* (e.g., for a single realization run the *gwp_ave.res* output results are provided for each time step and *gwppktim.res* provides only the peak result among all time steps for each realization so the visual inspection will check whether the *gwppktim.res* shows the true maximum values and correct time step for each result computed for the single realization that was run).

Pass/fail criteria:
Test passes if:

Criterion 1 (from SCR-563, PL-2 test): Test is passed if spreadsheet computed alpha concentration, Ra226 concentration, and organ and whole body doses match test run code output values.

Criterion 2 (from SCR-563, PL-2 test): Test is passed if all the output results of *gwppktim.res* file are consistent with results reported in *gwp_ave.res*.

Criterion 3 (from SCR-563, PL-3 test): Test is passed if spreadsheet computed values match test run TPA51BetaW code output for:

i) gross alpha and Ra226 concentrations by realization and
ii) average alpha concentration, Ra226 concentration, and organ and whole body doses

Test Results
Deviations from planned test:

Because changes to groundwater protection computations were acceptance tested under SCR-563, and one of the SCR acceptance tests (PL-2) was identical to the planned validation test, this validation report references the SCR tests for the applicable test results. An additional test (PL-3) under SCR-563 goes beyond the initial planned validation test for this report but results are included because they are consistent with the intent of the validation and provide additional confidence the code is operating as designed.

Archived on CD accompanying SCR-563, tests PL-2 and PL-3 results

Criterion 1: **PASSED**
Criterion 2: **PASSED**
Criterion 3: **PASSED**
Files *tpa51.validation.gwprot.xls* and *tpa51.validation.gwprot.pl3.xls* included with SCR-563 file archive demonstrate agreement in results

Overall Test Status PASS

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: **20.06002.01.354**
Software Name: **TPA**	Versions: **5.1BetaU, 4.2r, 5.0.0b**
Test ID: **P-18**	Test Series Name: **Atmospheric Transport and Deposition of Radionuclides**

Test Method

x code inspection	☐ spreadsheet
x output inspection	☐ graphical
☐ hand calculation	x comparison with external code results

Test Objective: See Attachment A

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): WindowsXP (SP2)

Input Data (files, data base, mode settings): See Attachments A–C

Assumptions, constraints, and/or scope of test: ASHPLUMO and ASHRMOVO modules have not been modified since the last validated code version. Scope of test is to verify that the ASHPLUMO and ASHRMOVO modules remain functional.

Test Procedure: See Attachments A–C

Test Results

Location: see attached CD labeled "TPA Version 5.1 Validation Task P-18"

Test Criterion and Analysis of Results: See attachments A–C.

Test Evaluation (Pass/Fail): Pass

Notes:

Tester: M. Necsoiu	Date: 4/27/2007

Attachment A

Task P-18 Test Plan
Objectives, Assumptions, Planned Tests

The following describes the objectives, assumptions, and planned tests for Task P-18 of the TPA Version 5.1 code Software Validation. The test procedures described in this attachment supplement the TPA Version 5.1 Software Validation Plan.

OBJECTIVES

The objective of Software Validation Task P-18 is to verify that the alternative model that utilizes the *ashplumo.f* and *ashrmovo.f*, as implemented in previous version of the TPA code, is still functional.

ASSUMPTIONS

For the purposes of this validation test, it is assumed:

1. The input parameters and their distributions supplied by tpa.inp are consistent with the abstractions of the modeled processes.
2. Previous validation testing of this module and testing of subsequent SCRs affecting this module have been properly performed, and may be cited as evidence of module performance.

TESTS

The following tests sequentially address the objectives of this SVR. Criteria are also specified at the end of the test description.

Test 1

Execute the TPA code for single reference case realization of 10,000 yrs, appending all files and modify the tpa.inp file in accordance with the following table. Redirect the screen output to a *tpa.out* file for inspection.

Parameter	Value
AshEvolutionMode[0=no_ashremob,1=ashremob]	0
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
ModeFuelParticulateSize[cm]	0.001

Test 1 Criteria: ASHPLUMO and ASHRMOVO modules are called by TPA with the above specified settings, and the following files are generated: *ashplume.out, ashplumo.ech, ashplumo.rlt, ashrmovo.ech* and *ashrmovo.rlt*

Test 2

For similar ASHPLUMO parameters values, TPA 51Beta U and a previous version (i.e., TPA version 4.2r) generates identical values except for the total fuel mass available parameter.

Replace the tpa.inp with the tpameans.inp and re-run the TPA 51Beta U. Set up the environmental variables for TPA 4.2r and execute the code for single reference case realization of 10,000 yrs, appending all files and set the following flag as below:

Parameter	Value
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
DistanceToReceptorGroup[km]	18.0

Rename the generated tpameans.inp as tpa.inp and update the ASHPLUMO and ASHRMOVO parameters definitions with the ones generated by TPA version 5.1betaU. Calculate the ratios of xfuel and total fuel mass available parameter values (from *ashplume.out*) obtained with these versions and verify that they are similar.

Test 2 Criteria: The ratios of xfuel and total fuel mass available parameter values (from *ashplume.out*) obtained with the TPA 51Beta U and TPA version 4.2r are identical to at least 2 significant figures.

Test 3
Use a file comparison test between ashrmovo.f TPA version 5.00b and 5.1betaU.

Test 3 Criteria: The test should reveal no code changes.

Test 4.
An additional ASHPLUME mass balance test (Attachment C) was conducted in 2003 for the Validation of the TPA Version 5.0 code. This mass balance test was not included in that validation report. The TPA Version 5.0 report noted the ASHPLUME mass balance did not satisfy the 10 percent acceptance criterion for a passing test. The analysis provided in Attachment C, however, shows that the ASHPLUME model does, in fact, satisfy the mass balance criterion. See Attachment C for criterion.

Attachment B

TPA 5.1 Software Validation
Task P-18 Test Results

Test 1. Test that ashplumo and ashrmovo are called by the TPA program.

Path for run directory:
Test case: Olympus: L\TPA\ValidationTPA\Task18_case1

Environment variable:
Test case: TPA_DATA=L:\TPA\tpa51betaU
TPA_TEST=L:\TPA\tpa51betaU

Path for archive of results
Test case: [CD: titled P18 Testing]: \SVT18\test1

Special diagnostic code modifications required: None

Program modes to be used (append flags, scenario/model switches, etc.):
Test case: append all, and the following

Table 1: Test1

Parameter	Value
AshEvolutionMode[0=no_ashremob,1=ashremob]	0
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
ModeFuelParticulateSize[cm]	0.001

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: Ensure that ASHPLUMO and ASHRMOVO were called by the TPA program. The desire is to make sure these modules still work since the implementation of the ASHREMOB module.

Assumptions None, other than those made within the TPA code.

Constraints None

Output files to compare or examine: Screen output (tpa.exe>tpa.*out*)

Test Procedure
1.Execute the TPA code for single reference case realization of 10,000 yrs, appending all files and modify the tpa.inp file in accordance with table 1.

2.Redirect the output to tpa.out file and verify that ASHPLUMO and ASHRMOVO modules were called by the program.

3.Verify that the following files were generated: ashplume.out, ashplumo.ech, ashplumo.rlt, ashrmovo.ech and ashrmovo.rlt.

Pass/Fail criteria

ASHPLUMO and ASHRMOVO modules are called by TPA with the above specified settings, and the following files are generated: *ashplume.out, ashplumo.ech, ashplumo.rlt, ashrmovo.ech* and *ashrmovo.rlt*

Test results:

The test case realization was successfully executed under the above conditions. The 15 last lines of the tpa.out file include two statements that shows that ashplumo and ashrmovo were called by the program.

```
exec: calling ashplumo
exec: calling ashrmovo
exec: calling dcags
          Highest annual dose from GS
      Pu239  1.6283E+03 [mrem/yr] at  9.107E+03 yr
      Pu240  1.4003E+03 [mrem/yr] at  9.107E+03 yr
      Am243  1.5910E+02 [mrem/yr] at  9.107E+03 yr
       Nb94  4.9914E+01 [mrem/yr] at  9.107E+03 yr
      Sn126  4.1995E+01 [mrem/yr] at  9.107E+03 yr
      Pu242  2.2077E+01 [mrem/yr] at  9.107E+03 yr
exec: end realizations

exec: Peak Mean Dose is 3.31880E+00 rem/yr at    9107.2 yr, based on     1 realizations.

exec:  Run Successfully Completed
```

An examination of the Task18_case1 directory revealed that ashplume.out, ashplumo.ech, ashplumo.rlt, ashrmovo.ech and ashrmovo.rlt were generated.

These results are submitted as evidence that test 1 of Task P-18 has been successfully tested.

Test 1 Results (PASS/FAIL): **PASS**

Test 2. For similar ASHPLUMO parameters values, TPA version 5.1 and TPA version 4.2.r generates identical values except for the total fuel mass available parameter

Path for run directory:

Reference case: Olympus: L\TPA\ValidationTPA\Task18_case1
Test case : Olympus: L\TPA\ValidationTPA\Task18_case2

Environment variable:

Reference case: TPA_DATA=L:\TPA\tpa51betaU
TPA_TEST=L:\TPA\tpa51betaU
Test case: TPA_DATA=L:\TPA\tpa42r
TPA_TEST=L:\TPA\tpa42r

Path for archive of results

Reference case: [CD: titled P18 Testing]: \SVT18\test1\mean values
Test case: [CD: titled P18 Testing]: \SVT18\test2 and
[CD: titled P18 Testing]: \SVT18\test2\mean values

Special diagnostic code modifications required: None

Program modes to be used (append flags, scenario/model switches, etc.):

Reference case: append all
Test case: append all, and the following

Table 2: Test2

Parameter	Value
VolcanismDisruptiveScenarioFlag(yes=1,no=0)	1
DistanceToReceptorGroup[km]	18.0

Utility scripts needed to perform the test: None

Utility codes needed in the analysis of the test data: None

Objective: For similar ASHPLUMO parameters values, TPA version 5.1 and TPA version 4.2.r generates identical values except for the total fuel mass available parameter.

Assumptions None, other than those made within the TPA code.

Constraints None

Output files to compare or examine: Screen output (tpa.exe>tpa.*out*)

Test Procedure

1.Replace the tpa.inp with the tpameans.inp and re-run the TPA 51Beta U in a new directory (i.e., ..Task18_case1\mean values).

2. Set up the environmental variables for TPA 4.2r and execute the code for single reference case realization of 10,000 yrs, appending all files and set the flags in accordance with table 2.
3. Rename the generated tpameans.inp as tpa.inp and update the ASHPLUMO and ASHRMOVO parameters definitions with the ones generated by TPA version 5.1betaU. Re-run the TPA 4.2r in a new directory (i.e., ..Task18_case2\mean values).
4. Calculate the ratios of xfuel and total fuel mass available parameter values (from ashplume.out) obtained with these versions and verify that they are similar.

Pass/Fail criteria

The ratios of xfuel and total fuel mass available parameter values (from *ashplume.out*) obtained with the TPA 51Beta U and TPA version 4.2r are identical to at least 2 significant figures.

Test results:

The test case realizations were successfully executed under the above conditions.

The ASHPLUMO and ASHRMOVO parameters definitions for TPA version 5.1betaU are listed below:

```
**        ***>>> ASHPLUMO <<<***
**
constant
DensityOfAirAtSTP[g/cm3]
0.00129
**
constant
ViscosityOfAirAtSTP[g/cm-s]
0.00017
**
constant
ConstantRelatingFallTimeToEddyDiffusivity[cm2/s5/2]
400.0
**
constant
MaximumParticleDiameterForParticleTransport[cm]
10.0
**
constant
MinimumFuelParticulateSize[cm]
0.0001
**
constant
ModeFuelParticulateSize[cm]
0.001
**
constant
MaximumFuelParticulateSize[cm]
```

0.01
**
constant
MinimumAshDensityForVariationWithSize[g/cm3]
0.8
**
constant
MaximumAshDensityForVariationWithSize[g/cm3]
1.6
**
constant
MinimumAshLogdiameterForDensityVariation
-2.0
**
constant
MaximumAshLogdiameterForDensityVariation
-1.0
**
constant
ParticleShapeParameter
0.5
**
constant
IncorporationRatio
0.3
**
constant
WindDirection[degrees]
-90.0
**
constant
WindSpeed[cm/s]
913.9638942540339
**
constant
VolcanicEventDuration[s]
149591.4436055754
**
constant
VolcanicEventPower[W]
67082039324.99380
**
constant
VolcanicColumnConstantBeta
10.0
**
constant
AshMeanParticleLogDiameter[d_in_cm]
0.1000000000000000

**
constant
AshParticleSizeDistributionStandardDeviation
1.0
**
** ***>>> ASHRMOVO <<<***
**
constant
RelativeRateOfBlanketRemoval[1/yr]
0.0007
**
constant
FractionOfPrecipitationLostToEvapotranspiration
0.68
**
constant
FractionOfIrrigationLostToEvapotranspiration
0.5
**
constant
FractionOfYearSoilIsSaturatedDueToPrecipitation
0.0054
**
constant
FractionOfYearSoilIsSaturatedDueToIrrigation
0.2
**
constant
AshBulkDensity[g/cm3]
1.2
**
constant
AshVolumetricMoistureFractionAtSaturation
0.4
**
constant
DepthOfTheRootingZone[m]
0.15
**
constant
KdOfUraniumInVolcanicAsh[cm3/g]
607.5725249999998
**
constant
KdOfCuriumInVolcanicAsh[cm3/g]
21184.64190000000
**
constant
KdOfPlutoniumInVolcanicAsh[cm3/g]

23004.92565000000
**
constant
KdOfAmericiumInVolcanicAsh[cm3/g]
22660.12145000000
**
constant
KdOfThoriumInVolcanicAsh[cm3/g]
16938.40890000000
**
constant
KdOfRadiumInVolcanicAsh[cm3/g]
134453.1526000000
**
constant
KdOfLeadInVolcanicAsh[cm3/g]
22487.07940000000
**
constant
KdOfProtactiniumInVolcanicAsh[cm3/g]
5074.097500000000
**
constant
KdOfActiniumInVolcanicAsh[cm3/g]
4175.509400000000
**
constant
KdOfNeptuniumInVolcanicAsh[cm3/g]
69.05746000000001
**
constant
KdOfSamariumInVolcanicAsh[cm3/g]
48668.43320000000
**
constant
KdOfCesiumInVolcanicAsh[cm3/g]
9312.037150000000
**
constant
KdOfIodineInVolcanicAsh[cm3/g]
11.10399500000000
**
constant
KdOfTinInVolcanicAsh[cm3/g]
1450.512050000000
**
constant
KdOfSilverInVolcanicAsh[cm3/g]
1817.317050000000

**
constant
KdOfPaladiumInVolcanicAsh[cm3/g]
 506.8169500000000
**
constant
KdOfTechnetiumInVolcanicAsh[cm3/g]
 0.6252075000000001
**
constant
KdOfMolybdenumInVolcanicAsh[cm3/g]
 342.7308500000000
**
constant
KdOfNiobiumInVolcanicAsh[cm3/g]
 1520.427400000000
**
constant
KdOfZirconiumInVolcanicAsh[cm3/g]
 6168.347700000000
**
constant
KdOfStrontiumInVolcanicAsh[cm3/g]
 147.9783000000000
**
constant
KdOfSeleniumInVolcanicAsh[cm3/g]
 58.97800000000000
**
constant
KdOfNickelInVolcanicAsh[cm3/g]
 1355.639300000000
**
constant
KdOfChlorineInVolcanicAsh[cm3/g]
 0.1447565000000000
**
constant
KdOfCarbonInVolcanicAsh[cm3/g]
 51.26751000000000
**
constant
SolubilityOfUraniumInVolcanicAsh[moles/liter]
3.20E-05
**
constant
SolubilityOfCuriumInVolcanicAsh[moles/liter]
1.0e-6
**

constant
SolubilityOfPlutoniumInVolcanicAsh[moles/liter]
1.00E-07
**
constant
SolubilityOfAmericiumInVolcanicAsh[moles/liter]
1.00E-07
**
constant
SolubilityOfThoriumInVolcanicAsh[moles/liter]
3.2e-9
**
constant
SolubilityOfRadiumInVolcanicAsh[moles/liter]
1.0e-7
**
constant
SolubilityOfLeadInVolcanicAsh[moles/liter]
3.2e-7
**
constant
SolubilityOfProtactiniumInVolcanicAsh[moles/liter]
3.2e-8
**
constant
SolubilityOfActiniumInVolcanicAsh[moles/liter]
1.0E-10
**
constant
SolubilityOfNeptuniumInVolcanicAsh[moles/liter]
1.0e-4
**
constant
SolubilityOfSamariumInVolcanicAsh[moles/liter]
5.10E-08
**
constant
SolubilityOfCesiumInVolcanicAsh[moles/liter]
1.0
**
constant
SolubilityOfIodineInVolcanicAsh[moles/liter]
1.0
**
constant
SolubilityOfTinInVolcanicAsh[moles/liter]
5.0e-8
**
constant

SolubilityOfSilverInVolcanicAsh[moles/liter]
1.0
**
constant
SolubilityOfPaladiumInVolcanicAsh[moles/liter]
9.5e-4
**
constant
SolubilityOfTechnetiumInVolcanicAsh[moles/liter]
1.0
**
constant
SolubilityOfMolybdenumInVolcanicAsh[moles/liter]
1.0
**
constant
SolubilityOfNiobiumInVolcanicAsh[moles/liter]
1.0e-8
**
constant
SolubilityOfZirconiumInVolcanicAsh[moles/liter]
3.2e-10
**
constant
SolubilityOfStrontiumInVolcanicAsh[moles/liter]
1.00E-04
**
constant
SolubilityOfSeleniumInVolcanicAsh[moles/liter]
1.0
**
constant
SolubilityOfNickelInVolcanicAsh[moles/liter]
1.80E-03
**
constant
SolubilityOfChlorineInVolcanicAsh[moles/liter]
1.0
**
constant
SolubilityOfCarbonInVolcanicAsh[moles/liter]
1.0
**

The ASHPLUME output file generated with TPA 51Beta U and TPA 4.2r mean values are listed below. Differences in parameter values are highlighted.

TPA 51Beta U
ASHPLUME version 1.1 output file.

Run started: Mon Mar 26 11:16:18 2007
iseed= 10
Validation nominal scenario reference case.

```
*******************************************************************
*                                                                 *
*              realization number             1        *
*               wind speed (cm/s)        914.0000      *
*             wind direction (deg)       -90.0000      *
*      mean particle diameter (cm)         0.1000      *
*                 log- std dev        1.0000      *
*                column ht (km)        4.1730      *
*             event duration (s)      0.1496E+06      *
*                  ash mass (g)      0.1367E+14      *
*               event power (W)      0.6707E+11      *
*                       beta      10.0000      *
*       vent exit velocity (cm/s)        688.3000      *
*         particle shape parameter         0.5000      *
*            air density (g/cc)      0.1290E-02      *
*         air viscosity (g/cm-s)      0.1700E-03      *
*   eddy diff. constant (cm2/s5/2)        400.0000      *
*              size cutoff (cm)        10.0000      *
*            incorporation ratio        0.3000      *
*   fuel particle minimum log-diam         -4.0000      *
*    fuel particle median log-diam         -3.0000      *
*   fuel particle maximum log-diam         -2.0000      *
*     total fuel mass available (g)      0.3004E+08      *
*                                                                 *
*******************************************************************
```

x (km)	y (km)	xash (g/cm^2)	xfuel (g/cm^2)
0.000	-18.000	0.2631E+01	0.6157E-05

TPA 4.2r
ASHPLUME version 1.1 output file.
Run started: Mon Mar 26 14:21:00 2007
iseed= 10
Base case.

```
*******************************************************************
*                                                                 *
*              realization number             1        *
*               wind speed (cm/s)        914.0000      *
*             wind direction (deg)       -90.0000      *
*      mean particle diameter (cm)         0.1000      *
*                 log- std dev        1.0000      *
*                column ht (km)        4.1730      *
*             event duration (s)      0.1496E+06      *
```

```
*                    ash mass (g)        0.1367E+14        *
*                 event power (W)        0.6707E+11        *
*                          beta        10.0000        *
*           vent exit velocity (cm/s)          688.3000        *
*            particle shape parameter            0.5000        *
*                 air density (g/cc)        0.1290E-02        *
*              air viscosity (g/cm-s)        0.1700E-03        *
*        eddy diff. constant (cm2/s5/2)          400.0000        *
*                  size cutoff (cm)          10.0000        *
*                 incorporation ratio          0.3000        *
*        fuel particle minimum log-diam            -4.0000        *
*         fuel particle median log-diam            -3.0000        *
*        fuel particle maximum log-diam            -2.0000        *
*         total fuel mass available (g)        0.3252E+08        *
*                                            *
*****************************************************************

   x (km)     y (km)    xash (g/cm^2)   xfuel (g/cm^2)

   0.000    -18.000       0.2631E+01        0.6665E-05
```

The xfuel and total fuel mass available parameter values obtained using TPA 51Beta U and TPA 4.2r are listed in Table 3.

Table 2: xfuel and total fuel mass available parameter values

Parameter	TPA 51Beta U	TPA 4.2r
xfuel (g/cm^2)	0.6157E-05	0.6665E-05
total fuel mass available(g)	0.3004E+08	0.3252E+08

The ratios of xfuel and total fuel mass available parameter values are identical to the third decimal (i.e., 2.049E-13).

These results are submitted as evidence that test 2 of Task P-18 has been successfully tested.

Test 2 Results (PASS/FAIL): **PASS**

Test 3. **ASHRMOVO code did not change between TPA version 5.00b (SCR 482 changes implemented) and TPA version 5.1betaU.**

Objective: ASHRMOVO code did not change between TPA version 5.00b (SCR 482 changes implemented) and TPA version 5.1betaU.

Utility scripts needed to perform the test:
xdiff - X11/Motif based file comparator and merge tool. Version 3.4

Utility codes needed in the analysis of the test data:
None

Test Procedure
Use a file comparison test between ashrmovo.f TPA version 5.00b and 5.1betaU.

Pass/Fail criteria
The test should reveal no code changes.

Test results:

The test used xdiff utility program on “raven” machine (Sun Fire V880Z SunOS 5.9) using the following command:

raven:/work2/TPA/ValidationTPA/Task18_case3 {553} xdiff ashrmovo_500b.f ashrmovo_51betaU.f

As seen in the following figure, the file comparison test revealed no code change between TPA version 5.00b and 5.1betaU.

xdiff

```
c Program Name:       TPA - Total-System Performance Assessment Code
c File Name:          ashrmovo.f
c File Date:          09/23/04
c Release Version:    5.0
c
c Client Name:        USNRC
c                     U. S. Nuclear Regulatory Commission
c                     NRC Office of Nuclear Material Safety and Safeguard
c                     Division of Waste Management
c Contract Number:    NRC 02-02-012
c
c NRC Contact         Tim McCartin (301) 415-6681
c
c CNWRA Contact:      Sitakanta Mohanty (210) 522-5185
c                     Center for Nuclear Waste Regulatory Analyses
c                     San Antonio, Texas 78238-5166
c                     smohanty@swri.edu
c
c Documentation:      Predecisional "Total-System Performance Assessment
c                     (TPA) Version 4.0 Code: Module Description and
c                     User's Guide", Center for Nuclear Waste Regulatory
c                     Analyses
c NUREG-Series Designator: N/A
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
c
c                       D I S C L A I M E R
c
c = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
c
c    "This computer code/material was prepared as an account of work
c performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA)
c for the Division of Waste Management of the Nuclear Regulatory
c Commission (NRC), an independent agency of the United States
c Government.  Neither the developer(s) of the code nor any of their
c sponsors make any warranty, expressed or implied, or assume any legal
c liability or responsibility for the accuracy, completeness, or
c usefulness of any information, apparatus, product or process
c disclosed, or represent that its use would not infringe on privately-
c owned rights."
c
c    "In no event unless required by applicable law will the sponsors
c or those who have written or modified this code, be liable for
c damages, including any lost profits, lost monies, or other special,
c incidental or consequential damages arising out of the use or
c inability to use the program (including but not limited to loss of
c data or data being rendered inaccurate or losses sustained by third
c parties or a failure of the program to operate with other programs),
c even if you have been advised of the possibility of such damages or
c for any claim by any other party."
c
c = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
c
c    CONTENTS:
c             subroutine ashrmovo
c             subroutine leachrate
c
c=========================================================================
      subroutine ashrmovo(gramsfpercm2,
     &                    nt,time,
     &                    ciperm2)
c-------------------------------------------------------------------------
```


```
c Program Name:       TPA - Total-System Performance Assessment Code
c File Name:          ashrmovo.f
c File Date:          09/23/04
c Release Version:    5.0
c
c Client Name:        USNRC
c                     U. S. Nuclear Regulatory Commission
c                     NRC Office of Nuclear Material Safety and Safeguarc
c                     Division of Waste Management
c Contract Number:    NRC 02-02-012
c
c NRC Contact         Tim McCartin (301) 415-6681
c
c CNWRA Contact:      Sitakanta Mohanty (210) 522-5185
c                     Center for Nuclear Waste Regulatory Analyses
c                     San Antonio, Texas 78238-5166
c                     smohanty@swri.edu
c
c Documentation:      Predecisional "Total-System Performance Assessment
c                     (TPA) Version 4.0 Code: Module Description and
c                     User's Guide", Center for Nuclear Waste Regulatory
c                     Analyses
c NUREG-Series Designator: N/A
cccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c
c = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
c
c                       D I S C L A I M E R
c
c = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
c
c    "This computer code/material was prepared as an account of work
c performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA)
c for the Division of Waste Management of the Nuclear Regulatory
c Commission (NRC), an independent agency of the United States
c Government.  Neither the developer(s) of the code nor any of their
c sponsors make any warranty, expressed or implied, or assume any legal
c liability or responsibility for the accuracy, completeness, or
c usefulness of any information, apparatus, product or process
c disclosed, or represent that its use would not infringe on privately-
c owned rights."
c
c    "In no event unless required by applicable law will the sponsors
c or those who have written or modified this code, be liable for
c damages, including any lost profits, lost monies, or other special,
c incidental or consequential damages arising out of the use or
c inability to use the program (including but not limited to loss of
c data or data being rendered inaccurate or losses sustained by third
c parties or a failure of the program to operate with other programs),
c even if you have been advised of the possibility of such damages or
c for any claim by any other party."
c
c = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
c
c    CONTENTS:
c             subroutine ashrmovo
c             subroutine leachrate
c
c=========================================================================
      subroutine ashrmovo(gramsfpercm2,
     &                    nt,time,
     &                    ciperm2)
c-------------------------------------------------------------------------
```


Figure 1. Screen capture showing no change in code between TPA version 5.00b and 5.1betaU

This result is submitted as evidence that test 3 of Task P-18 has been successfully tested.

Test 3 Results (PASS/FAIL): **PASS**

Attachment C

Previous Analysis with TPA Version 5.0g
Demonstration of Mass Balance for ASHPLUME Model

<table>
<tr><td colspan="2" align="center">Test Method
☐ code inspection ☒ spreadsheet
☒ output inspection ☐ graphical
☒ hand calculation ☒ comparison with external code results</td></tr>
<tr><td colspan="2">Test Objective: Account for ash and fuel entering volcano by integrating areal depositions.</td></tr>
<tr><td colspan="2">Test Environment Setup
Hardware (platform, peripherals): SUN Ultra 10 nmss16, Dell PC room T7F8 and SUNW, Ultra-4, “SPOCK”
Software: Sun OS, F90 compiler, S-Plus, MATHCAD 2000 and SUN-OS 5.8; f77 version 5.0
Input Data (files, data base, mode settings): ashplume.out, ashplume.in, infile.ash with TPA settings activated for volcanism and direct-release only flags for extrusive volcanism.</td></tr>
<tr><td colspan="2">Assumptions, constraints, and/or scope of test: See following pages of this attachment.</td></tr>
<tr><td colspan="2">Test Procedure: The test procedures for the preliminary and additional analyses are presented in the following pages of this attachment.</td></tr>
<tr><td colspan="2">Test Results
Location: For the preliminary analysis, test results are located in nmss16:/rbc/local1/tpa50g/, in the subdirectory .Data for Splus results, and in the directory rbc/tpa50g for FORTRAN results. For the additional analyses, test results are on the CD attached to this SVTR. The SVTR and Attachment C, which are contained in the SVTR_C14-2_and_REPORT.wpd file, are also included on the attached CD.
Test Criterion or Expected Results: The integrated depositions of fuel and ash should match the input masses of fuel and ash to within 10%.
Test Evaluation (Pass/Fail): Pass.</td></tr>
<tr><td colspan="2">Notes: See Attachment 3 for details and interpretation.</td></tr>
<tr><td>Testers: Richard Codell and Rob Rice</td><td>Date: 7/17/03 and 7/25/03</td></tr>
</table>

ASHPLUME Model: Test for Ash and Fuel Mass Balance

Integration of Volcanic Plume for Ash and Fuel Recovery

The validation report for the previous TPA version 5.0 indicated that the ASHPLUME model may not meet the specified fuel and ash mass balance criterion. The analyses presented in this attachment were performed with TPA version 5.0 as a follow up test to demonstrate appropriate mass balance; however, that analysis was never included in a validation report. Although the analyses in this report are not part of the TPA Version 5.1 planned validation tests, they are included because they address the question raised during the validation of the previous code version. Since the ASHPLUME code has not changed substantively since the TPA Version 5.0m used in this analysis, the results also provides confidence that the code is working properly in TPA Version 5.1.

Introduction

The purpose of this test was to simulate the ground-surface ash and fuel deposition from a extrusive volcanic event with the *ASHPLUME* code and determine whether mass is conserved in computing the areal ash and fuel densities. The TPA Code Version 5.0g with volcanism activated was utilized to generate the ASHPLUME input file parameters. This report describes the test procedure, the TPA simulation used to determine these *ASHPLUME* input parameters, and the integration methods developed to compute the ash and fuel deposition associated with the plume.

In the preliminary analyses, the *ASHPLUME* code from the TPA Code Version 5.0g was used and the ash and fuel deposition integrated to estimate how much of the input ash and fuel was recovered. The presumption was that the *ASHPLUME* model would conserve the mass of ash and fuel, so that all ash and fuel leaving the volcanic vent would be recovered on the ground.

Additional analyses were conducted with the *ASHPLUME* code from the TPA Code Version 5.0m because the preliminary results did not meet the *Test Criterion or Expected Results* described in the Software Validation Test Report (SVTR) for TPA Version 5.0. An expanded grid and EXCEL spreadsheet calculations equivalent to the integration methods employed in the preliminary analyses were used in the additional analyses, which are also described here. The approach of the additional analyses is to model a larger fuel and ash deposition area that was not modeled in the preliminary analyses, and then reevaluate whether the mass of the fuel and ash meet the 10% maximum error in the mass balance that were specified in the *Test Criterion or Expected Results* for TPA Version 5.0.

Test Procedure for Preliminary Testing

1. Run a representative ashplume case from a sampled data set. Use the first vector of a data set, and a few additional cases can be run , if necessary.
2. Using the input files *infile.ash* and *ashplume.in* that are generated in the Monte Carlo run for the chosen vector, re-run the ASHPLUME.E code after modifying the file *ashplume.in* to generate a grid of reference points down-wind of the volcano.
3. At each reference point, ASHPLUME.E will calculate an areal ash density and fuel density in grams/cm^2.

4. Read output into code S-Plus, MATHCAD, and EXCEL to perform an areal integration of the ash and fuel. Use simple integration schemes or, if necessary, fit a smooth surface or splines to surfaces. Also, construct FORTRAN codes for performing integration, if necessary.
5. Compare integrated outputs for fuel and mass to the input values of fuel and mass.

Test Case Input

The TPA5.0g code was run with the sample input for one Monte Carlo vector. The relevant parameters for the ASHPLUME code are described in Table 1 below, which is taken directly from the beginning of an output table from the code.

Table 1 - Parameters for ASHPLUME

ASHPLUME version 1.1 output file.		Run started: Tue Jul 15 17:09:32 2003	
iseed=	10	Very fine area right around vent rbc 7/15/03	
realization number	1	wind speed (cm/s)	1299.0000
wind direction (deg)	-90.0000	mean particle diameter (cm)	0.0593
log- std dev	1.0000	column ht (km)	6.1990
event duration (s)	0.5089E+06	ash mass (g)	0.2265E+15
event power (W)	0.3266E+12	beta	10.0000
vent exit velocity (cm/s)	1406.0000	particle shape parameter	0.5000
air density (g/cc)	0.1290E-02	air viscosity (g/cm-s)	0.1800E-03
eddy diff. constant (cm2/s5/2)	400.0000	size cutoff (cm)	10.0000
incorporation ratio	0.3000	fuel particle minimum log-diam	-4.0000
fuel particle median log-diam	-3.0000	fuel particle maximum log-diam	-2.0000
total fuel mass available (g)	0.6343E+08		

Initial integration

A grid of points surrounding the volcanic vent was laid out and the ASHPLUME code was executed to generate ash and fuel deposits. The grid had a spacing of 2 km in the x direction (perpendicular to plume direction) and 2.45 km in the y direction (parallel to plume). It stretched for -20 to +20 km perpendicular to the plume and 0 to -50 km parallel to the plume. This seems to capture the majority of the deposits. All of these calculations used the Mathcad 2000 program, and the output of these calculations is attached (file ashplume1.mcd). The area under the plume was calculated by developing a two-dimensional cubic spline function and performing a double integral of the function. The integration yielded a total of 1.478E14 grams of ash. The input quantity of ash was 0.2265E15 grams, so the recovery was only 65.2%. A similar integration of fuel yielded a recovery of 72.3%.

Refined calculations

Subsequent analyses attempted to refine the estimate. One possibility was that some of the plume went behind or upwind of vent, so the grid was extended upwind. Another possibility was that locations close to the vent would account for the greatest ash deposition, so the grid in this area should be finer.

In order to accommodate both a coarse grid for the large area and a fine grid close to the vent, a Fortran program ashnn.f given in Figure 1 was developed for ash deposition, and a similar program ashnnf.f for fuel deposition. These programs perform a fine scale integration of a symmetrical plume by interpolating an ash or fuel deposition from a spatial, irregular grid of points produced by ASHPLUME. First, establish a regular, fine grid encompassing the plume. For the center of each rectangular grid cell, get an interpolated ash deposition value from the irregular grid of points from ASHPLUME using the "nearest neighbor" approach. This was accomplished by calculating the distance between the center of the grid cell and all of the ASHPLUME points, and then selecting the closest 3 points. The interpolated value of deposition was then calculated using inverse square weighting of the 3 points; i.e., the weight of each of the three points was proportional to the inverse of the squared distance from that point to the center of the grid cell. This procedure was repeated for all grid cells in the fine grid.

The results from this procedure yielded an ash recovery of 64.3% and a fuel recovery of 70.7%, which is close to the original estimate. Therefore, it does not appear that the concerns about fineness of the grid or upwind deposition was responsible for the descrepancy.

Integration limits on ASHPLUME

One possible explanation for the discrepancy between the input and recovered amounts of ash and fuel is the outer integration limits for the Suzuki model shown in Equation 2-1 of the ASHPLUME model report (Jarzemba, 1997). The outer integral integrates over the minimum to maximum particle diameter limits set in the input file. The minimum diameter is essentially zero, 10^{-9} cm, but the upper limit is 10 cm. For this run, the geometric mean diameter was 0.0593 cm, and the $\log_{10}$ standard deviation was 1.0. The cumulative distribution of the lognormal function from 0 to 10 cm would be 0.98.7; i.e., the equation integrates only over 98.7% of the possible ash mass. This is slightly lower than 100%, but does not explain the large difference with the recovered ash and fuel amounts.

Conclusions from Preliminary Analyses

The ASHPLUME model does not appear to preserve the mass of ash and fuel inputted to the code for the conditions tested. The best estimate of ash and fuel recovery were 64.3% and 70.7%, respectively. There are several possible reasons for the low ash and fuel recovery including the explanations discussed previously, coding error, and grid spacing and dimensions.

Additional analyses was conducted to evaluate grid spacing and dimensions. The test procedure for this analyses is provided below.

Test Procedure for Additional Testing

1. Using the ashplume input files *infile.ash* and *ashplume.in* from the preliminary testing, run the ASHPLUME.E code with a grid expanded to -40 to 0km (x-direction) and -90 to 10km (y-direction) and a grid spacing of 1 km (note: this is a decrease in the x- and y-grid spacing from 2km to 1km and increase in the modeled area of -20 to 0km [x-direction] and -50 to 0km [y-direction])

2. To capture satisfactorily capture the spent fuel and ash mass, continue with expanded grids for 8 other areas: (1) "more_grid1" of -40 to 0km (x-direction) and -100 to -90km (y-direction); (2) "more_grid2" -40 to 0km (x-direction) and -110 to -100km (y-direction); (3) "more_grid3"-40 to 0km (x-direction) and -120 to -110km (y-direction); (4) "more_grid4" -40 to 0km (x-direction) and -220 to -120km (y-direction); (5) "more_grid5" -40 to 0km (x-direction) and -320 to -220km (y-direction); (6) "more_grid6" -50 to -40km (x-direction) and -320 to 0km (y-

direction); (7) “more_grid7" -50 to 0km (x-direction) and -420 to -320km (y-direction); (8) “more_grid8" -60 to -50km (x-direction) and -420 to 0km (y-direction).

3. Utilize an EXCEL spreadsheet to compute the total mass of fuel and ash in the *ashplume.out* file by integrating (i.e., using an computing the average mass/unit area in a 1km grid block and multiplying by the area [1e10 cm^2/km^2]) and then doubling this value because of symmetry.

4. Compare integrated outputs for fuel and mass to the input values of fuel and mass by computing the % difference between these values and determine whether the *Test Criterion or Expected Results* are met.

Results from Additional Testing

The ashplume code was executed using the same input files utilized in the Preliminary Testing except with the expanded grids described in Step 2 of the Section *Test Procedure for Additional Testing*. Results from these ashplume runs are provided on the CD attached to this report in the subdirectory “Ashplume_Matching_Preliminary_Analyses.”

The spent fuel and ash results (g/cm^2) in the ashplume output file *ashplume.out* were extracted into the EXCEL spreadsheet file *Results_Matching_Preliminary_Analyses.xls* also included on the attached CD. Consistent with Step 3 of the Section *Test Procedure for Additional Testing*, the total mass of spent fuel and ash were computed for the initial grid and each of the 8 additional grids. The cumulative totals of the total mass of spent fuel and ash with each additional grid are provided in the “ashplume” worksheet of the file *Results_Matching_Preliminary_Analyses.xls* together with a % error computed relative to the initial spent fuel and ash mass (as provided in the header section of the ashplume output file *ashplume.out*). There are separate worksheets in this file for each of initial grid and each of the 8 additional grids. The “grid-cumulative” computed total mass of spent fuel and ash are presented below.

(During this analyses, it was observed that for the first grid, ashplume output did not include a spent fuel and ash mass result for the origin [0,0]. Since the origin is the location of the event, an ashplume run was conducted for a location very close to this origin [i.e., at (0, -0.01) or 10 m directly downwind from the event] and the spent fuel and ash mass deposited at this location was used in the EXCEL spreadsheet integration computations.)

Mass of Spent Fuel and Ash and % Differences from Additional Analyses *ashplume* Runs

totals	**g ash**	**kg fuel**
	8.96129E+13	**27536548.49**
	kg ash	**kg fuel**
kg total (x 2 with symmetry)	**1.79226E+11**	**5.50731E+04**
kg initial	**2.26500E+11**	**6.34300E+04**
% difference - first grid	**20.9%**	**13.2%**
total with more grid 1	**1.81797E+11**	**5.58497E+04**
% difference with more grid 1	**19.7%**	**12.0%**
total with more grids 1-2	**1.83983E+11**	**5.65006E+04**

% difference with more grids 1-2	**18.8%**	**10.9%**
total with more grids 1-3	**1.85837E+11**	**5.70477E+04**
% difference with more grids 1-3	**18.0%**	**10.1%**
total with more grids 1-4	**1.95586E+11**	**5.98149E+04**
% difference with more grids 1-4	**13.6%**	**5.7%**
total with more grids 1-5	**1.99739E+11**	**6.09188E+04**
% difference with more grids 1-5	**11.8%**	**4.0%**
total with more grids 1-6	**2.01254E+11**	**6.13330E+04**
% difference with more grids 1-6	**11.1%**	**3.3%**
total with more grids 1-7	**2.03709E+11**	**6.19555E+04**
% difference with more grids 1-7	**10.1%**	**2.3%**
total with more grids 1-8	**2.05049E+11**	**6.23104E+04**
% difference with more grids 1-8	**9.5%**	**1.8%**

Conclusions from Additional Analyses

From the results above for the first grid, the % difference between the initial and the computed deposited spent fuel and ash masses was **13.2%** and **20.9%**, respectively. This is a reasonable result and demonstrates consistency with the Preliminary Testing results (which showed approximately **30%** and **35%** differences), because, since the grid expanded from -20 to 0km (x-direction) and -50 to 0km (y-direction) to -40 to 0km (x-direction) and -90 to 0km (y-direction), it is expected more mass will be captured in the total mass computations.

Moreover, with each additional grid, the accumulated amount of computed deposited spent fuel and ash increases and results in the following decrease in the % difference between the initial and deposited spent fuel and ash masses. (Note that the % difference from first grid followed by the % difference for each of the additional 8 grids is shown.)

Spent Fuel: 13.2%, 12.0%, 10.9%, 10.1%, 5.7%, 4.0%, 3.3%, 2.3%, and **<u>1.8%</u>**

Ash: 20.9%, 19.7%, 18.8%, 18.0%, 13.6%, 11.8%, 11.1%, 10.1%, and **<u>9.5%</u>**

Therefore, this Additional Analyses determines a less than 10% difference between the initial and deposited spent fuel and ash masses and thus the *Test Criterion or Expected Results* are met.

Overall Status

The *Test Criterion or Expected Results* for a less than 10% difference between the initial and deposited spent fuel and ash masses are met and the test is successfully **PASSED.**

Reference

Jarzemba, M, P. LaPlante, K. Poor, "ASHPLUME version 1.0 - a code for contaminated ash dispersal and deposition", CNWRA 97-004, Center for Nuclear Waste Regulatory Analyses, San Antonio, TX, February 1997.

Figure 1 - ashnn.for computer code

```
      program ashnn
c     integration of ash plume total deposition
c     using nearest neighbor with random locations for
c     ash densities rbc 7/15/03
c     variables in code
c     x,y = location of points of ash deposition,
c       with respect to vent, km
c     ashden = ash deposit density, gm/cm^2
c     fuelden = fuel deposit density, gm/cm^2
c     xnn,ynn = 3 nearest neighbors to an integration point
c     wt = weights for each nearest neighbor
      real x(6000),y(6000),ashden(6000),fuelden(6000)
      real xs(6000),ys(6000),ashds(6000),fuelds(6000)
      real xnn(3),ynn(3),d2nn(3),w(3),wt(3)
      real d2(6000),d2s(6000),ashdnn(3),fueldnn(3)
      open(1,file='ashtot.dat')
      open(2,file='ashsave.tmp')
      i=0
  1   continue
      i=i+1
c     read the location, ash and fuel density from ASHPLUME
      read(1,*,end=200) x(i),y(i),ashden(i),fuelden(i)
      go to 1
 200  continue
      npts=i-1
c     max and minimum of x for plume, km. Just half of symmetric plume here
c     xmin=0
      xmax=25
c     number of x locations for fine grid integration
      nx=200
c     max an min of y direction for plume, km
      ymin=-50
      ymax=10
c     number of y locations for fine grid integration
      ny=200
c     start nearest neighbor procedure
      sum=0
c     the x,y increments and the area of a patch for fine grid integration
      dx=(xmax-xmin)/nx
      dy=(ymax-ymin)/nx
      darea=dx*dy
      write(6,*) 'dx,dy,darea=',dx,dy,darea
c     start fine points grid
```

```
        l=0
        do j=1,nx
          xp=(j-1)*dx+xmin+dx/2
          do i=1,ny
            yp=(i-1)*dy + ymin+dy/2
            l=l+1
            do k=1,npts
c             calculate distances
              d2(k)=(xp-x(k))**2+(yp-y(k))**2
            end do
c           sort the distances and pick the 3 nearest neighbors
            do k=1,npts
              d2s(k)=d2(k)
              xs(k)=x(k)
              ys(k)=y(k)
              ashds(k)=ashden(k)
              fuelds(k)=fuelden(k)
            end do
            call sort2(npts,d2s,xs,ys,ashds,fuelds)
c           pick the three nearest neighbors
            do k=1,3
              d2nn(k)=d2s(k)
              xnn(k)=xs(k)
              ynn(k)=ys(k)
              ashdnn(k)=ashds(k)
              fueldnn(k)=fuelds(k)
            end do
c           calculate the weighted average from 3 nearest neighbors
c           using inverse square distance
            do k=1,3
              if(d2nn(k).gt.0.0) then
                w(k)=1.0/d2nn(k)
              else
                w(k)=1.0e20
              end if
            end do
            do k=1,3
              wt(k)=w(k)/(w(1)+w(2)+w(3))
            end do
c         the ash deposition for the grid cell
            ashe=wt(1)*ashdnn(1)+wt(2)*ashdnn(2)
     1      + wt(3)*ashdnn(3)
            write(2,'(i5,2f9.3,e13.3)') l,xp,yp,ashe
c         accumulate the ash
            cumash=cumash+ashe
          end do
        end do
c       convert the sum to grams, and use factor of 2 for symmetric plume
        cumash=cumash*2e10*darea
        write(6,*) 'cumash = ', cumash
        stop
        end

      SUBROUTINE SORT2(N,RA,RB,rc,rd,re)
c       sort RA from largest to smallest, and resort RB, RC, RD
c       using the same order
       real RA(6000),RB(6000),rc(6000),rd(6000),
     1  re(6000)
      L=N/2+1
```

```
      IR=N
10    CONTINUE
        IF(L.GT.1)THEN
          L=L-1
          RRA=RA(L)
          RRB=RB(L)
              rrc=rc(l)
              rrd=rd(l)
              rre=re(l)
        ELSE
          RRA=RA(IR)
          RRB=RB(IR)
              rrc=rc(ir)
              rrd=rd(ir)
              rre=re(ir)
          RA(IR)=RA(1)
          RB(IR)=RB(1)
              rc(ir)=rc(1)
              rd(ir)=rd(1)
              re(ir)=re(1)
          IR=IR-1
          IF(IR.EQ.1)THEN
            RA(1)=RRA
            RB(1)=RRB
                rc(1)=rrc
                rd(1)=rrd
                re(1)=rre
            RETURN
          ENDIF
        ENDIF
        I=L
        J=L+L
20        IF(J.LE.IR)THEN
          IF(J.LT.IR)THEN
            IF(RA(J).LT.RA(J+1))J=J+1
          ENDIF
          IF(RRA.LT.RA(J))THEN
            RA(I)=RA(J)
            RB(I)=RB(J)
                rc(i)=rc(j)
                rd(i)=rd(j)
                re(i)=re(j)
            I=J
            J=J+J
          ELSE
            J=IR+1
          ENDIF
        GO TO 20
        ENDIF
        RA(I)=RRA
        RB(I)=RRB
            rc(i)=rrc
            rd(i)=rrd
            re(i)=rre
      GO TO 10
      END
```

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 20.06002.01.354	
Software Name: TPA		Version: 5.1 BetaU
Test ID: **S-1**	Test Series Name: **Waste Package Failure Modes**	

Test Method

☐ code inspection
■ output inspection
☐ hand calculation
☐ spreadsheet
■ graphical
☐ comparison with external code results

Test Objective:
The TPA code includes a number of processes leading to failure of the waste packages. This task seeks to understand the timing of waste package failure and identification of dominant failure modes.

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): Microsoft Windows XP; in addition to FORTRAN scripts supplied by the CNWRA (Osvaldo Pensado), R scripts were written to display graphically timing and magnitude of failure modes. Mathematica 5.1 was used to display data in graphic form and post-process the data.

Input Data (files, data base, mode settings): Nominal case tpa.inp for 10,000, 100,000 and 1,000,000 years. For disruptive scenarios, modifications to the nominal case tpa.inp included switching on the flags VolcanismDisruptiveScenarioFlag and FaultingDisruptiveScenarioFlag, in addition to change of the NumberOfTimeStepsAfterCompliancePeriod. 500 realizations were used for all simulations. The maximum time for faulting and igneous activities for the 100,000 and 1,000,000 years simulations were set to the simulation times respectively. The VolcanoModel was set to 1 = Geometric.

Assumptions, constraints, and/or scope of test: See Attachments A–C.

Test Procedure: See Attachments A–C.

Test Results

Location: See attached CD labeled “TPA Version 5.1 Validation Task S-1"

Test Criterion and Analysis of Results: The dominant failure modes for various time periods of interest must agree with conceptual understandings. The mean failure fractions must agree with input values in tpa.inp. There should not be double counting of waste package failures in realizations that return multiple failure modes in a single subarea. See Attachments A–C for results.

Test Evaluation (Pass/Fail): Pass

Notes:

Testers: C. Grossman, J. Gwo, O. Pensado	Date: 4/18/2007

Attachment A
TPA Version 5.1 Validation Task S-1

Scope of Test

1. For the nominal scenario, reference case, determine the dominant failure modes (i.e., initial defects, localized corrosion, mechanical, or general corrosion) for various time periods of interest (e.g., 10,000 years or 1,000,000 years) and input data that have the greatest effect on occurrence of those failure modes.
2. For the disruptive scenario, both igneous and faulting cases, determine the dominant failure modes for various time periods of interest (e.g., 10,000 years or 1,000,000 years) and input data that have the greatest effect on occurrence of those failure modes.
3. For realizations that return multiple failure modes in a single subarea (e.g., initial defects, localized corrosion, and mechanical), resulting source terms should be consistent with the numbers of packages failed by each mode (i.e., no double counting).
4. Identify systematic bias of waste package failures in all subareas.

Test Procedure

1. Identify waste package failure modes for nominal-seismic scenario

   Run three 500-realization runs, nominal-seismic scenario, with append flags on, 10^4, 10^5 and 10^6 years.

   Compare the normalized number of waste packages failed per subarea (normalized to the total number of waste packages in a subarea). The normalized number of waste packages failed per subarea may not be different from subarea to subarea. If differences are noted, rationalize any differences. Also, identify the predominant failure modes and the times they occur from wpsfail2.res. Identify an differences for the various simulation periods.

2. Identify waste package failure modes for faulting and igneous scenarios

   Run three 500-realization runs, faulting-igneous scenarios, with append flags on, 10^4, 10^5 and 10^6 years. Compare normalized number of waste packages failed per subarea. Identify the predominant failure modes and the times they occur. Identify an differences for the various simulation periods.

   Run multiple 500-realizations runs with faulting-igneous scenarios for 10^4 years using different random seeds. Compare normalized number of waste packages failed in the subareas. Identify any systematic bias of waste packages failed for all failure modes.

Test Results

1. Nominal Scenario

   Acceptance Testing for Software Change Report 663 (TPA 5.1 Version Beta O) checked in detail waste package counting and probability factors to scale the number of waste packages contributing to release. It was concluded that the number of waste packages contributing to release was properly defined in the TPA code (i.e., there is no double counting).

In the system level test it was concluded that he number of waste packages breached by localized corrosion and mechanical interaction with the drip shield shows consistent trends with expectations.

Scaling factors $P_{contact}$ and $P_{allowance}$ were properly implemented for the various waste package classes (initially defective, localized corrosion, and mechanical waste packages)

Dependence of results on the simulation time were noted, fully explainable a due to the waste package classification approach to define representative waste packages.

Detailed results on the testing were documented in the Power Point presentation, Attachment B. The presentation includes TPA output file names from which the data were read. Electronic files, Fortran scripts to read the data from TPA output files (located in the folder FortranScriptsTPA5.1), as well as the Mathematica 5.1 notebook (file name analysis.nb) for data post-processing and graphic display are included a CD accompanying this Software Validation Report.

2. Faulting-Igneous Scenarios

With the faulting and igneous flags on, the subarea fractions of waste packages failed due to localized corrosion are smaller in comparison with the nominal scenario (Attachment C, p. C-2), correctly reflecting the classification scheme of failed waste packages. Because of the longer simulation periods, mechanical failures for the 10^6 years run has the highest waste package failure fraction comparing with the other two runs for 10^4 and 10^5 years. The fractional mechanical failure history curves for the 10^5 and 10^6 years runs diverge slightly, caused by the waste package failure classification scheme (Attachment C, p. C-3). The detailed explanation of the dependence of the number of localized corrosion waste packages on the simulation time is provided in Attachment B, p. B-10.

The fractional faulting failure history curves for the 10^5 and 10^6 years runs also diverge slightly (Attachment C, p. C-7). These two history curves separate conspicuously from those of 10^4 years. The reason for the separation is the use of truncated exponential distributions (truncated at the end of the simulation) to define event times. Use of truncated exponential distributions is an appropriate approach to estimate conditional consequences. Conditional consequences should be multiplied by the probability of the scenario in the timeframe of interest (e.g., 10^5 or 10^6 years) to derive a dose risk. The probability weighted consequences produce comparable results, independent of the simulation time. Likewise, the conditional igneous consequence curves for the 10^4, 10^5 and 10^6 years runs separate from each other visibly (Attachment C, p. C-4). Probability weighted igneous consequences are independent of the simulation time.

Four random seeds, including the one used for the nominal scenario, were used to run four 10^4 year simulations. The results indicated that there is not statistically significant bias of waste package failure of all modes among the 10 subareas (Attachment C., p. C-4 – 8).

With the igneous flag on, the dominant failure mode is the volcanism, on the condition that an igneous event occur in a subarea. The EBS release rates for Am, Np and Pu may increase more than 2 orders of magnitude and more than 1 order of magnitude for Tc-99 and Th-230 should an igneous event occur (Attachment C, p. C-9).

Detailed results on the testing were documented in a Power Point presentation, Attachment C. Electronic files, R scripts to read the data from TPA output files for post-processing and graphic display are included a CD accompanying this Software Validation Report.

Attachment B

TPA Version 5.1 Beta U
Validation Testing
Task S-1
Nominal Scenario
Waste Package Failure Analysis

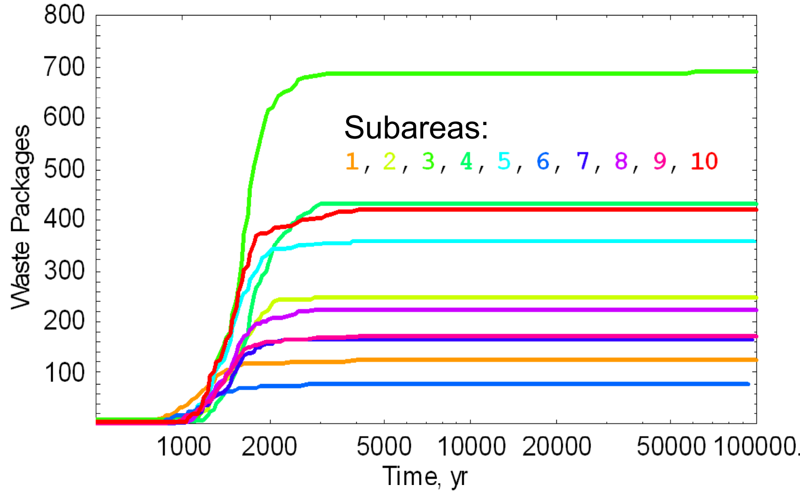
Osvaldo Pensado

March 28-29, 2007

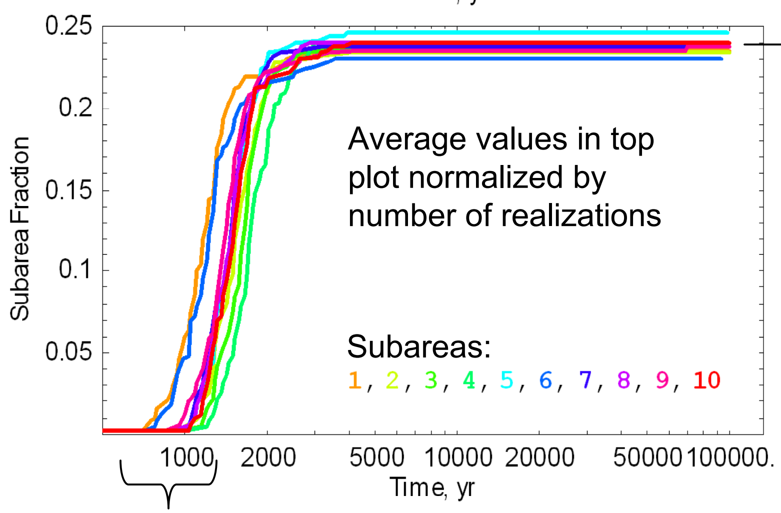
Team Members: T. Ghosh, C. Grossman,J. Gwo

Localized Corrosion

Data from wpsfail.res, 5th column. Average from 500 realizations. Nominal scenario



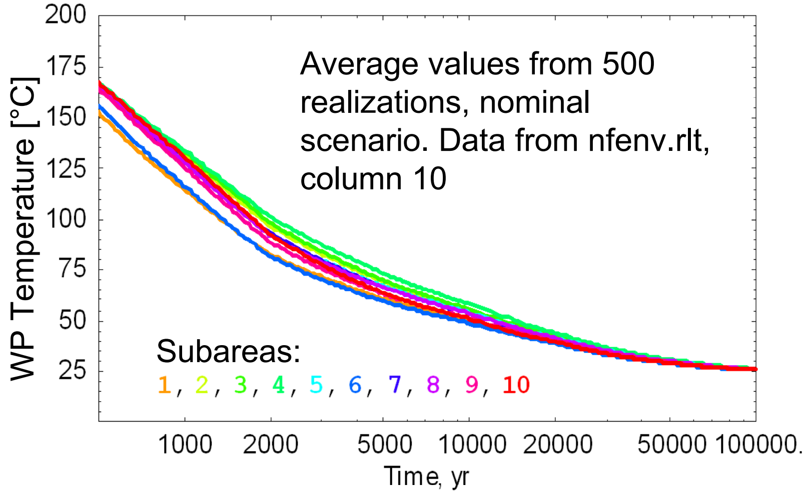
No WPs	Subarea
2904.	SA3
1793.	SA4
1747.	SA10
1452.	SA5
1062.	SA2
931.	SA8
723.	SA9
696.	SA7
526.	SA1
343.	SA6



Value consistent with localized corrosion estimates in the report CNWRA 2005-02, Passive and Localized Corrosion of Alloy 22 —Modeling and Experiments

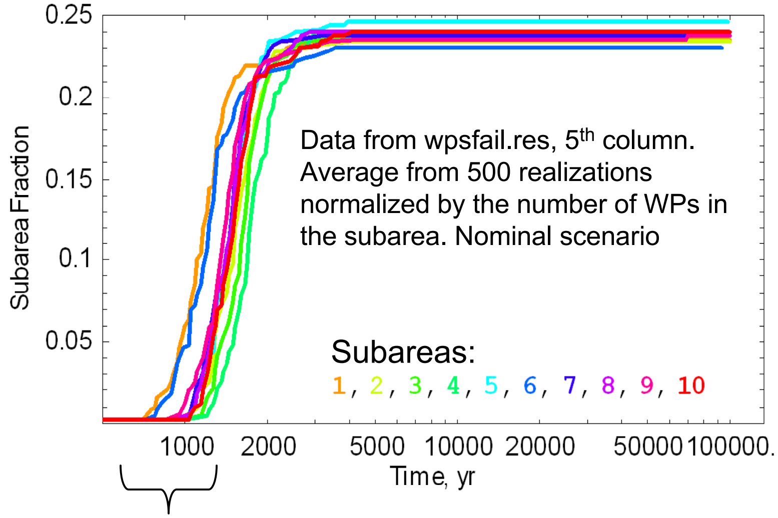
The order is consistent with subarea temperatures as shown in next slide

Localized Corrosion



No WPs	Subarea
2904.	SA3
1793.	SA4
1747.	SA10
1452.	SA5
1062.	SA2
931.	SA8
723.	SA9
696.	SA7
526.	SA1
343.	SA6

Subareas temperature tends to increase, in average, with increasing number of waste packages

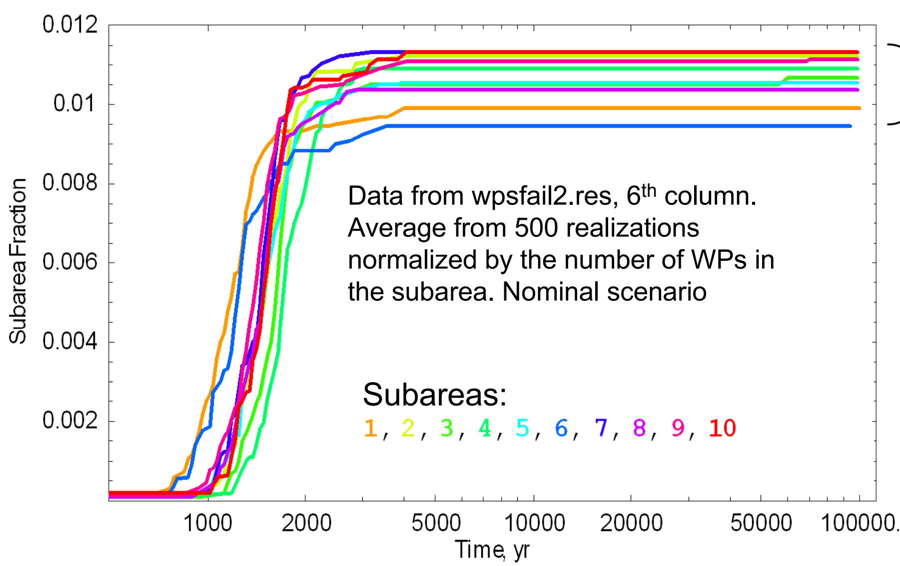


The initiation of localized corrosion is mainly controlled by the time of re-wetting. In the TPA code, re-wetting after reflux occurs when the waste package temperature drops below threshold values. Therefore, localized corrosion is initiated first in cooler subareas and later in hotter subareas.

Localized corrosion is first initiated in subareas of low temperature and later in hotter subareas

Localized Corrosion

- The number of WPs in the file wpsfail.res is scaled by the factor $P_{contact}$
- Probability_WPWaterContact_LC=uniform(1.0E-3, 1.0E-1)
- From data in the wpsfail.res
  - Maximum number of WPs affected by LC = 23% of WPs (see previous slide)
  - When the scale factor $P_{contact}$ is applied (data tracked in wpsfail2.res), the maximum average number of WPs contributing to radionuclide release should be approximately 1%



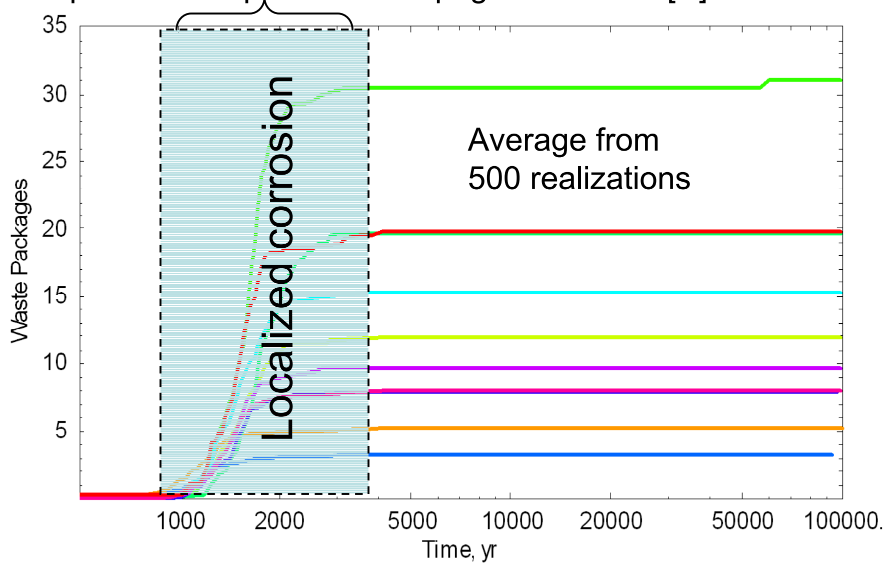
Maximum number of WPs affected by LC = 23% of WPs (from wpsfail.res)

Average $P_{contact}$ value: 0.05

The product is 0.0115, consistent with the plot

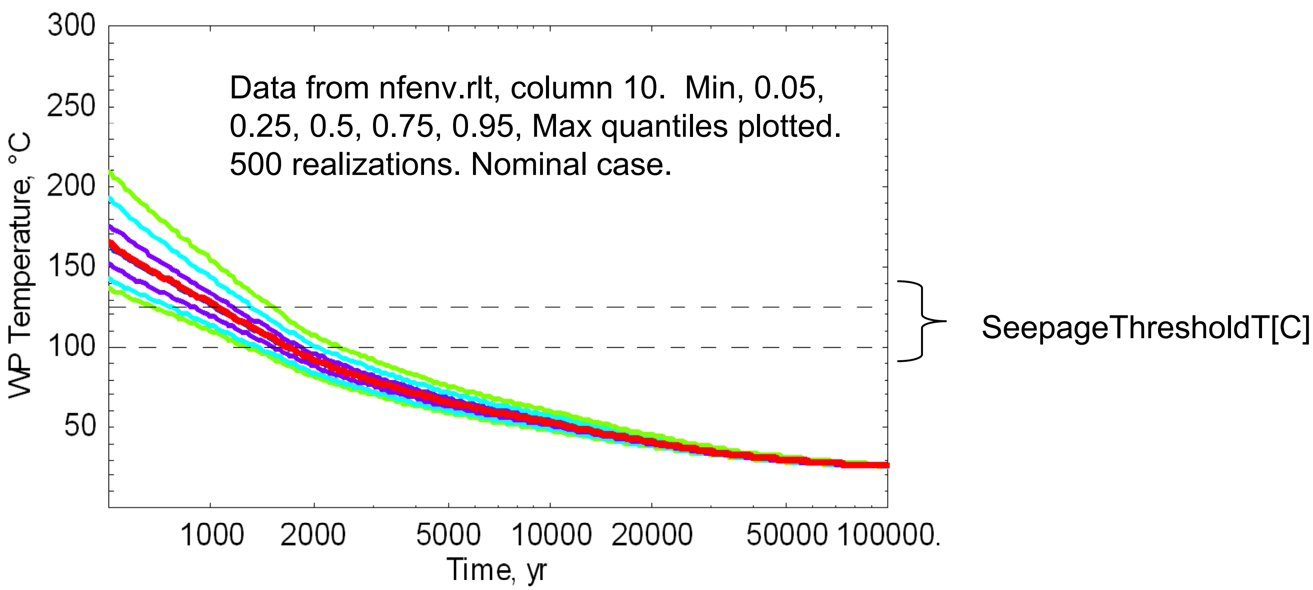
Localized Corrosion

Localized corrosion initiation consistent with time when WP temperature drops below SeepageThresholdT[C]

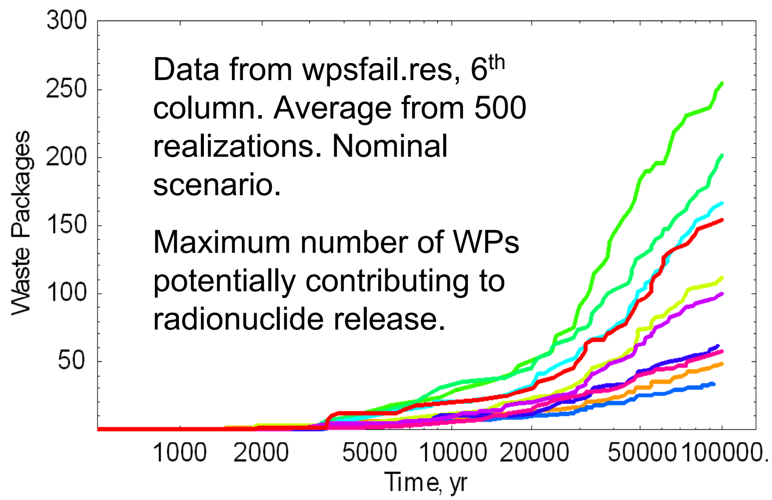


No WPs	Subarea
2904.	SA3
1793.	SA4
1747.	SA10
1452.	SA5
1062.	SA2
931.	SA8
723.	SA9
696.	SA7
526.	SA1
343.	SA6

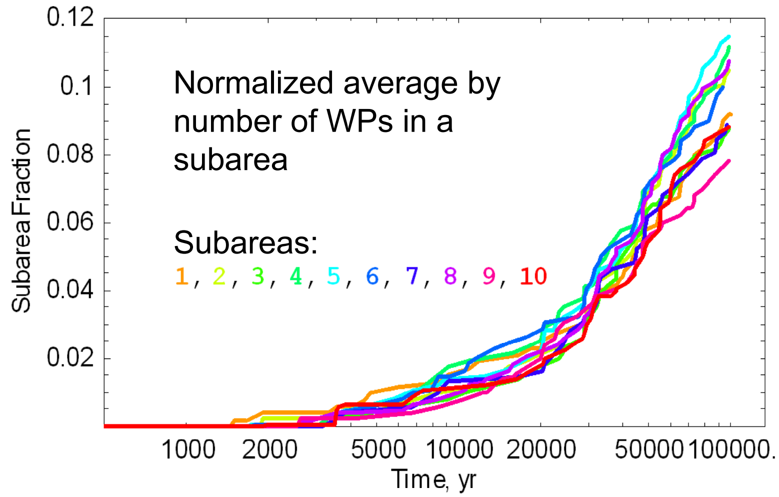
Data from wpsfail2.res ($P_{contact}$ applied to determine the number of WPs breached)



Mechanical Breach



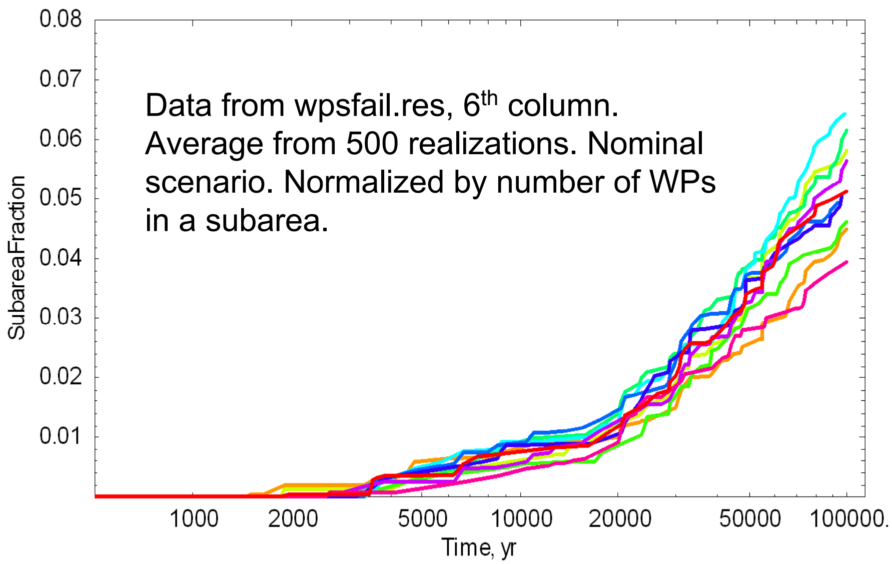
No WPs	Subarea
2904.	SA3
1793.	SA4
1747.	SA10
1452.	SA5
1062.	SA2
931.	SA8
723.	SA9
696.	SA7
526.	SA1
343.	SA6



The normalized number of WPs (i.e., subarea fraction) do not show any significant trend. From the point of view of seismic damage, all subareas are alike.

Mechanical Breach

- The number of WPs in the file wpsfail.res is scaled by the factor $P_{allowance}$
- Probability_WPWaterAllowance_MechFail=uniform(1.0E-2, 1.0)
- From data in the wpsfail.res
  - Maximum number of WPs contributing to release = ~10% of WPs in 10^5 years (see previous slide)
  - When the scale factor $P_{allowance}$ is applied (data tracked in wpsfail2.res), the maximum average number of WPs contributing to radionuclide release should be approximately 5%



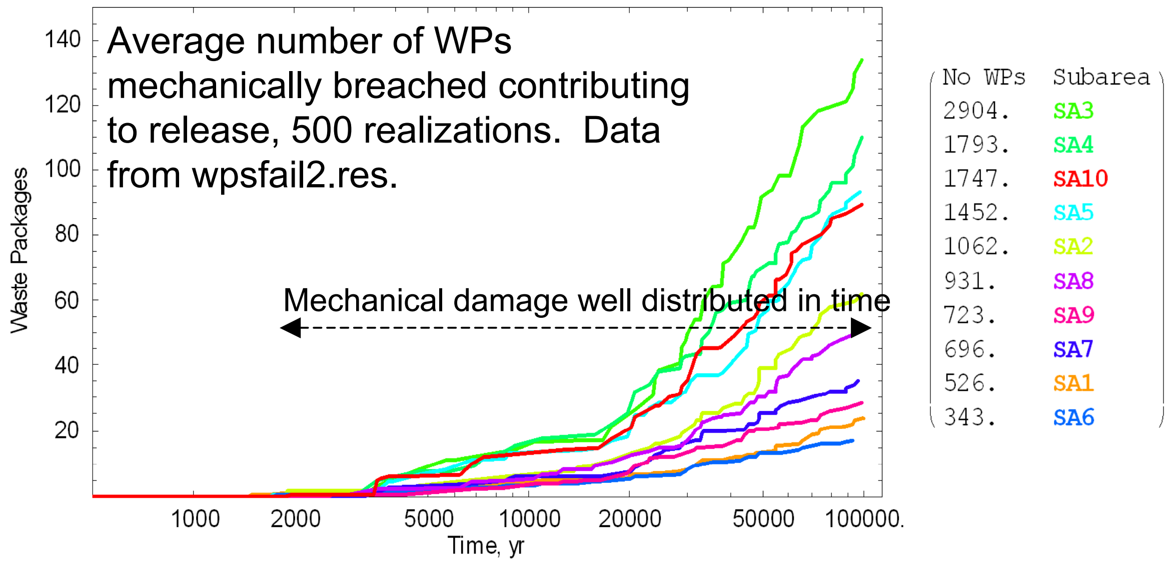
Maximum number of WPs contributing to release in 10^5 years: 10%

Mean $P_{allowance}$: 0.5

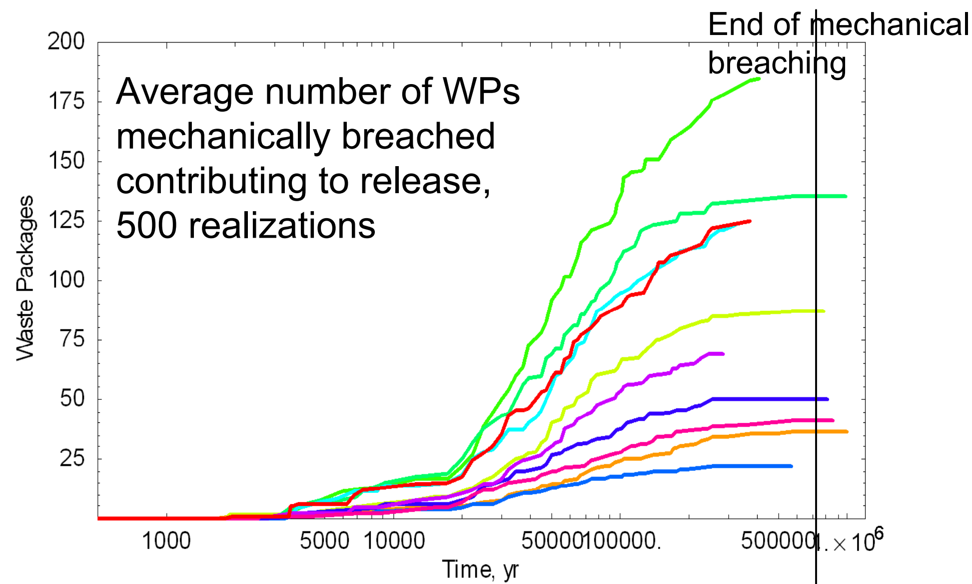
The product, 0.05, is consistent with end of plot

Thermal-hydrology plays minimal role in creating differences in WP failure from subarea to subarea.

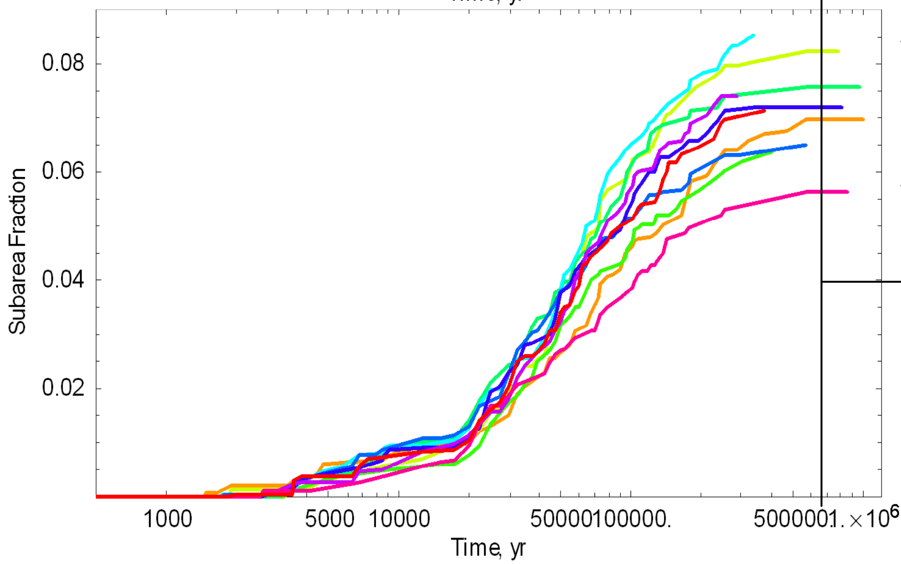
Mechanical Breach



Mechanical Breach, 10^6 years



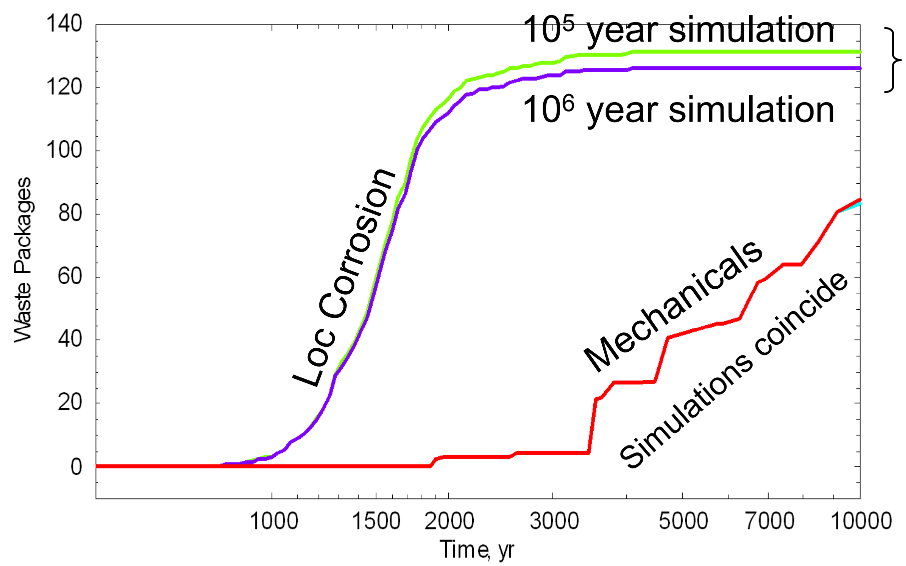
No WPs	Subarea
2904.	SA3
1793.	SA4
1747.	SA10
1452.	SA5
1062.	SA2
931.	SA8
723.	SA9
696.	SA7
526.	SA1
343.	SA6

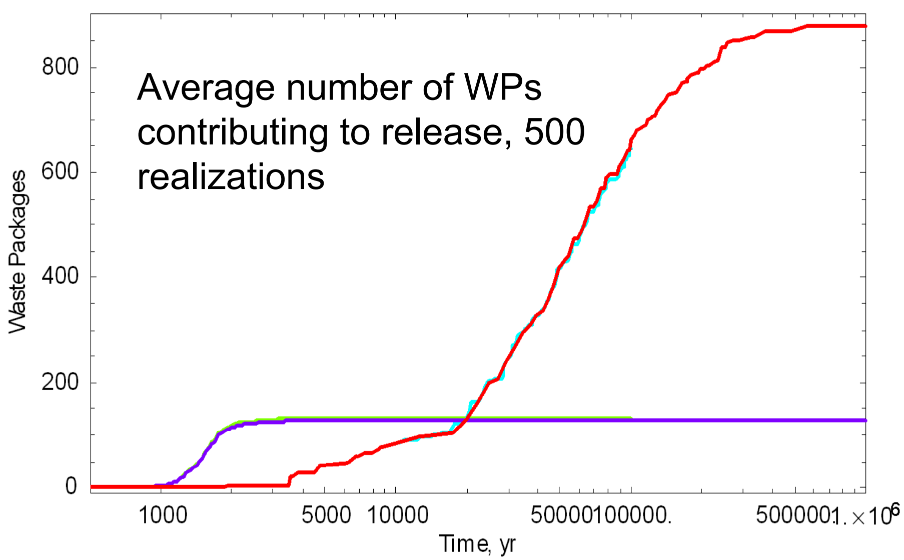


Variance is broader as time elapses

End of mechanical breaching is controlled by the drip shield corrosion rate:
DripShieldCorrosionRate[m/yr]=logtriangular(2.0e-8, 2.98e-7, 6.4e-7).
Maximum time = 0.015 m/(2E-8 m/yr) = 7.5E5 yr
After the drip shield is breached by corrosion it is assumed that it cannot efficiently transfer rock loads to the waste package (i.e., mechanical breaching of the WP is not longer possible)

Comparison of Simulation Times





} Small difference

The small difference is due to the WP classification approach.

WP classified as members of the LC class in 10^5 year simulations can be classified as belonging to the MECH class in 10^6 year simulations (the MECH class wins over the LC class).

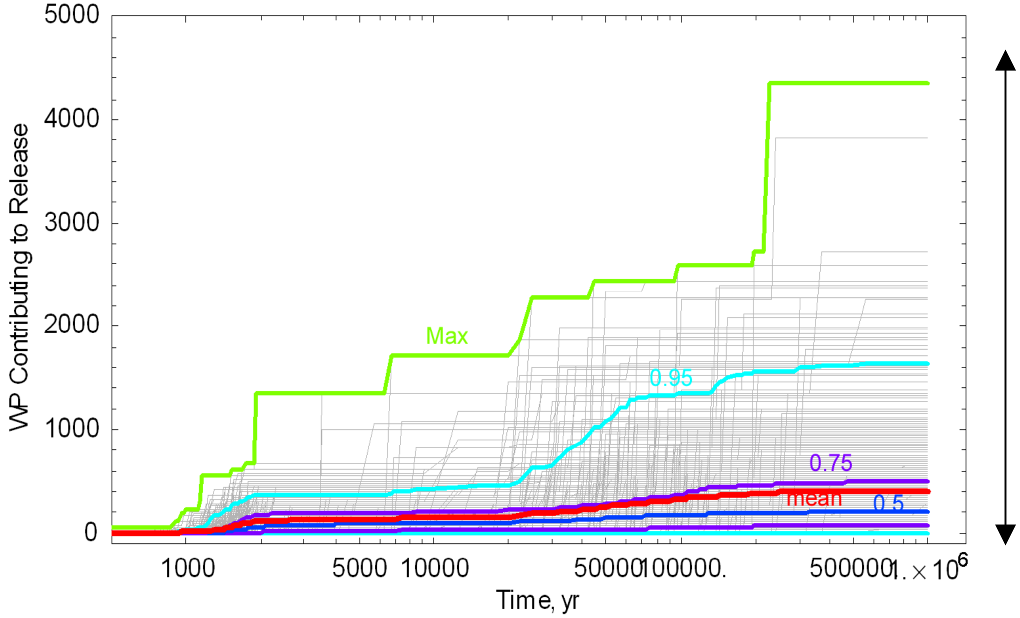
If mechanical breaching and LC occur in the same subarea, in the same realization, those WPs belong to the MECH class. However, it is assumed that those WPs also experience LC (LC seepage factors are used and releases are activated at the time of LC breaching).

In the end, the total number of WPs experiencing LC (in the LC and MECH classes) is larger for longer simulation times.

Therefore, different results are expected depending on the simulation time (but not too different), unless LC or mechanical breaching is deactivated in the simulation.

Waste Packages Contributing to Release

Initials, localized corrosion, and mechanicals
500 realizations



Lots of variance introduced by the $P_{contact}$ and $P_{allowance}$ factors

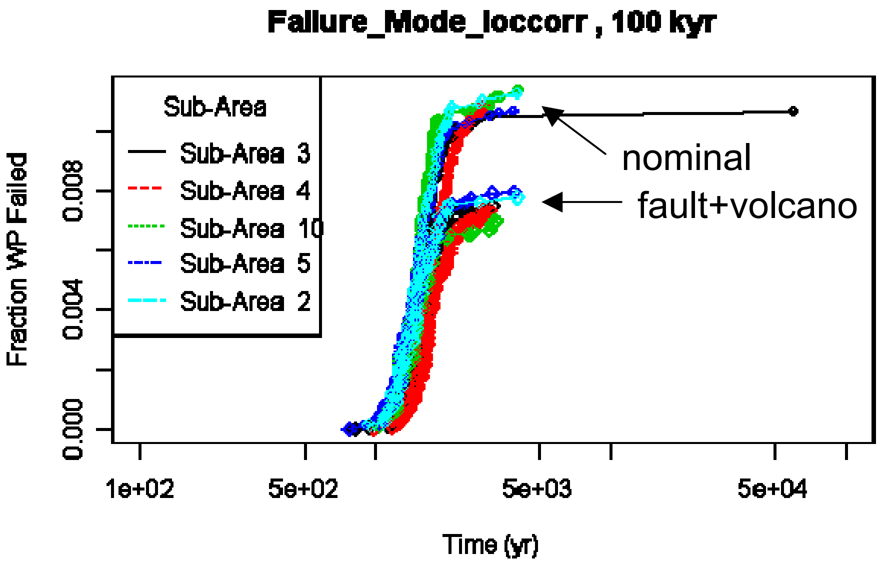
Conclusion

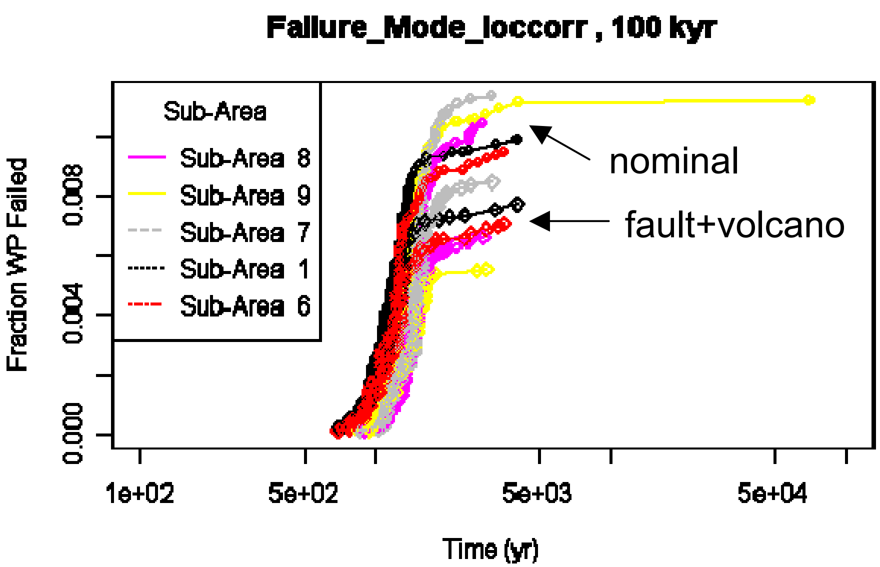
- The number of waste packages breached by localized corrosion and mechanical interaction with the drip shield shows consistent trends with expectations
- Scaling factors $P_{contact}$ and $P_{allowance}$ are properly implemented
- Dependence of results on the simulation time were noted, fully explainable a due to the waste package classification approach to define representative waste packages
- Acceptance testing for Software Change Report 663 checked in detail that $P_{contact}$ and $P_{allowance}$ factors were properly implemented in general.

Attachment C

TPA Version 5.1 Beta U
Validation Testing

System Level Task S-1
Failure Mode – Fault/Volcano
Jack Gwo

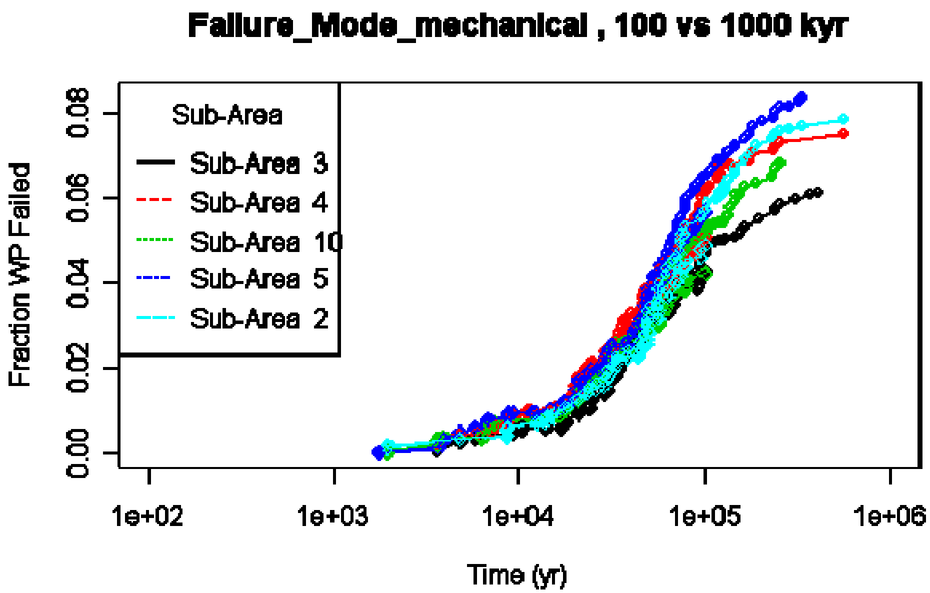




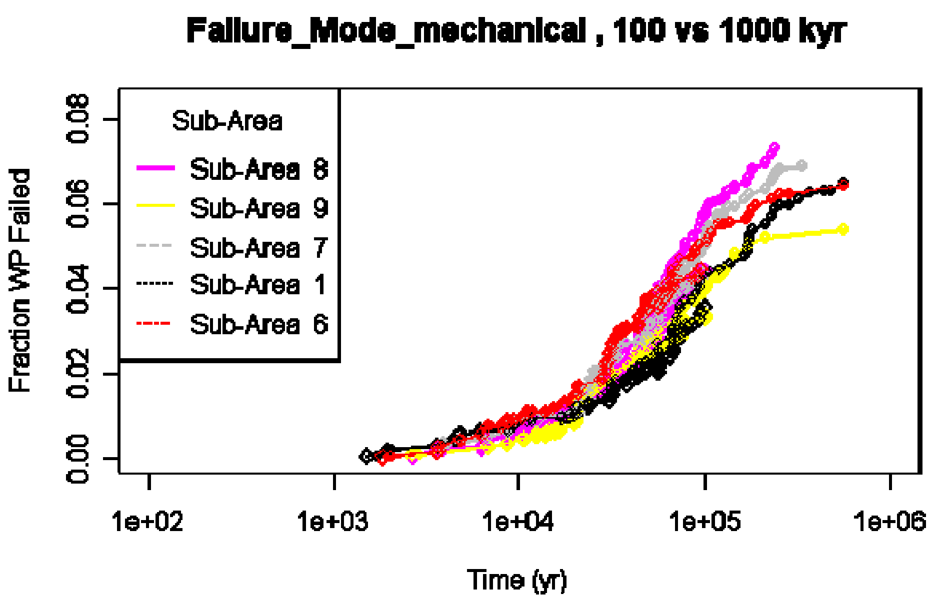
	nominal		fault/volcano 100 kyr	
Sub-Area	mean	std	mean	std
SA_1	0.0099	0.0231	0.0077	0.0208
SA_2	0.0112	0.0255	0.0078	0.0210
SA_3	0.0107	0.0241	0.0075	0.0174
SA_4	0.0109	0.0245	0.0073	0.0188
SA_5	0.0106	0.0243	0.0079	0.0211
SA_6	0.0094	0.0221	0.0071	0.0190
SA_7	0.0113	0.0250	0.0085	0.0213
SA_8	0.0104	0.0238	0.0066	0.0190
SA_9	0.0112	0.0246	0.0055	0.0179
SA_10	0.0113	0.0249	0.0070	0.0193

Observations:

1. **Fault/volcano (100 kyr and 1 myr) cases has lower fraction of localized corrosion in sub-areas.**
2. **Ditto mechanical failure for 100 kyr but not 1 myr which has the highest failure fractions among the three cases (nominal, 100 kyr and 1 myr) – caused by the longer simulation period.**

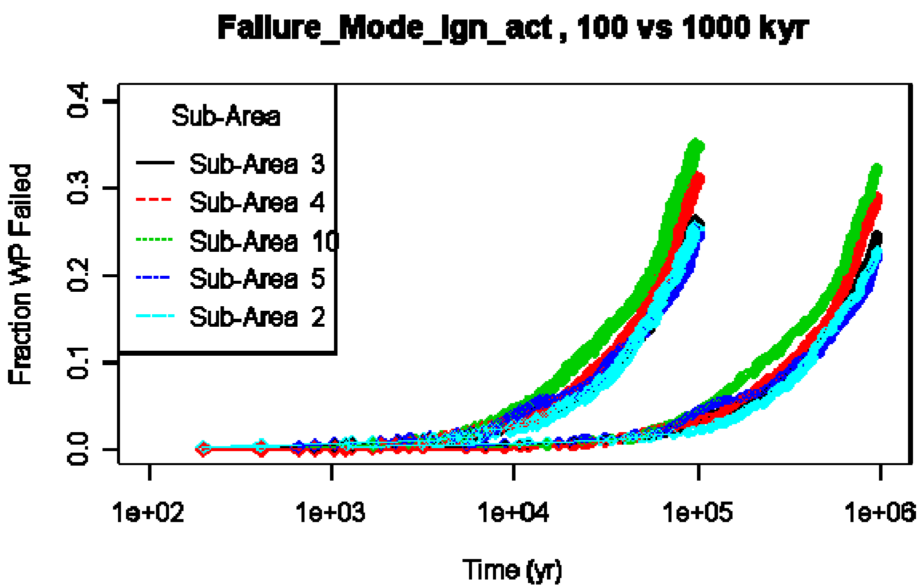


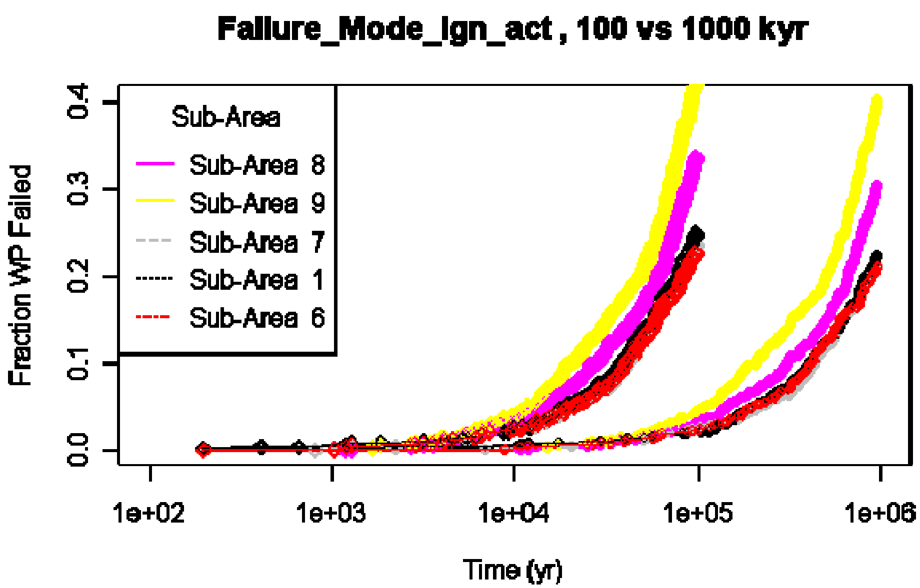
	nomin		fault/volcano 100 kyr		fault/volcano 1 myr	
fail mode	mean	std	mean	std	mean	std
loccorr	0.0107	0.0242	0.0073	0.0196	0.0069	0.0192
mech	0.0522	0.1786	0.0443	0.1629	0.0691	0.2025
fault			0.0007	0.0036	0.0007	0.0038
ign_act			0.2905	0.3995	0.2666	0.3900



Observations:

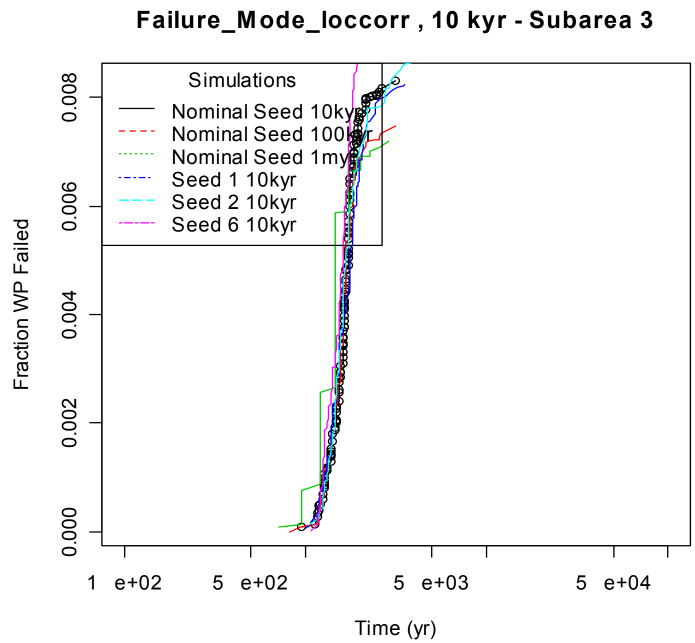
1. **1 myr and 100 kyr failure mode history diverges slightly for localized corrosion, mechanical and faulting.**

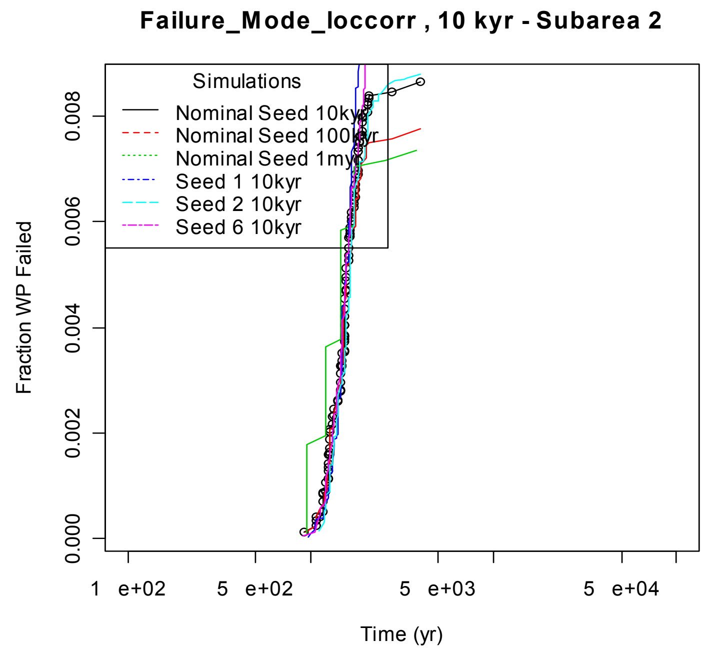


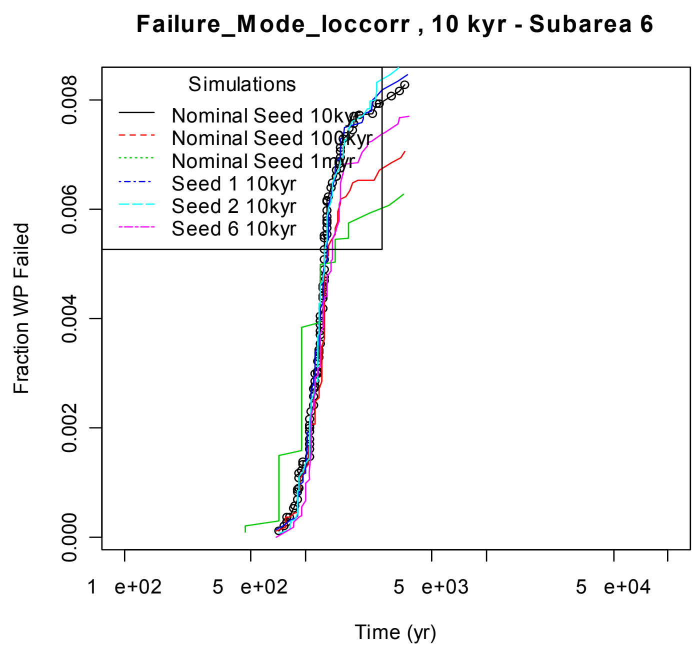


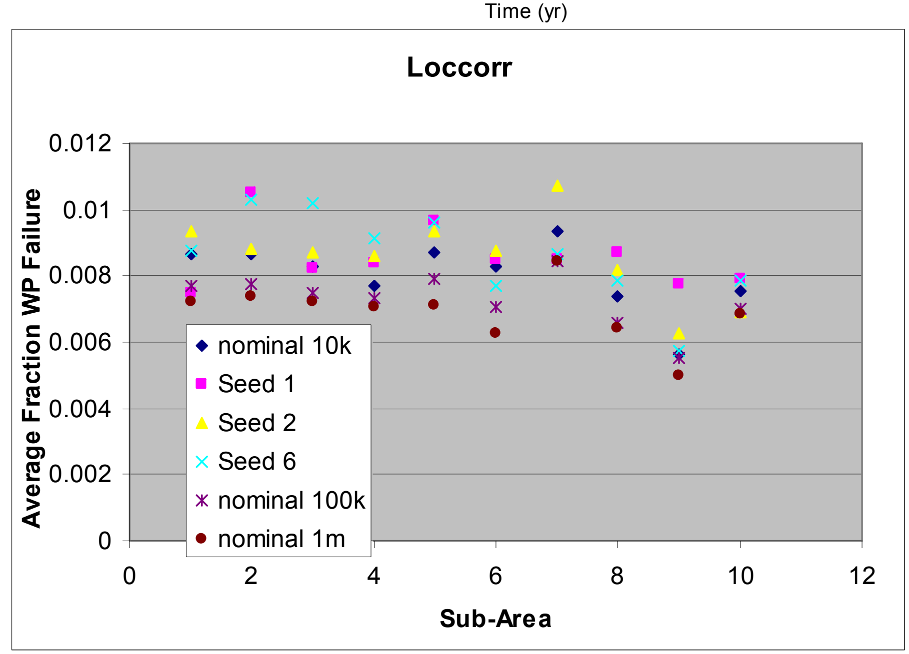
Observations:

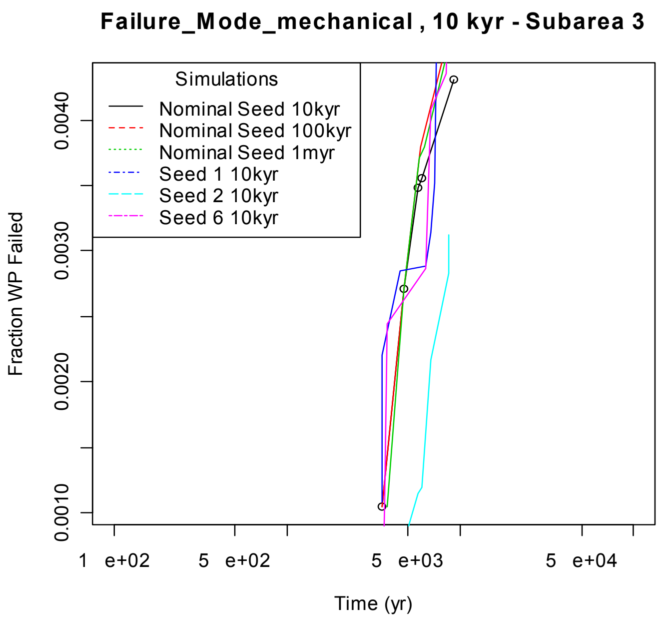
1. **The failure mode history curves of igneous activities for 100 kyr and 1 myr runs separate conspicuously.**
2. **The reason for the separation is the use of truncated exponential distributions (truncated at the end of the simulation) to define event times. Use of truncated exponential distributions is an appropriate approach to estimate conditional consequences. Conditional consequences should be multiplied by the probability of the scenario in the timeframe of interest (e.g., 10^5 or 10^6 years) to derive risk estimates. The probability weighted consequences produce comparable results, independent of the simulation time.**

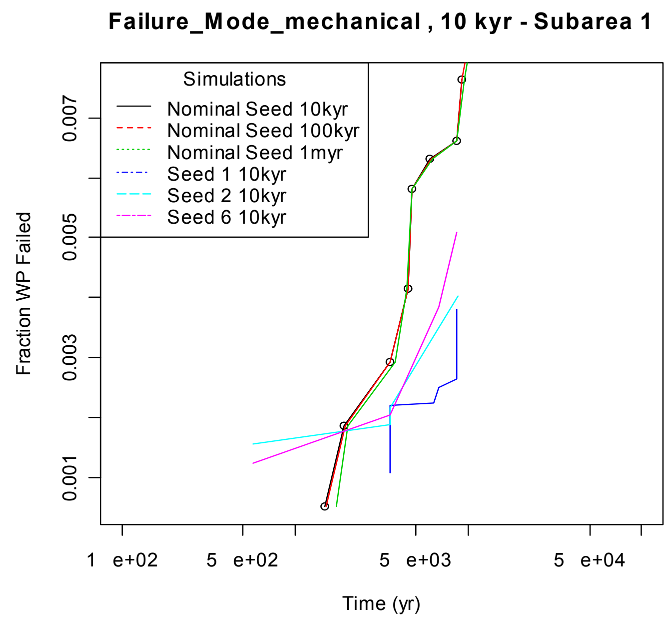

Failure_Mode_loccorr , 10 kyr - Subarea 3
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
0.000
0.002
0.004
0.006
0.008
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)

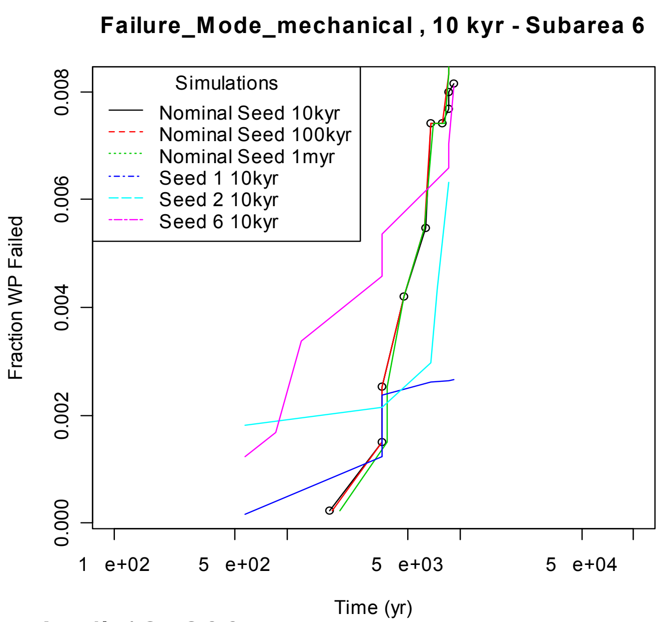

Failure_Mode_loccorr , 10 kyr - Subarea 2
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
0.000
0.002
0.004
0.006
0.008
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)

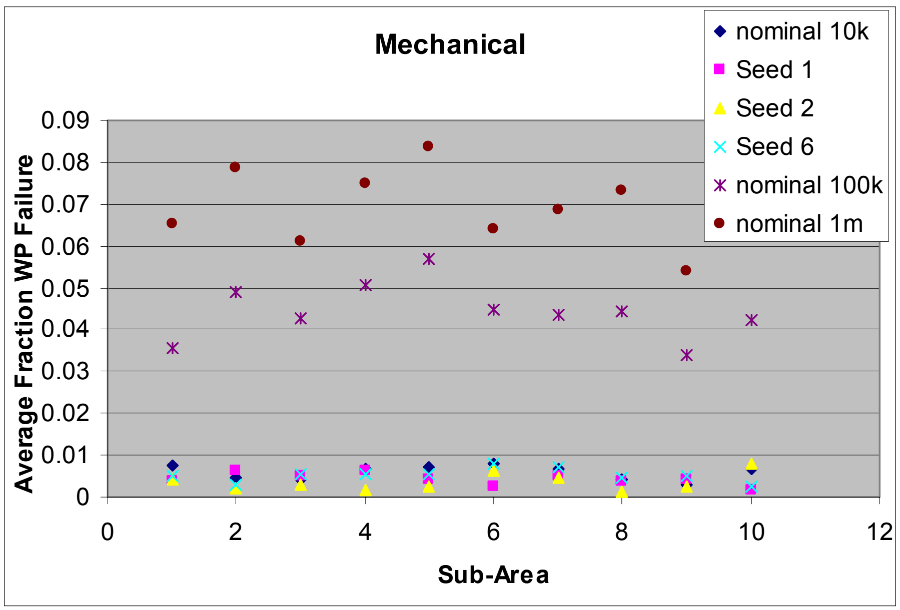

Failure_Mode_loccorr , 10 kyr - Subarea 6
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
0.000
0.002
0.004
0.006
0.008
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)

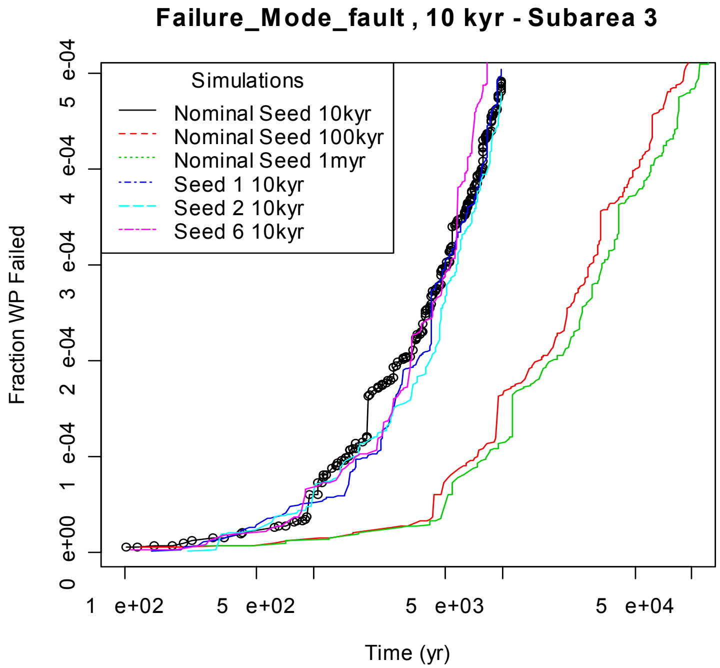

Loccorr
Average Fraction WP Failure
0.012
0.01
0.008
0.006
0.004
0.002
0
0
2
4
6
8
10
12
Sub-Area
nominal 10k
Seed 1
Seed 2
Seed 6
nominal 100k
nominal 1m


Failure_Mode_mechanical , 10 kyr - Subarea 3
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
0.0010
0.0020
0.0030
0.0040
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)

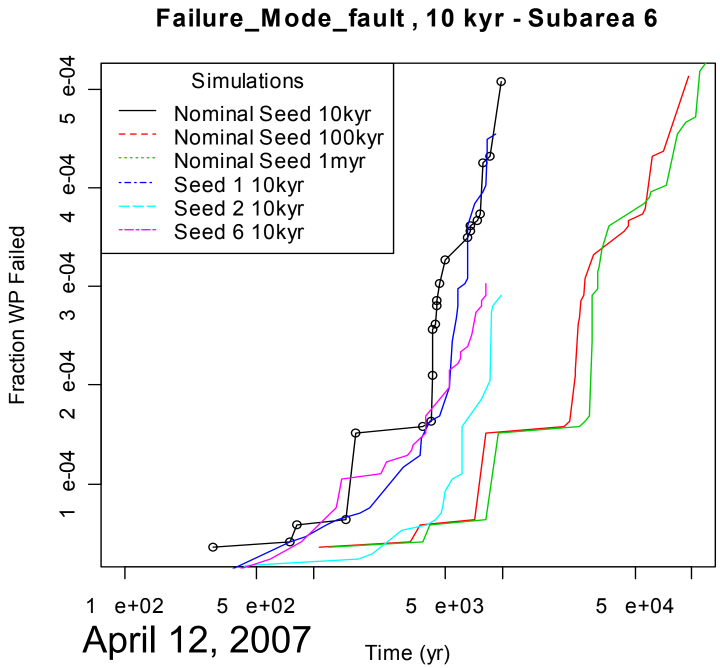

Failure_Mode_mechanical , 10 kyr - Subarea 1
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
0.001
0.003
0.005
0.007
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)


Failure_Mode_mechanical , 10 kyr - Subarea 6
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
0.000
0.002
0.004
0.006
0.008
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)

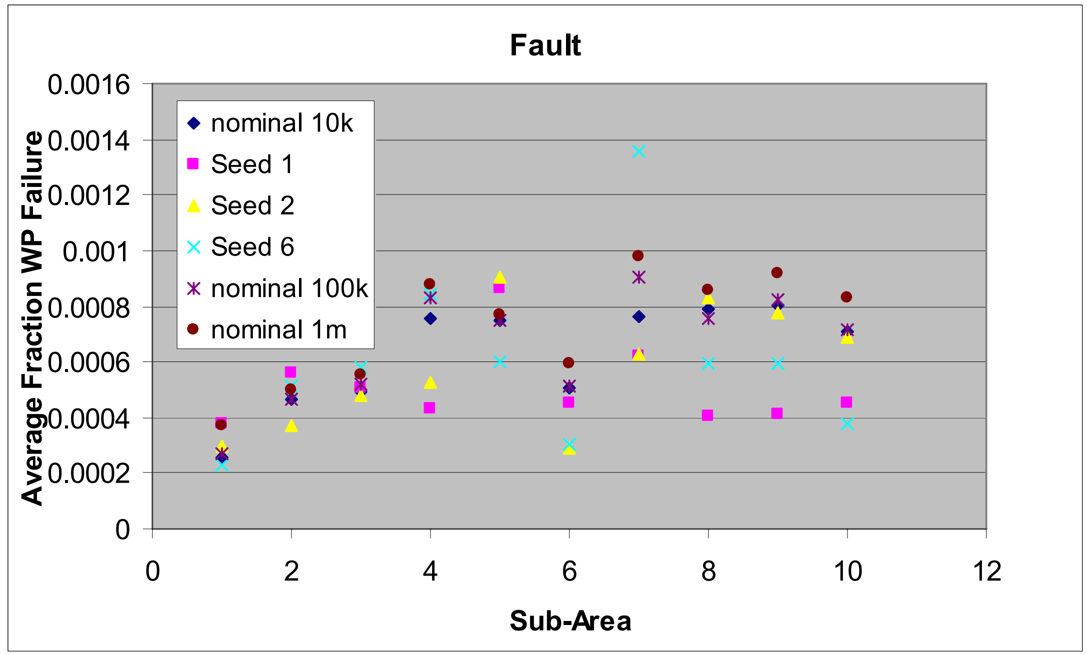

Mechanical
nominal 10k
Seed 1
Seed 2
Seed 6
nominal 100k
nominal 1m
Average Fraction WP Failure
0
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0.09
0
2
4
6
8
10
12
Sub-Area



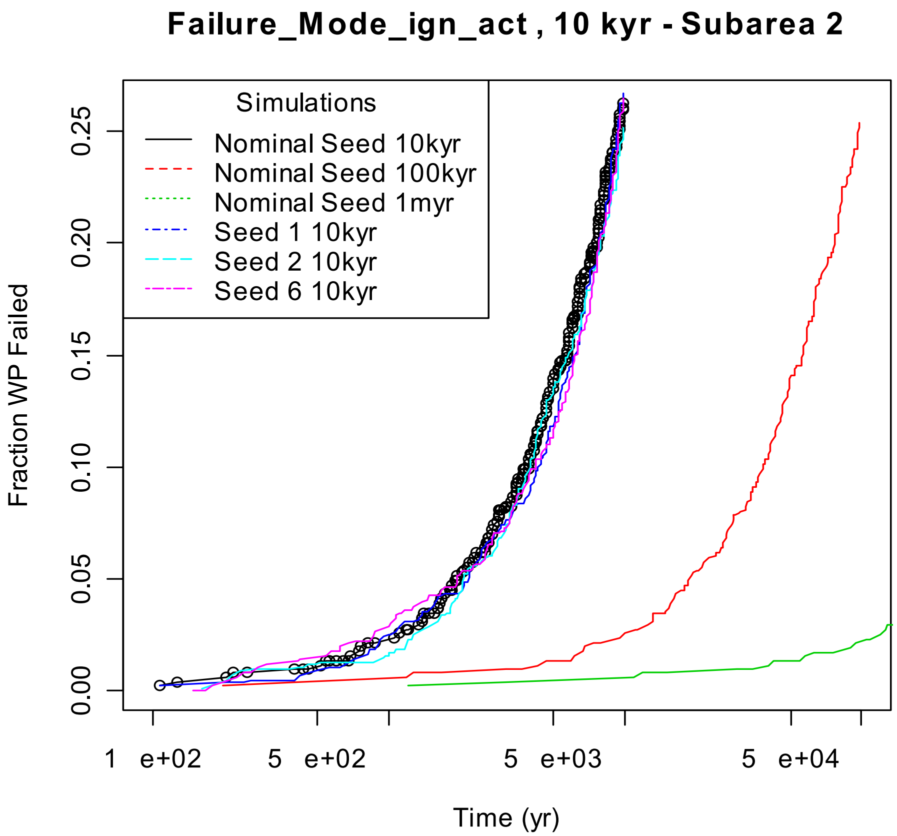
Failure_Mode_fault , 10 kyr - Subarea 3
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
0 e+00
1 e-04
2 e-04
3 e-04
4 e-04
5 e-04
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)

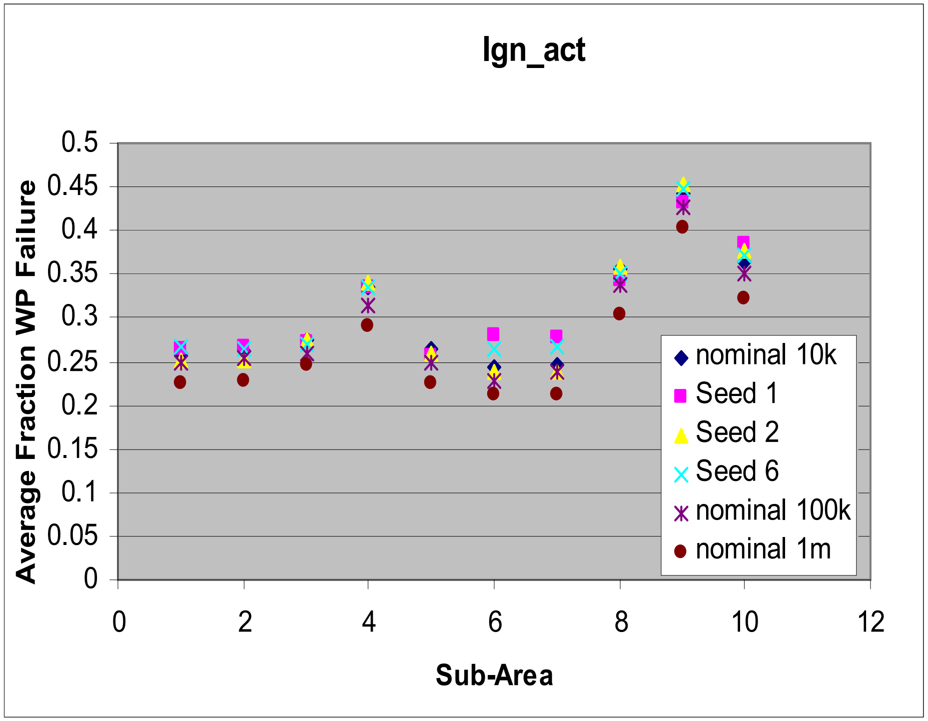


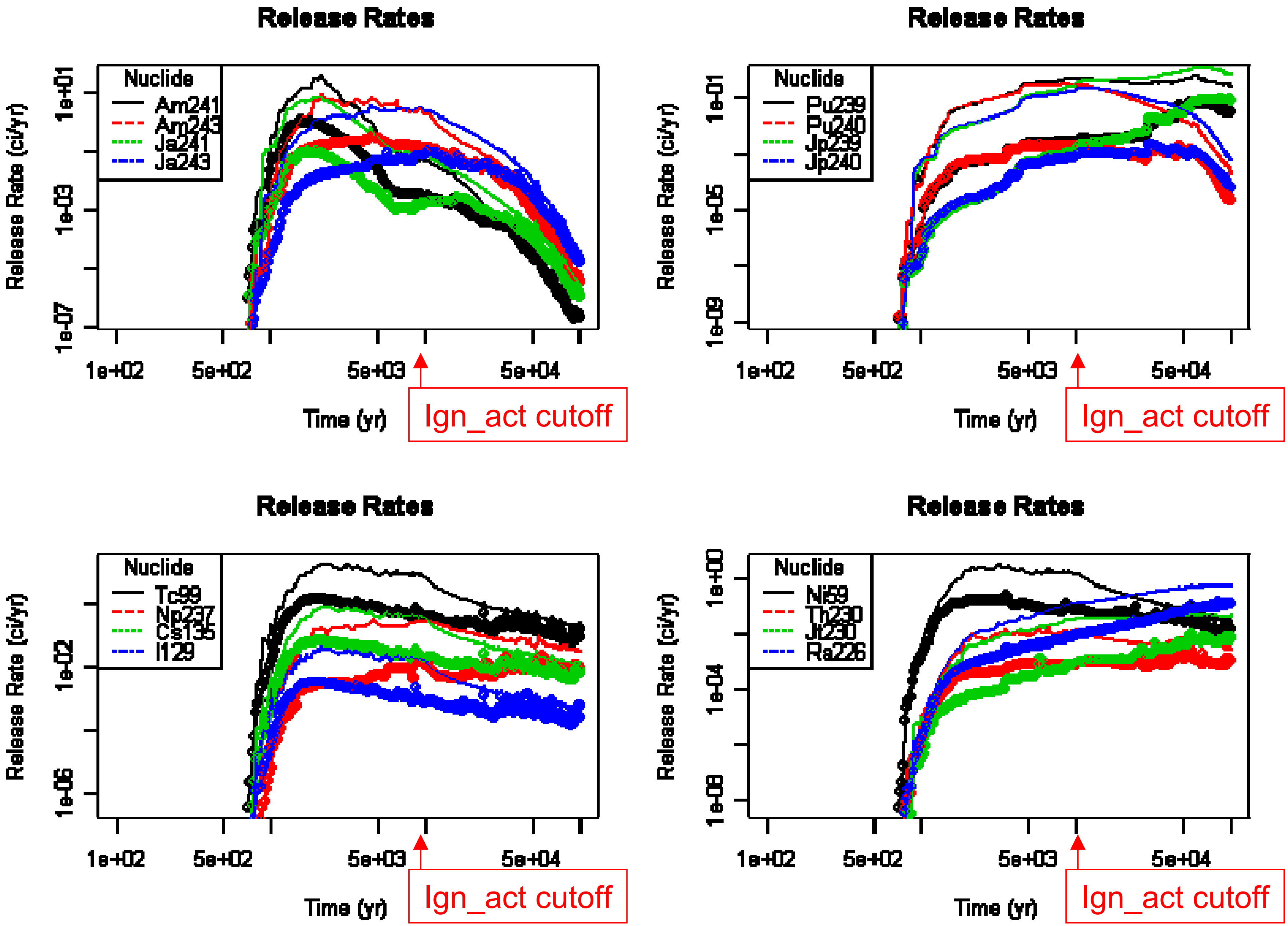
Failure_Mode_fault , 10 kyr - Subarea 6
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
1 e-04
2 e-04
3 e-04
4 e-04
5 e-04
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)



Fault
nominal 10k
Seed 1
Seed 2
Seed 6
nominal 100k
nominal 1m
Average Fraction WP Failure
0.0016
0.0014
0.0012
0.001
0.0008
0.0006
0.0004
0.0002
0
0
2
4
6
8
10
12
Sub-Area


Failure_Mode_ign_act , 10 kyr - Subarea 2
Simulations
Nominal Seed 10kyr
Nominal Seed 100kyr
Nominal Seed 1myr
Seed 1 10kyr
Seed 2 10kyr
Seed 6 10kyr
Fraction WP Failed
0.00
0.05
0.10
0.15
0.20
0.25
1 e+02
5 e+02
5 e+03
5 e+04
Time (yr)


Ign_act
Average Fraction WP Failure
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
2
4
6
8
10
12
Sub-Area
nominal 10k
Seed 1
Seed 2
Seed 6
nominal 100k
nominal 1m



marker = nominal 100 kyr
no marker = fault/volcano on

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 20.06002.01.354	
Software Name: **TPA**		Version: 5.1 BetaW
Test ID: **S-2**	Test Series Name: **System-Level Testing: Radionuclide Release Rates**	

Test Method

- ☐ code inspection
- ■ output inspection
- ☐ hand calculation
- ☐ spreadsheet
- ■ graphical
- ☐ comparison with external code results

Test Objective:
Understand radionuclide release rates at different breakthrough points in the system (engineered barrier system, unsaturated zone, saturated zone)

Test Environment Setup

Hardware (platform, peripherals): PC

Software (OS, compiler, libraries, auxiliary codes or scripts): Microsoft Windows XP. FORTRAN scripts were used to read data from TPA output files. Mathematica 5.1 was used to display data in graphic form and post-process the data.

Input Data (files, data base, mode settings): Nominal case tpa.inp for 100,000 and 1,000,000 years. 500 realizations were used for all simulations

Assumptions, constraints, and/or scope of test:
No special assumptions were considered as the test was aimed at rationalizing trends and behavior in release rates.

Test Procedure: See attachment A

Test Results

Location: Attached in a CD labeled “TPA Version 5.1 Validation Task S-2"

Results: See Attachment B for summary and analysis of results.

Test Criterion and Analysis of Results: Radionuclides release rates for various time periods of interest must agree with conceptual understandings. EBS, UZ, and SZ releases should be mutually consistent. Doses should be consistent with UZ releases. Specific test criteria are described in Attachment B.

Test Evaluation (Pass/Fail): **Pass**

Notes: None

Testers: O. Pensado	Date: April 30, 2007

Attachment A
TPA Version 5.1 Validation Task S-1

500-realization runs of the nominal scenario with seismic activity, with append flags on, 10^5 and 10^6 years were executed using TPA Version 5.1BetaW.

Files *ebsrel.rlt, uzft.rlt, szft.rlt* track releases per radionuclide per subarea. From these output files average releases per radionuclide can be abstracted. FORTRAN scripts were used to read the data from *rlt* files and compute radionuclide averages. The average dose per radionuclide is available in a small file, *rgwna.tpa*. A Mathematica notebook was used for data post-processing and for data plotting.

1. Identification of relevant radionuclides to dose estimates

Plots of the average release rate per radionuclide were used to identify the radionuclides most contributing to release. Results are included in the Attachment B, slides B-1 to B-20.

2. Analysis of the effect of colloids on releases and the dose

Radionuclides transported in intrinsic colloids are tracked as independent species labeled with a *J* character in the TPA output files tracking release rates. The main contributor (dissolved or colloidal) was identified and presented in graphic form. Results are included in the Attachment B, slides B-12 to B-20.

3. General mass balance analyzes of EBS releases

Since detailed mass balance analyzed are required in task P-10; this task was aimed at generic mass balance verifications from EBS releases.

Radionuclides were classified as “low” and “high” solubility. Average release rates were plotted to identify common features.

Radionuclide release rates of “high solubility” should show similar trends. Release rates normalized by the initial inventory should coincide for all radionuclides of high solubility. This expected result was verified. Results are included in the Attachment B, slide B-6.

For radionuclides that are solubility limited, the average release rate divided by the average solubility should be consistent with the average flow rate per waste package reported in the file *infilper.cum*. This expected result was verified. Results are included in the Attachment B, slides B-7, B-10, and B-11.

4. Comparison of radionuclide releases per subarea

Normalized releases (normalized by the number of waste packages in the subarea) were computed and subarea differences were rationalized. It was verified, for example, that cooler subareas exhibit earlier radionuclides releases from the EBS than hotter subareas. Releases from the unsaturated and saturated zones were rationalized as well. Results are included in the Attachment B, slides B-21 to B-25.

5. Evaluate the effect of the diffusive release model on release rates

The diffusive release model is turned off in the TPA version 5.1 reference case. NRC requested an analysis to check the effect of diffusion on release rates. Diffusive releases were turned on by setting the FractionOfWPsWithDiffusionTilt[] = 0.5. Results were compared to a multiple-realization run of the TPA code without diffusive release. It was concluded that, with the set of reference case parameters, diffusive releases are a minor contributor to the total release. Results are included in the Attachment B, slides B-27 to B-28.

TPA Version 5.1 Validation Testing
S-2 Task, Nominal Scenario
Radionuclide Release Rates

Attachment B

Osvaldo Pensado

April 30, 2007

Team Members: T. Ghosh, C. Grossman, J. Gwo

General Comments

- TPA 5.1 beta W
- 500-realization runs, 10^5 and 10^6 yr simulation periods
- Nominal scenario
- Scripts and files to reproduce plots in this presentation are included in an attached CD
- TPA file names with original data are mentioned inside plots

EBS Releases

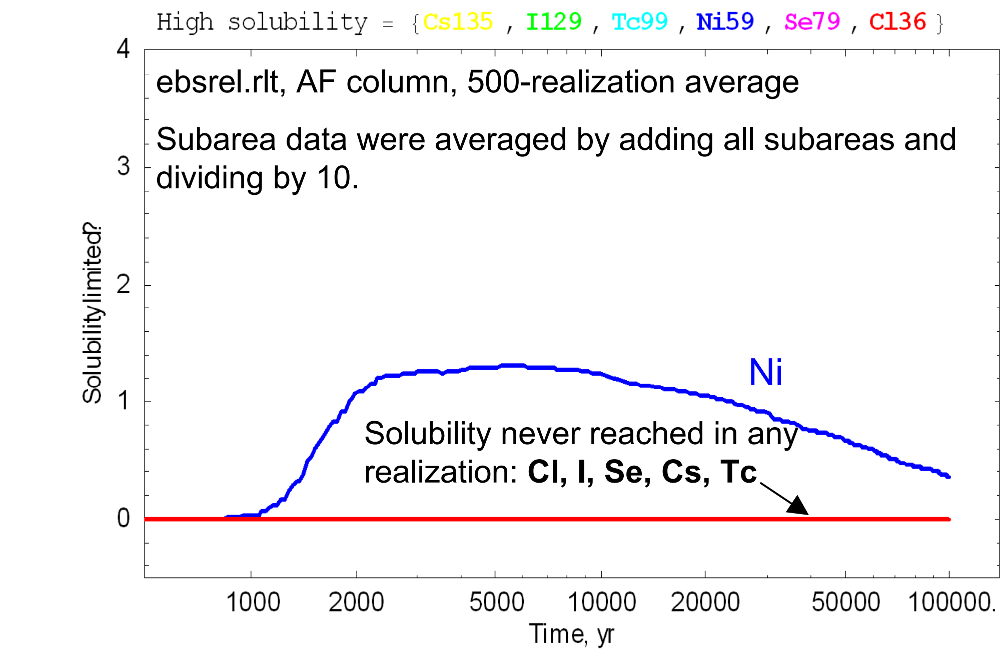
- Test for reasonableness of releases
  - Radionuclides not limited by solubility (e.g., ^{99}Tc)
    - EBS releases must be similar
  - Radiounuclides limited by solubility (e.g., U)
    - EBS release should follow trends dictated by waste package failure and water flow rates
    - Isotopes of an element must attain solubility constraints at the same time
  - For this test radionuclides were grouped in three sets: high solubility, low solubility, and short lived. These groups were also used to compare unsaturated zone and saturated zone releases.
- Identification of relevant radionuclides (Attachment A, test 1)
- Effect of colloids on releases and dose test (Attachment A, test 2)
- Mass balance test (Attachment A, test 3)

ebsrel.rlt: columns indicating whether the solubility limit is reached (no: 0; yes: 1)

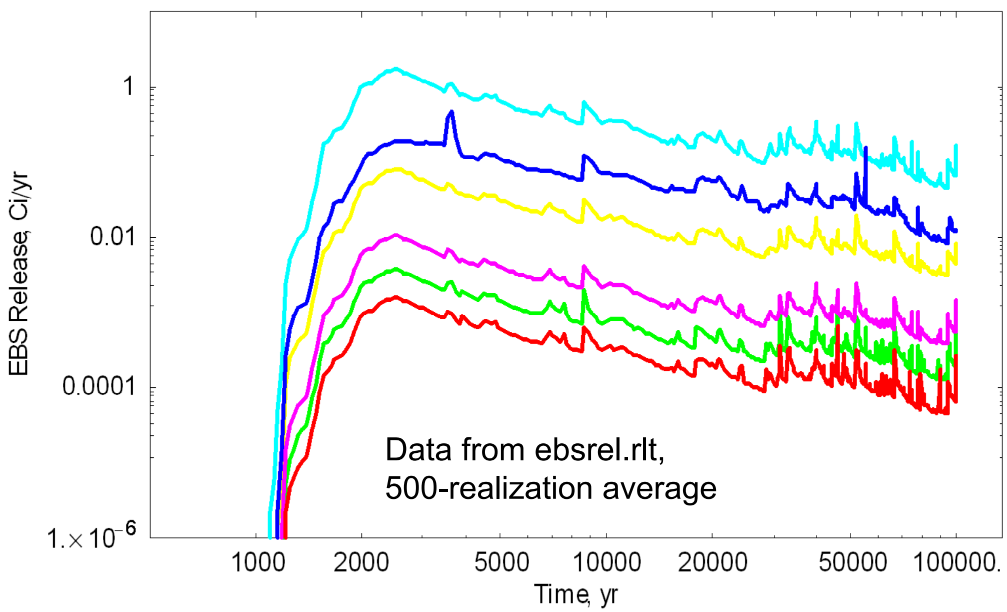
All nuclides - ciperyrinsaintoloweruz
(Ci/yr for this subarea from the ebs)
AF = Affected Flag: If this flag is set (1), then the release rate was affected by solubility.

	time	Cm246	AF	U238	AF	Cm245	AF	Am241	AF	Np237	AF
1	0.0000E+00	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
2	2.3102E+00	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
3	4.6744E+00	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
4	7.0940E+00	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
5	9.5702E+00	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
6	1.2104E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
7	1.4698E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
8	1.7352E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
9	2.0069E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
10	2.2849E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
11	2.5694E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
12	2.8605E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
13	3.1585E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
14	3.4635E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
15	3.7756E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
16	4.0950E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
17	4.4219E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
18	4.7564E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
19	5.0988E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
20	5.4492E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0
21	5.8078E+01	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0	0.0000E+00	0

Approach to compute averages per realization: for any radionuclide add subarea values and divide by 10. The same approach was followed to compute radionuclide release and treat values under the AF columns.



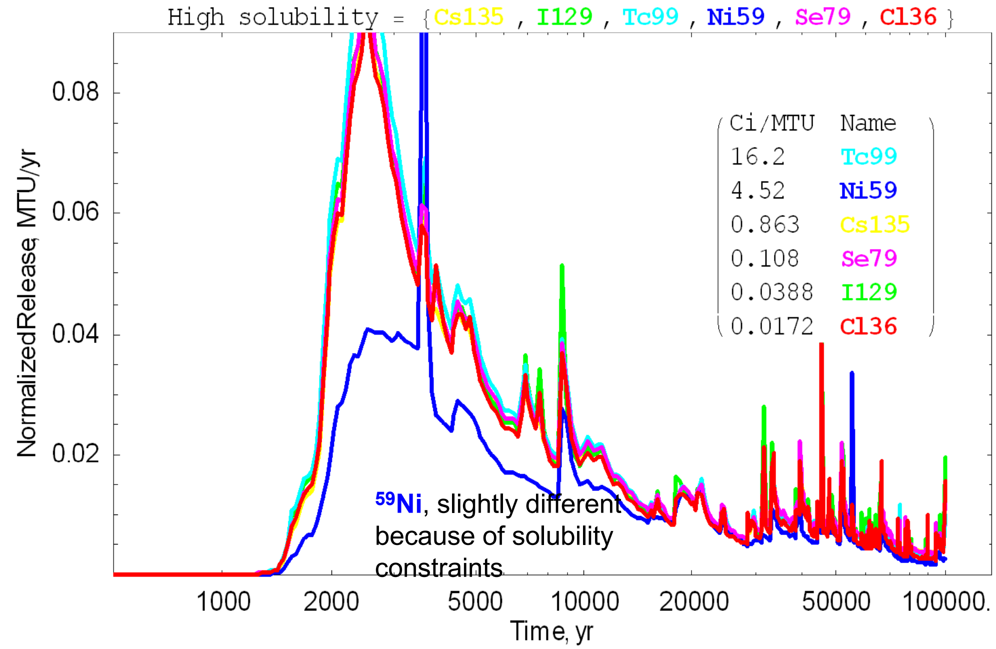
If a radionuclide never attains the solubility limit, then the AF column in ebsrel.rlt reports 0. In the case of Cl, I, Se, Cs, and Tc, only 0's are reported. In the case of Ni, some realizations report 1's (i.e., solubility limits are attained for some realizations).



In the release plot, it is noted that these radionuclides exhibit similar release behavior. The magnitude of the release is controlled by the initial inventory.

Initial Inventory

Ci/MTU	Name
16.2	Tc99
4.52	Ni59
0.863	Cs135
0.108	Se79
0.0388	I129
0.0172	Cl36

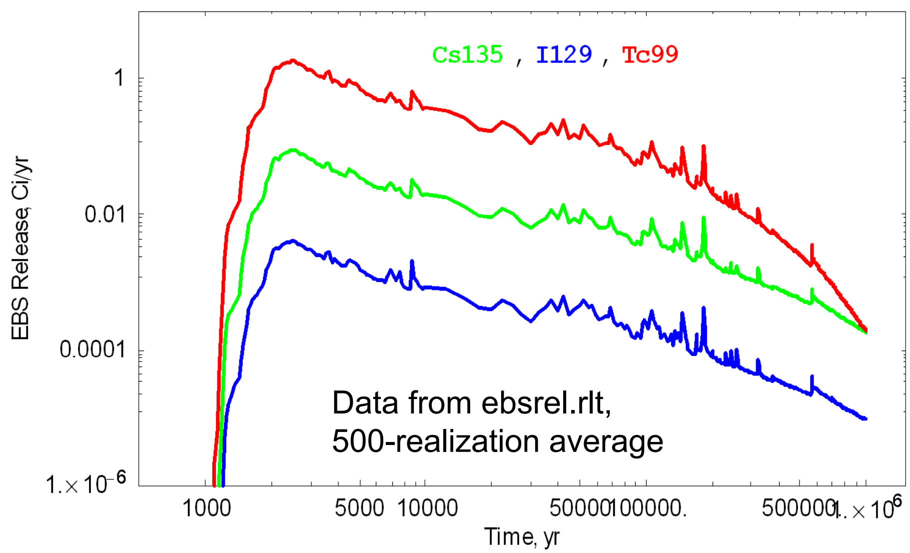


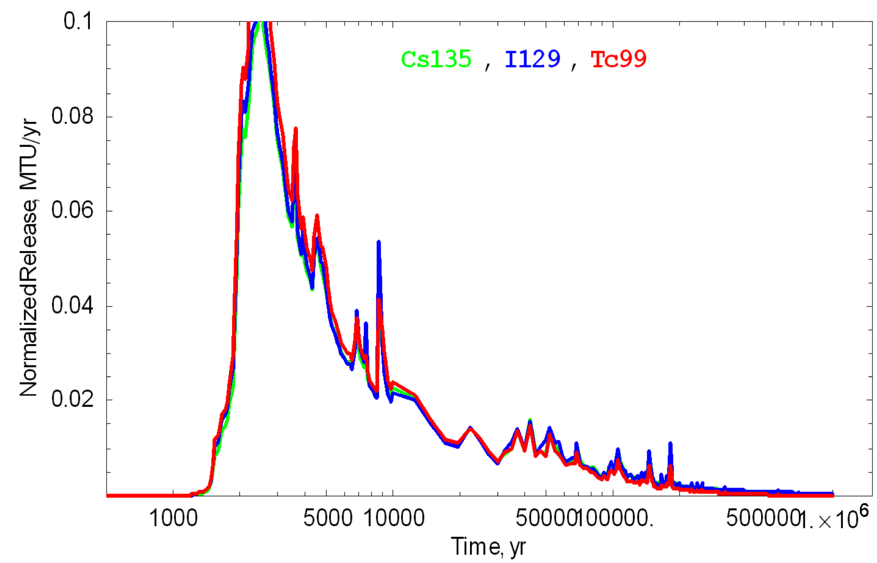
Release rates (Ci/yr) were normalized by the initial inventory (Ci/MTU). Normalized releases are practically identical (note that the vertical scale is linear). The exception is ^{59}Ni, due to the fact that Ni release is sometimes constrained by solubility.

The same analysis was repeated below with data from a 10^6-yr simulation. Releases normalized by the initial inventory are identical for radionuclides of high solubility.

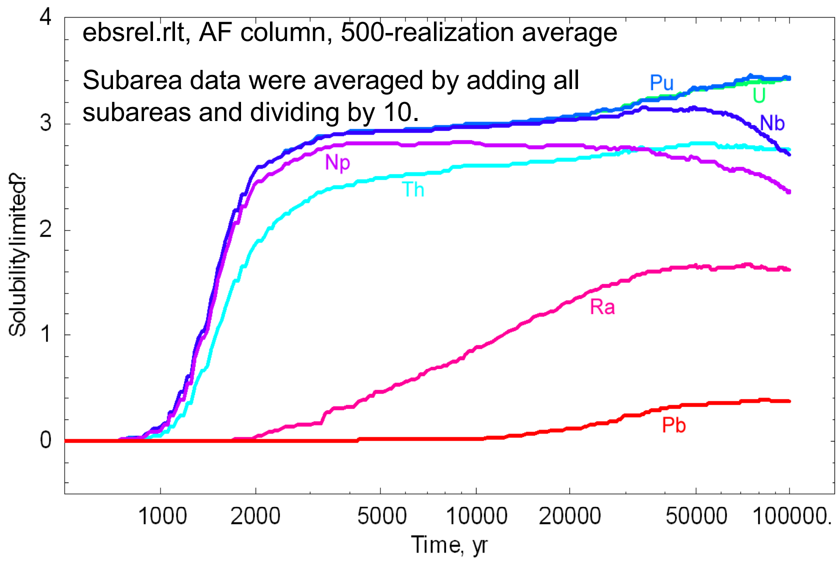
Therefore, the expected behavior is noted.

Mass balance test (Attachment A, test 3): **PASS**





Low solubility = {U238 , U233 , Th229 , U234 , Th230 , Pu239 , Nb94 , Np237 , Ra226 , Pb210 }



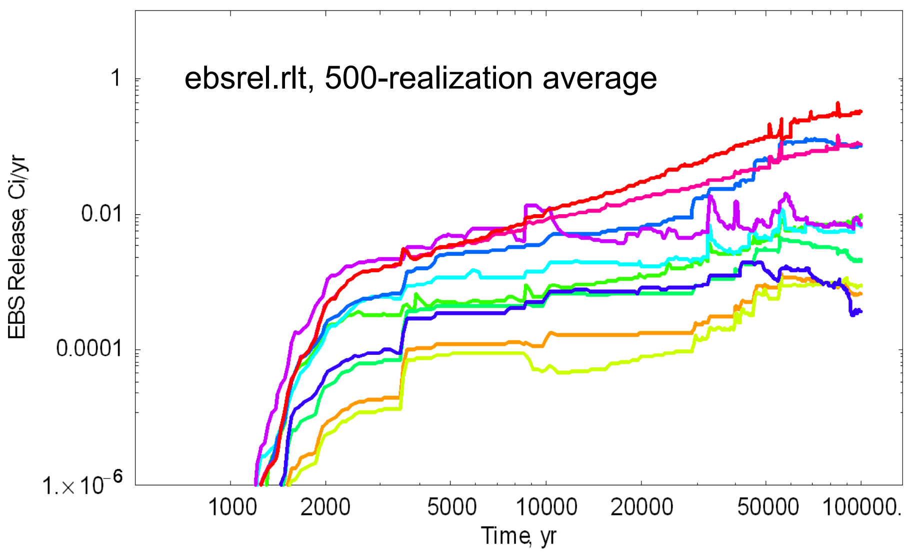
U attains the solubility limit most of the time and for most of the realizations. The upper value of the U-line can be interpreted as the average number of subareas with failed waste packages.

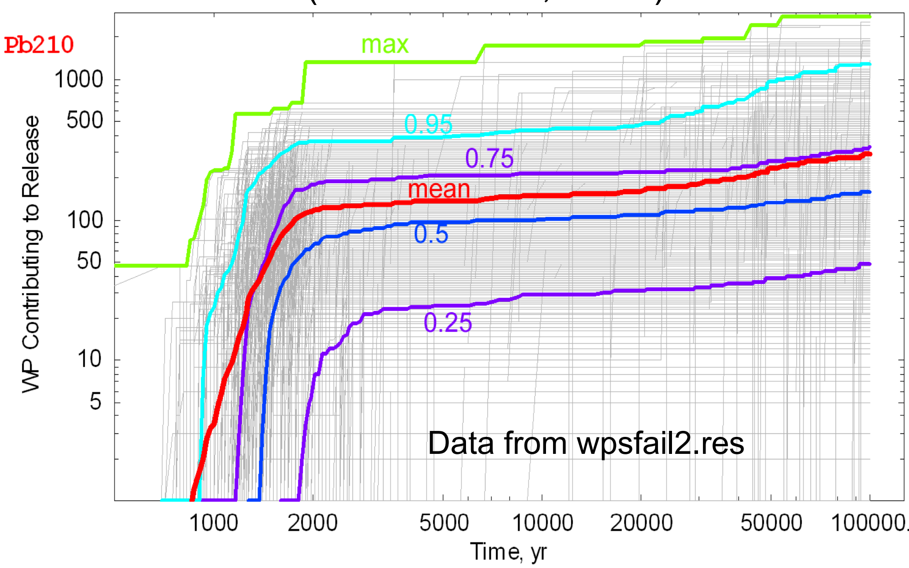
Isotopes of an element coincide on a single line. This is further indication that the solubility model was well implemented (isotopes of an element must attain solubility constraints at the same time).

In the plots below it is shown that the increasing trend in the releases tends to follow the waste package failure count.

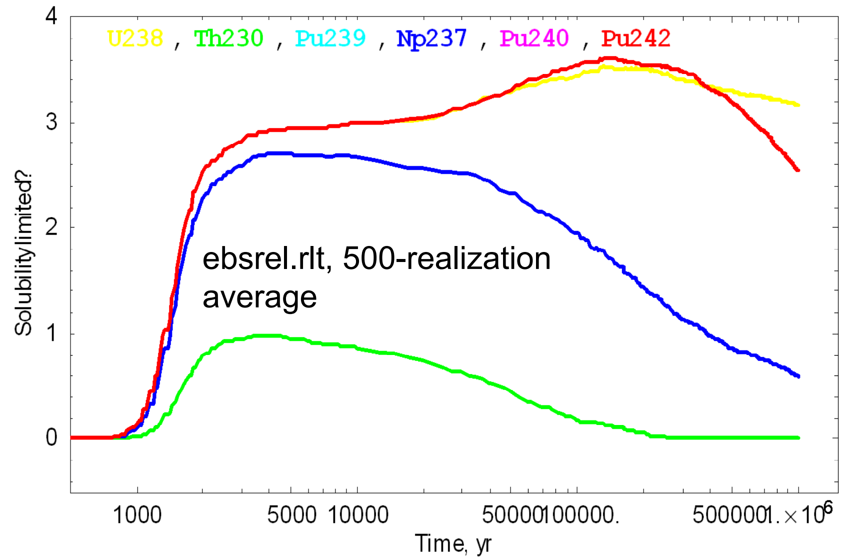
Mass balance test (Attachment A, test 3): **PASS**

U238 , U233 , Th229 , U234 , Th230 , Pu239 , Nb94 , Np237 , Ra226 , Pb210

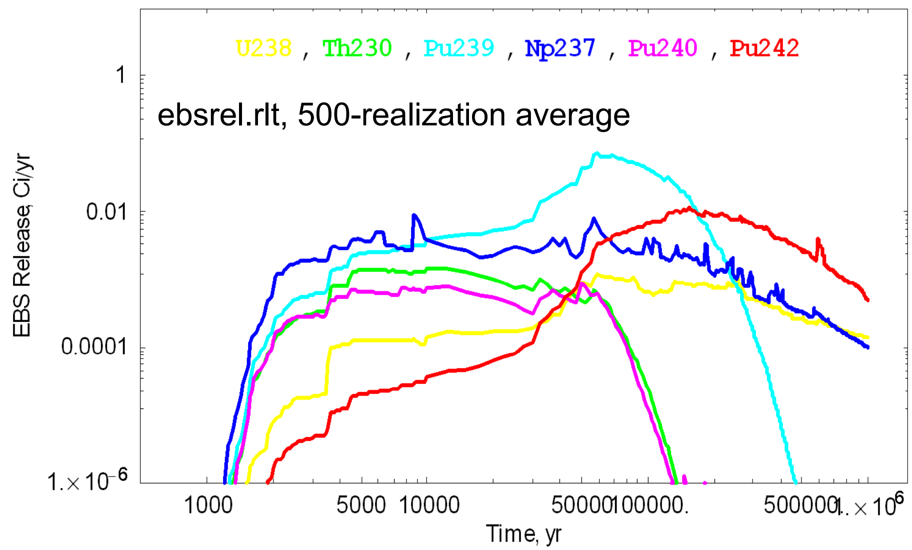




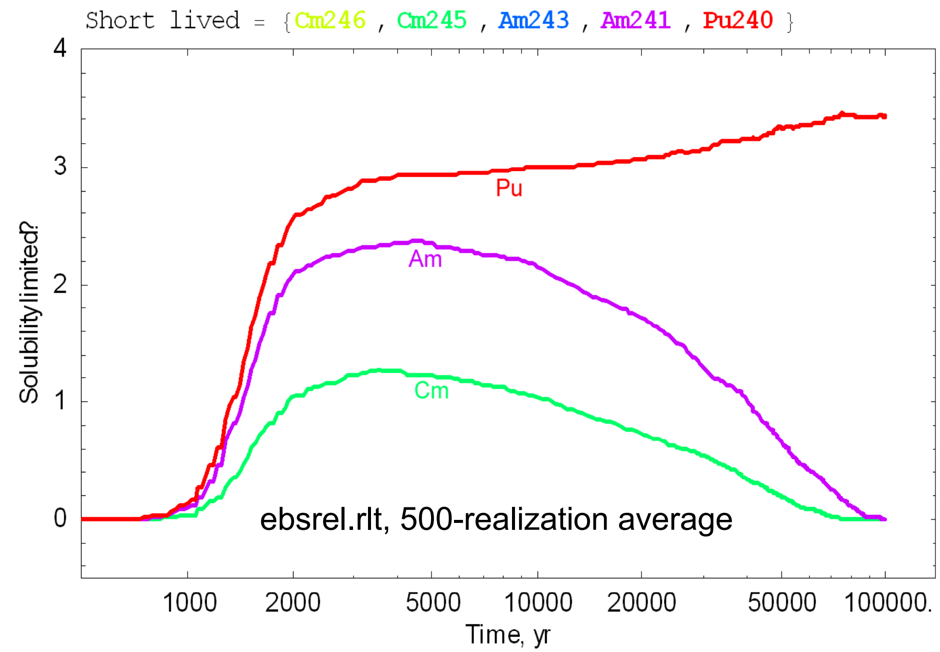
1-million year results

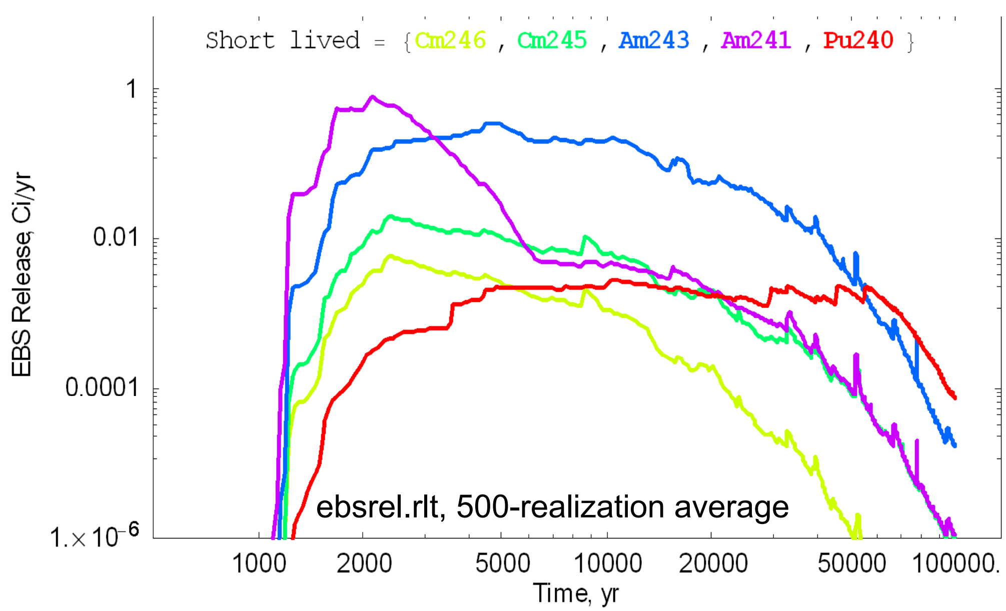


U and Pu are released at the solubility limit, most of the time. Isotopes of an element coincide on a single line.



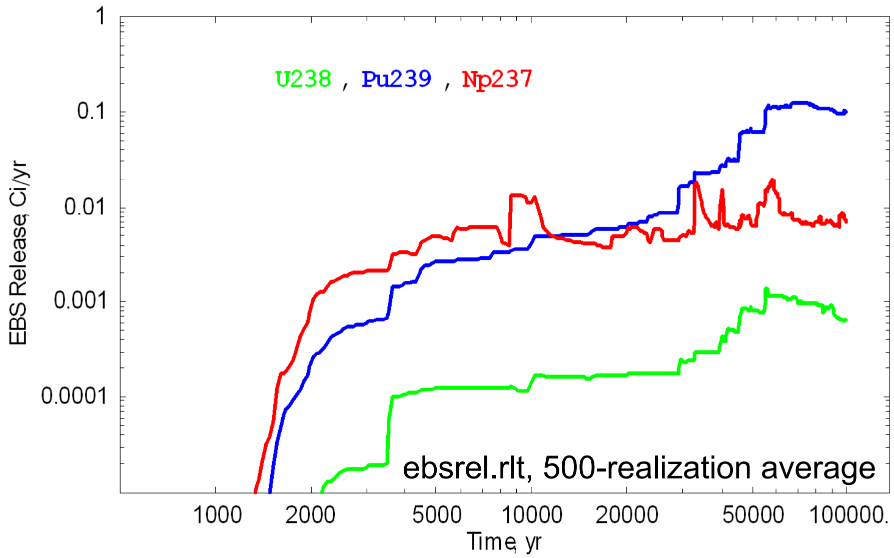
^{242}Pu is not considered in 10^4 year computations, but only in 10^6 year computations

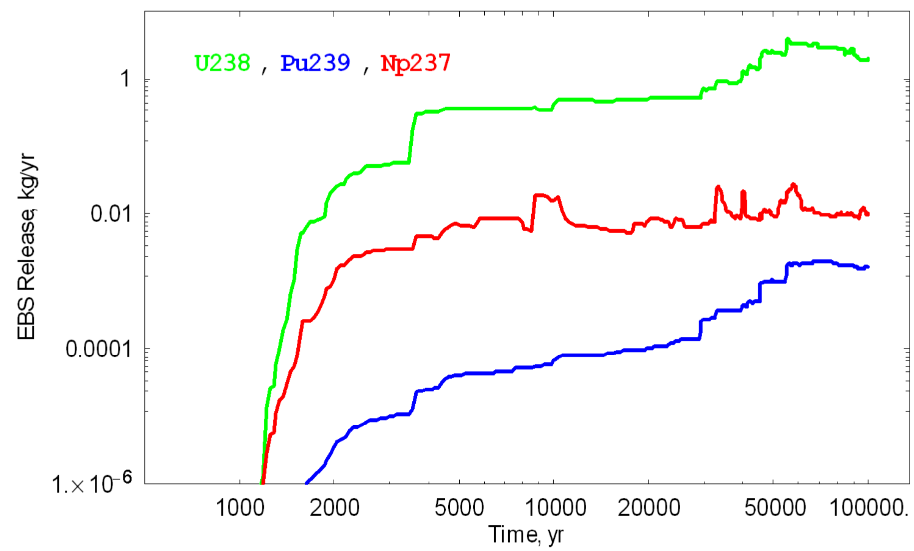


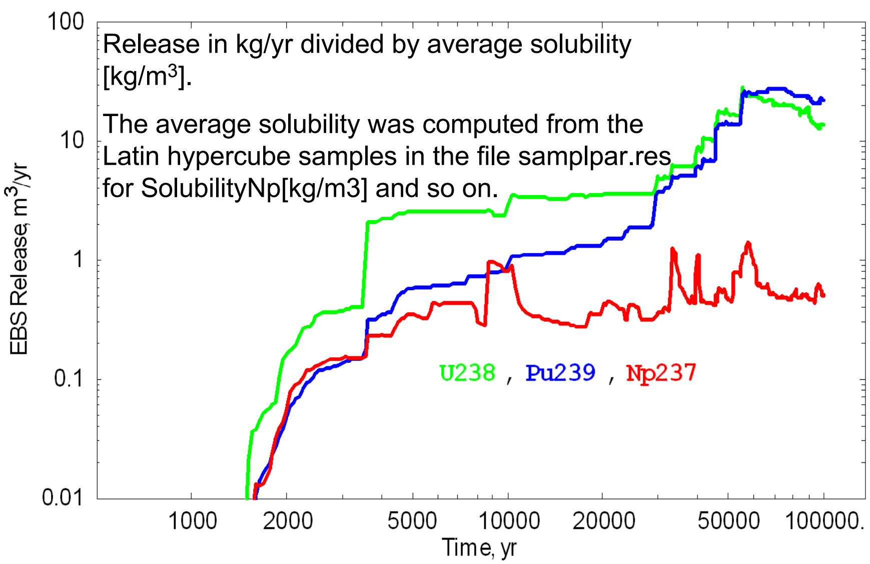


Short-lived radionuclides

Radionuclides with dominant isotopic mass and solubility controlled: ^{237}Np, ^{238}U, ^{239}Pu



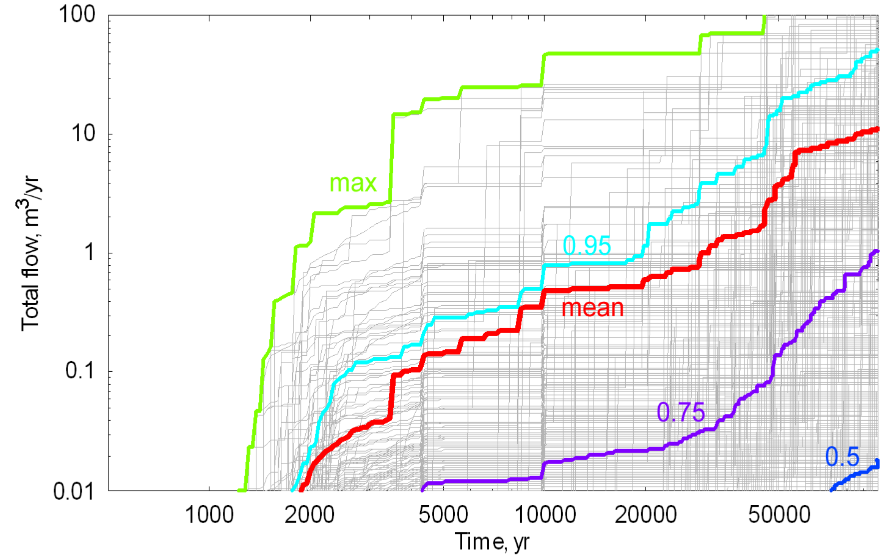


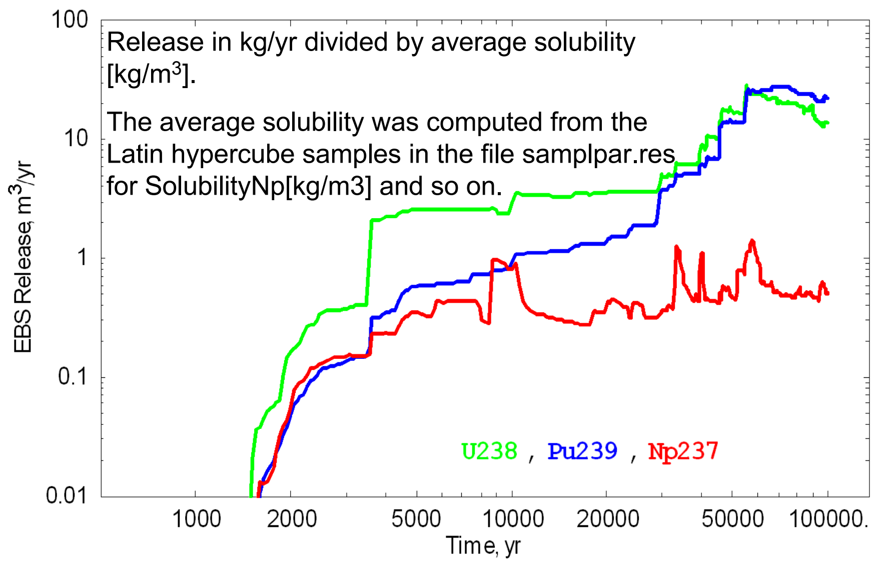


Normalized releases by the solubility produce comparable results. It is expected for the lines not to overlap because (i) isotopes of U and Pu with shared solubility, (ii) Np is of higher solubility than U and Pu, (iii) decay chain effects, and (iv) colloidal effects. Therefore, this test is only qualitative; aimed at identifying consistent trends and order of magnitude consistent with average flow rates.

Mass balance test (Attachment A, test 3): **PASS**

Average flow per breached WP, 10th column in infilper.cum





Flow rates in this plot were derived by multiplying the average flow rate per waste package (10th column in infilper.cum) by the total number of waste packages contributing to release (data from wpsfail2.res) for each realization. The red line is the mean from 500 realizations.

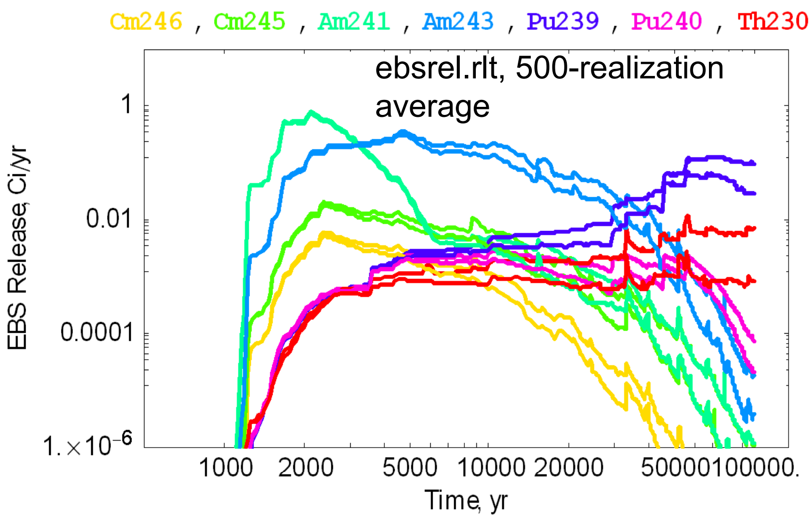
It is noted that ^{238}U and ^{239}Pu releases (plot below) are consistent with the total flow on the left. Therefore, release rates for radionuclides limited by solubility are consistent with total flow rates inside breached waste packages.

Therefore, the TPA code shows trends in EBS release rates consistent with expectations.

Mass balance test (Attachment A, test 3): **PASS**

Colloidal Radionuclides

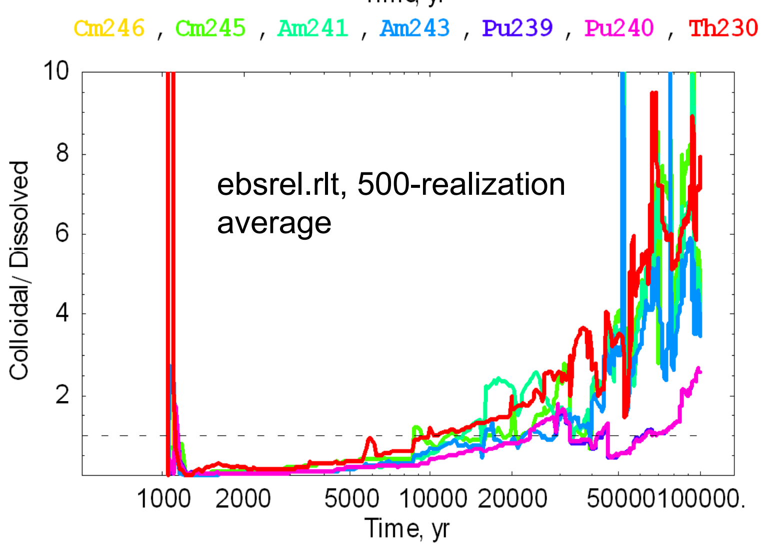
Test aimed at quantifying the relative contribution of colloids to total releases from the EBS



Upper lines: J-species added to dissolved radionuclides

500-realization average, TPA 5.1 beta W.

Data from ebsrel.rlt

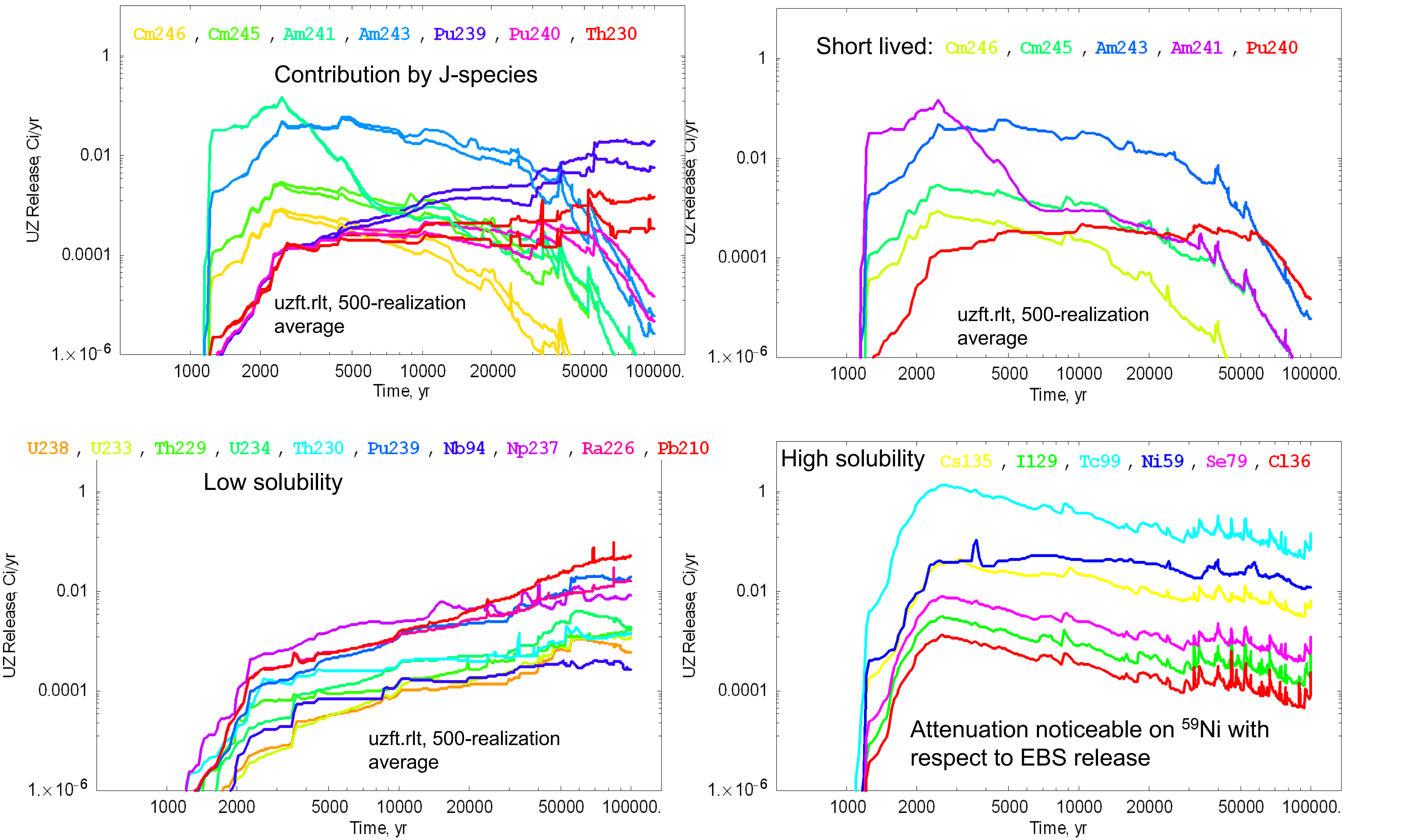


Ratio of colloidal to dissolved. Release in dissolved form is dominant up to 20,000 years, and then colloidal releases tend to dominate. However, note in the above plot that ^{245}Cm, ^{246}Cm, ^{241}Am, and ^{243}Am show significant decay after 20,000 years. For ^{239}Pu and ^{240}Pu, releases in colloidal form are always comparable to dissolved form releases after 20,000 years.

Colloidal release test (Attachment A, test 2)

UZ Releases

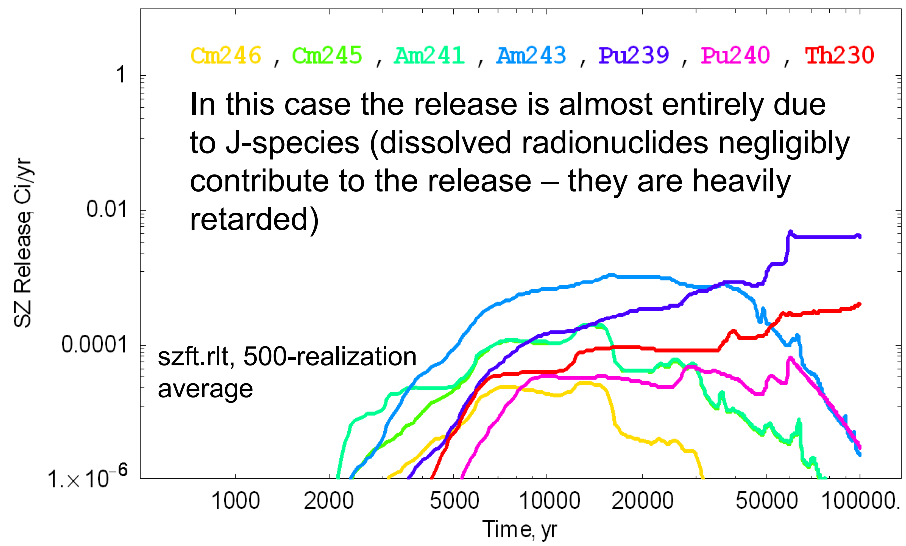
- UZ releases similarly grouped as EBS releases for this test
- UZ offers some attenuation/retardation effect
- UZ releases reported in the file uzft.rlt
- Identification of relevant radionuclides (Attachment A, test 1)
- Effect of colloids on releases and dose test (Attachment A, test 2)

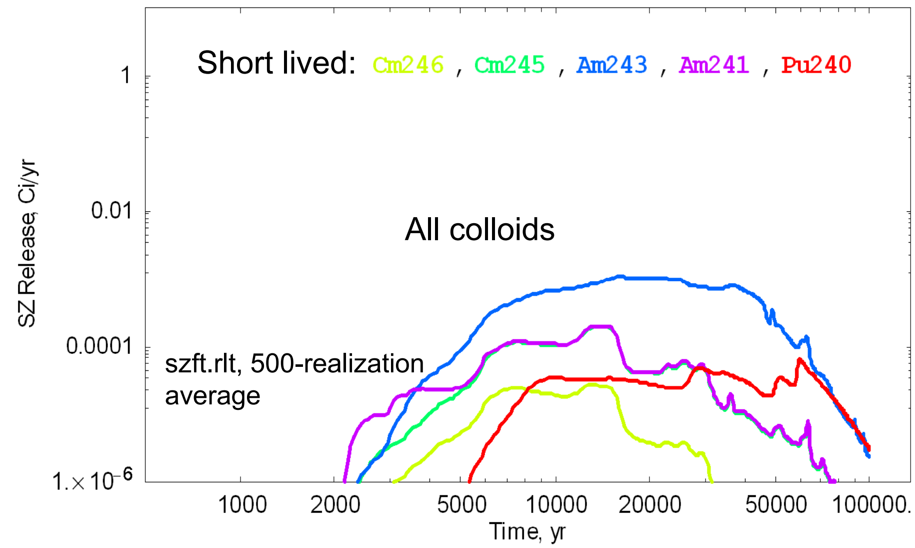

Cm246 , Cm245 , Am241 , Am243 , Pu239 , Pu240 , Th230
Contribution by J-species
uzft.rlt, 500-realization average
UZ Release, Ci/yr
Time, yr
Short lived: Cm246 , Cm245 , Am243 , Am241 , Pu240
uzft.rlt, 500-realization average
U238 , U233 , Th229 , U234 , Th230 , Pu239 , Nb94 , Np237 , Ra226 , Pb210
Low solubility
uzft.rlt, 500-realization average
High solubility Cs135 , I129 , Tc99 , Ni59 , Se79 , Cl36
Attenuation noticeable on 59Ni with respect to EBS release

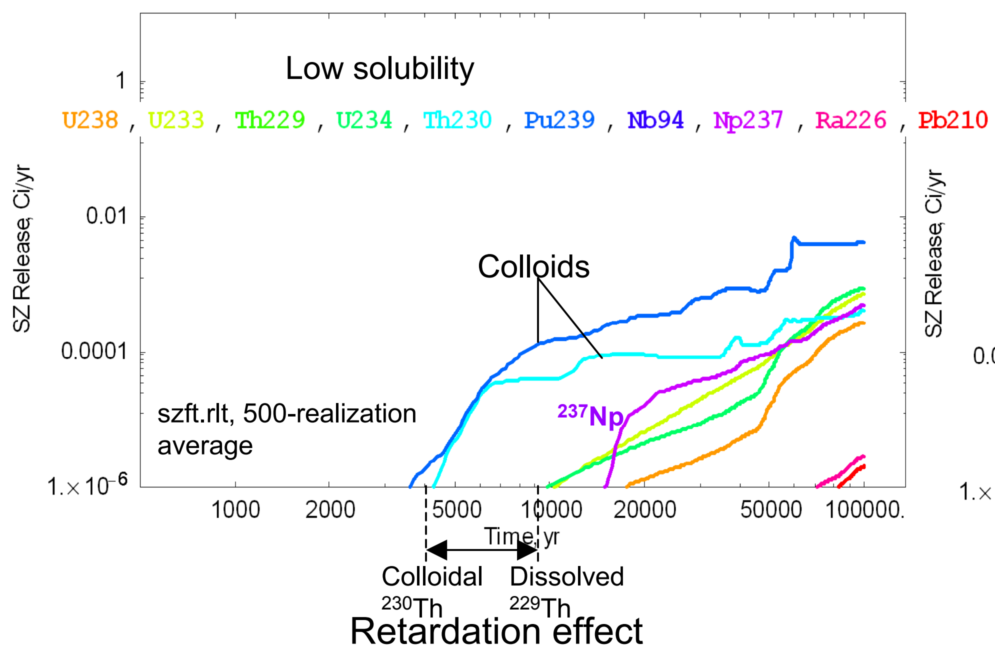
S2 B-14

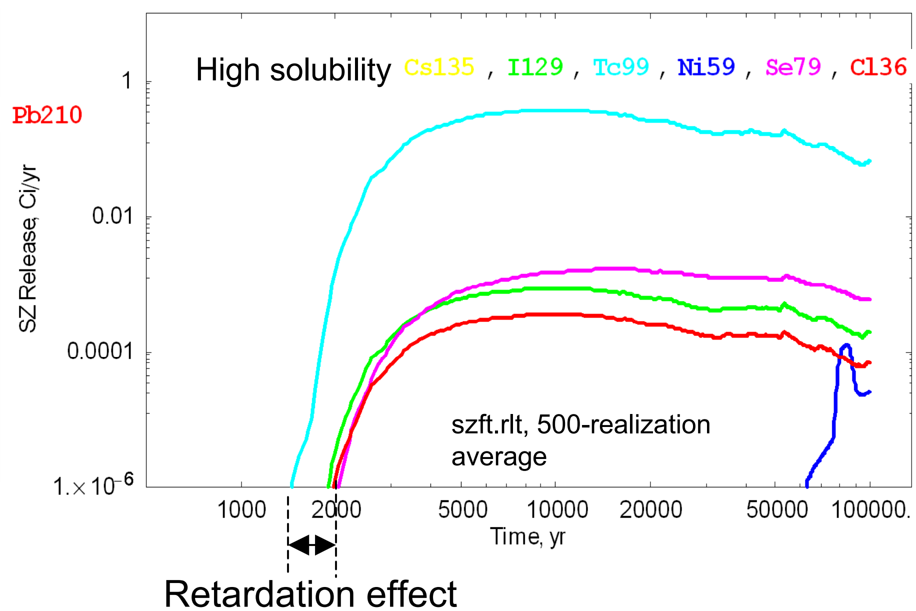
SZ Releases

- SZ releases similarly grouped as EBS releases for this test.
- SZ offers significant attenuation/retardation.
- Dissolved actinides are heavily retarded so that radionuclide release is dominated by colloids.
- The only dissolved actinides with significant release after transport through the SZ is ^{237}Np and U isotopes. All other actinides with significant releases are colloids.
- The fission products are less affected by retardation than the actinides. In particular ^{99}Tc travels fast through the SZ.
- SZ releases are reported in the file szft.rlt.
- Identification of relevant radionuclides (Attachment A, test 1)
- Effect of colloids on releases and dose test (Attachment A, test 2)

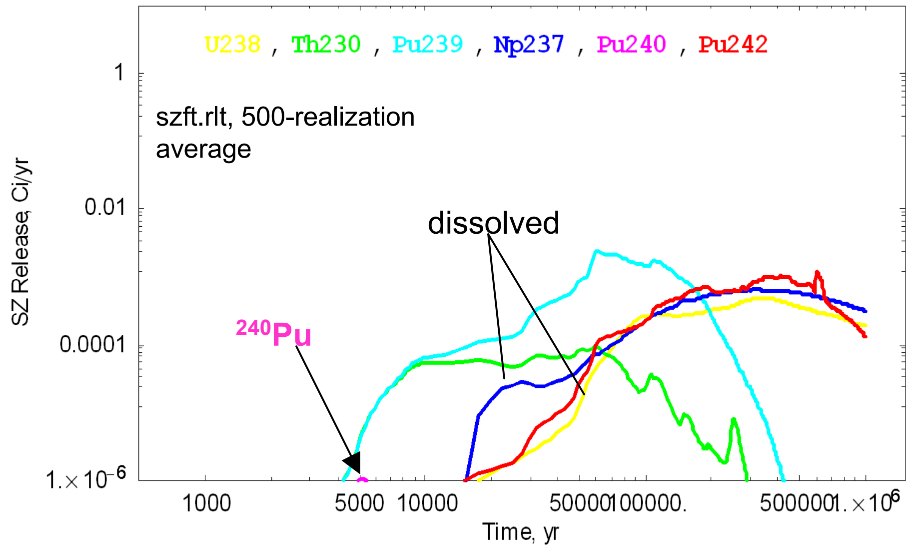

Cm246 , Cm245 , Am241 , Am243 , Pu239 , Pu240 , Th230
In this case the release is almost entirely due to J-species (dissolved radionuclides negligibly contribute to the release – they are heavily retarded)
szft.rlt, 500-realization average
SZ Release, Ci/yr
1
0.01
0.0001
1.×10^-6
1000
2000
5000
10000
20000
50000
100000.
Time, yr

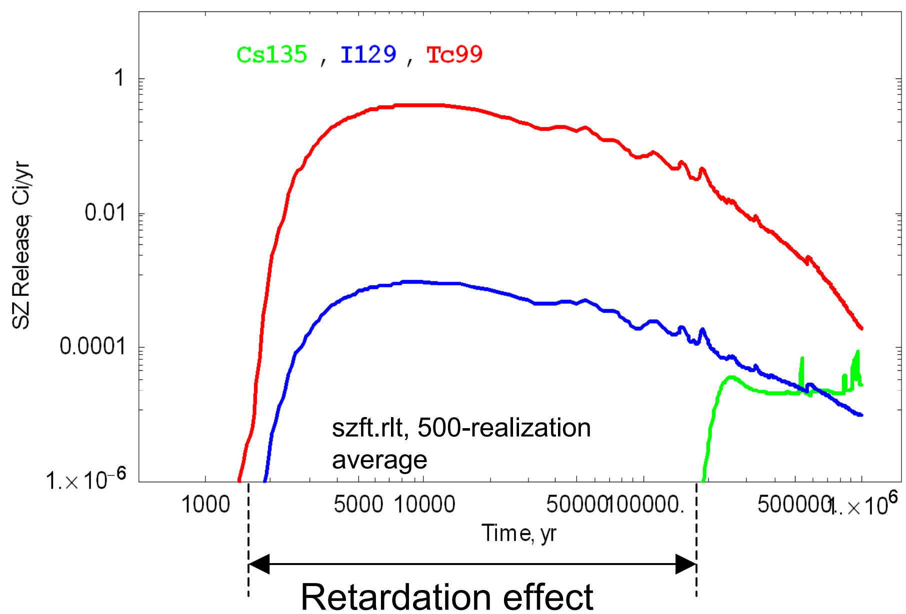

Short lived: Cm246 , Cm245 , Am243 , Am241 , Pu240
All colloids
szft.rlt, 500-realization average
SZ Release, Ci/yr
1
0.01
0.0001
1.×10^-6
1000
2000
5000
10000
20000
50000
100000.
Time, yr


Low solubility
U238 , U233 , Th229 , U234 , Th230 , Pu239 , Nb94 , Np237 , Ra226 , Pb210
Colloids
237Np
szft.rlt, 500-realization average
SZ Release, Ci/yr
1
0.01
0.0001
1.×10^-6
1000
2000
5000
10000
20000
50000
100000.
Time, yr
Colloidal 230Th
Dissolved 229Th
Retardation effect


High solubility Cs135 , I129 , Tc99 , Ni59 , Se79 , Cl36
szft.rlt, 500-realization average
SZ Release, Ci/yr
1
0.01
0.0001
1.×10^-6
1000
2000
5000
10000
20000
50000
100000.
Time, yr
Retardation effect

S2 B-16



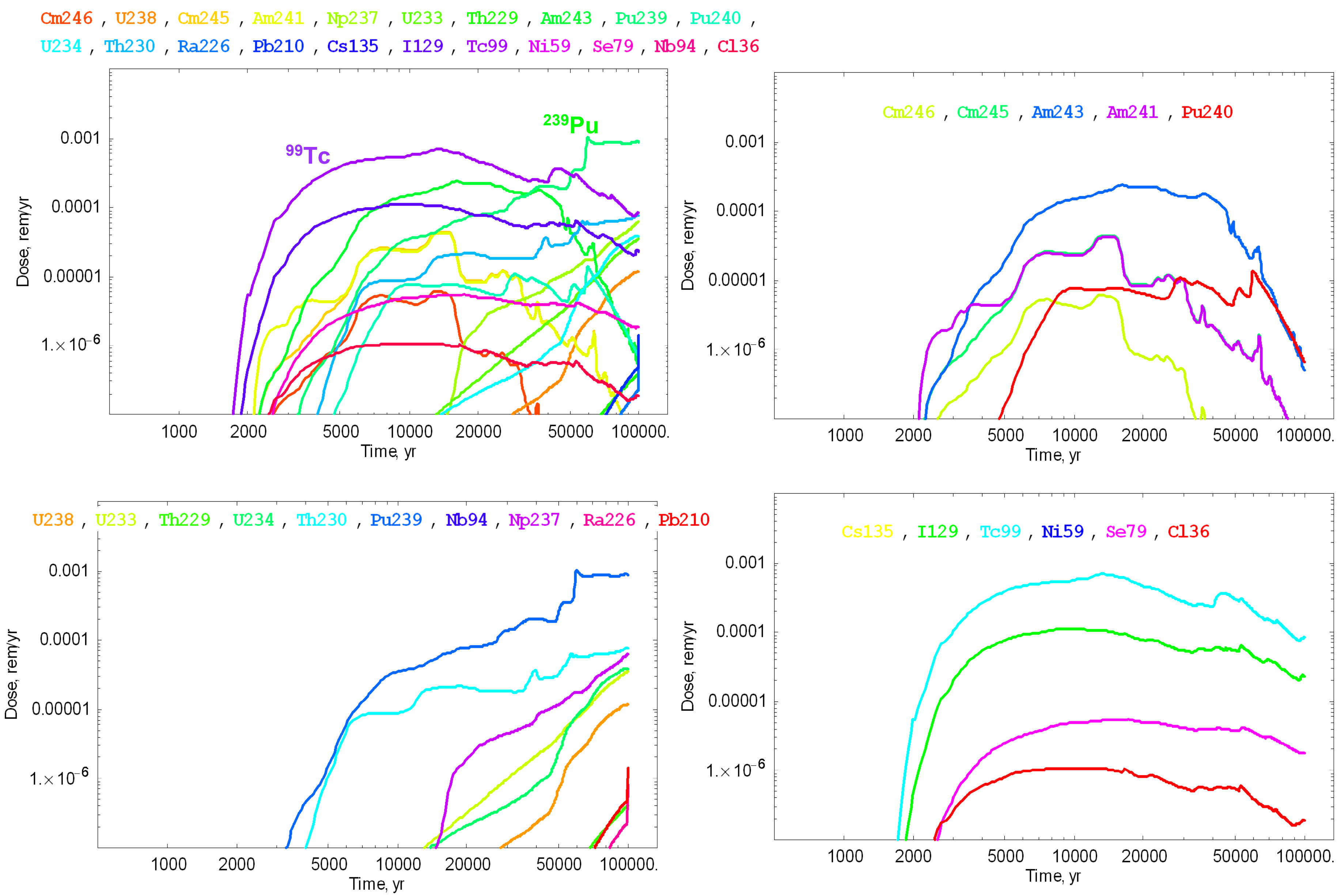


Releases of ^{230}Th, ^{239}Pu, ^{240}Pu, and ^{242}Pu come entirely from colloids. ^{237}Np and ^{238}U are dissolved.

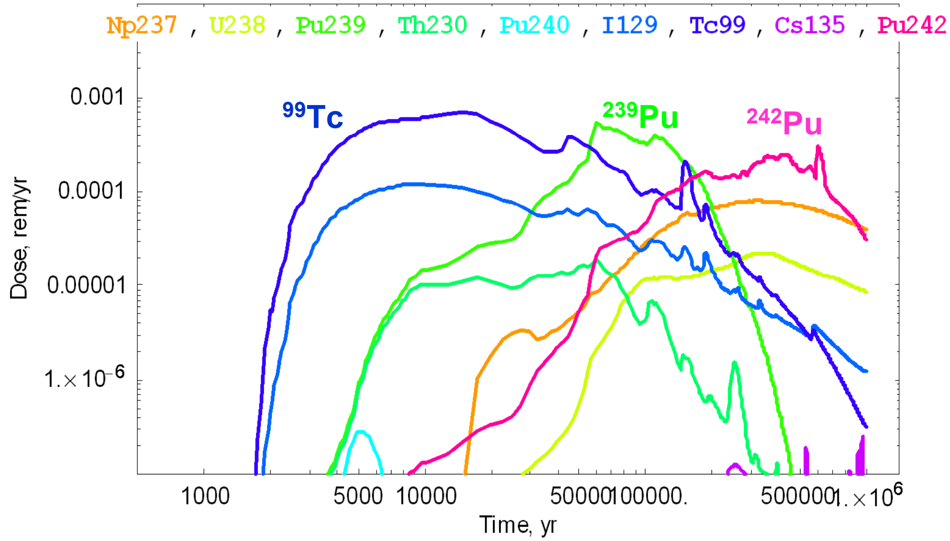
Retardation causes major attenuation of release of dissolved actinides. Only ^{237}Np "survives" the SZ retardation.

Doses

- Doses similarly grouped as EBS releases for this test.
- Doses per radionuclide are consistent with SZ releases.
- Identification of relevant radionuclides (Attachment A, test 1)
- Effect of colloids on releases and dose test (Attachment A, test 2)

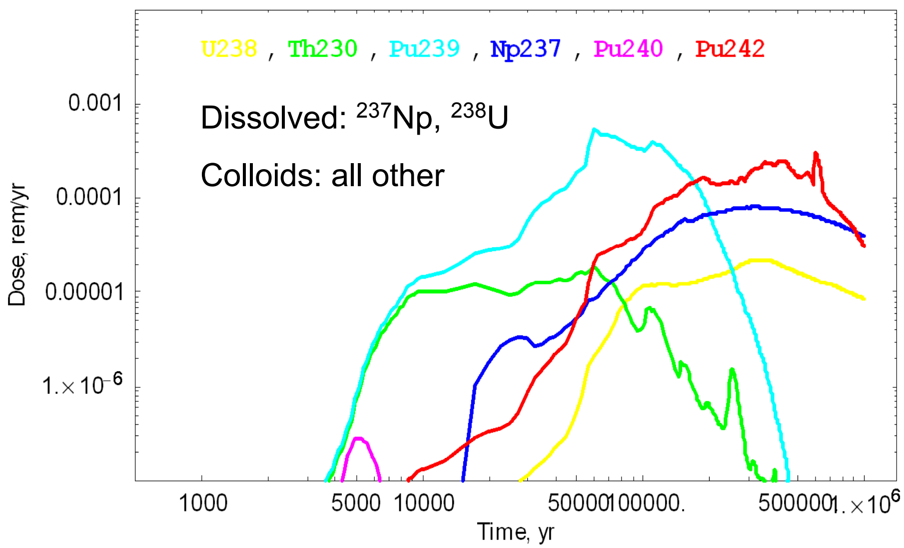


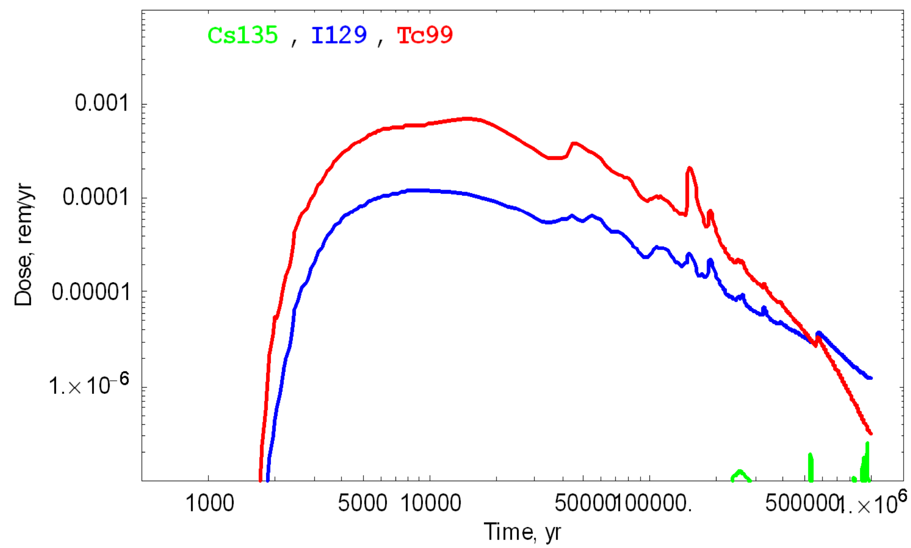
Data from rgwna.tpa, average from 500 realizations. Doses are consistent with the SZ release data.



Doses of ^{230}Th, ^{239}Pu, ^{240}Pu, and ^{242}Pu come entirely from colloids.

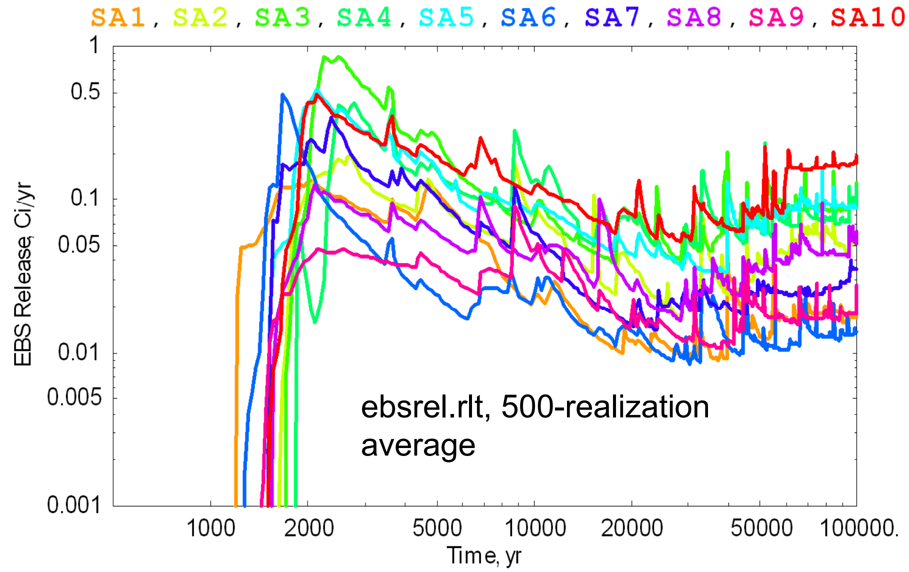
Data from rgwna.tpa, average from 500 realizations



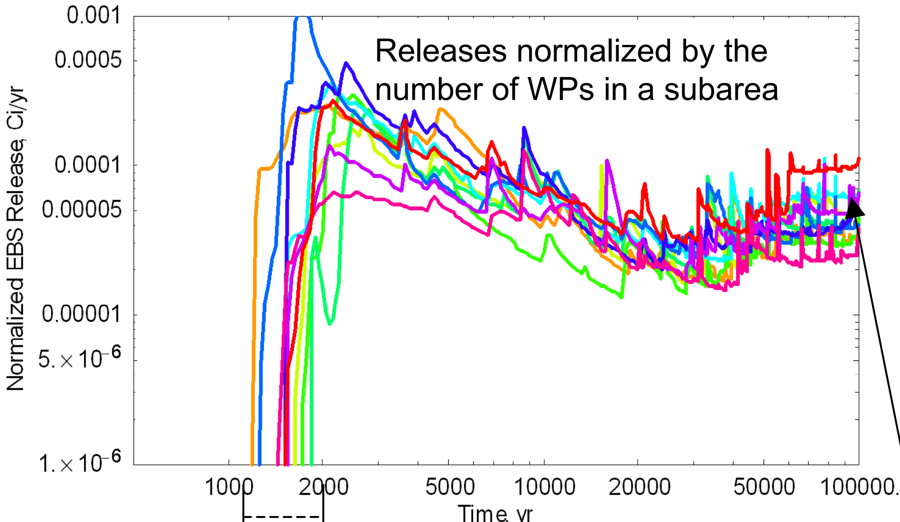


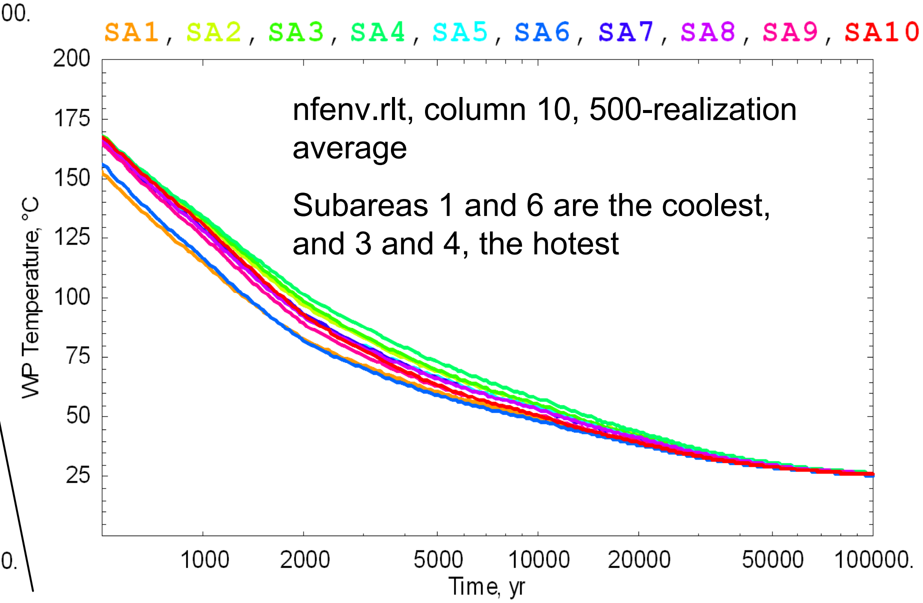
Subarea Analysis

- Compare EBS, UZ, and SZ releases per subarea, normalized by the number of waste packages in a subarea
- Trends, similitude, and differences should be explainable as function of subarea features
- Subarea release test (Attachment A, test 4)



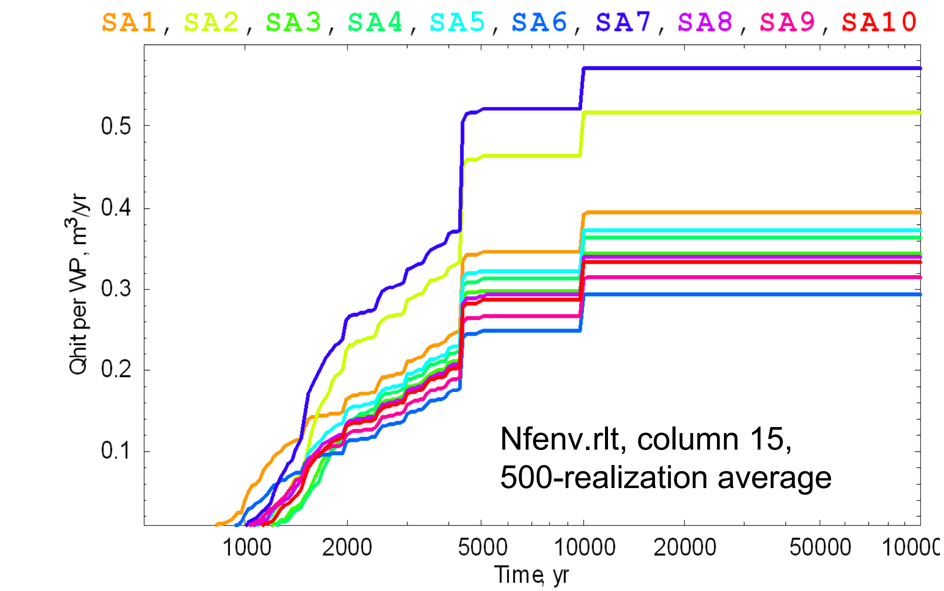
No WPs	Subarea
2904.	SA3
1793.	SA4
1747.	SA10
1452.	SA5
1062.	SA2
931.	SA8
723.	SA9
696.	SA7
526.	SA1
343.	SA6

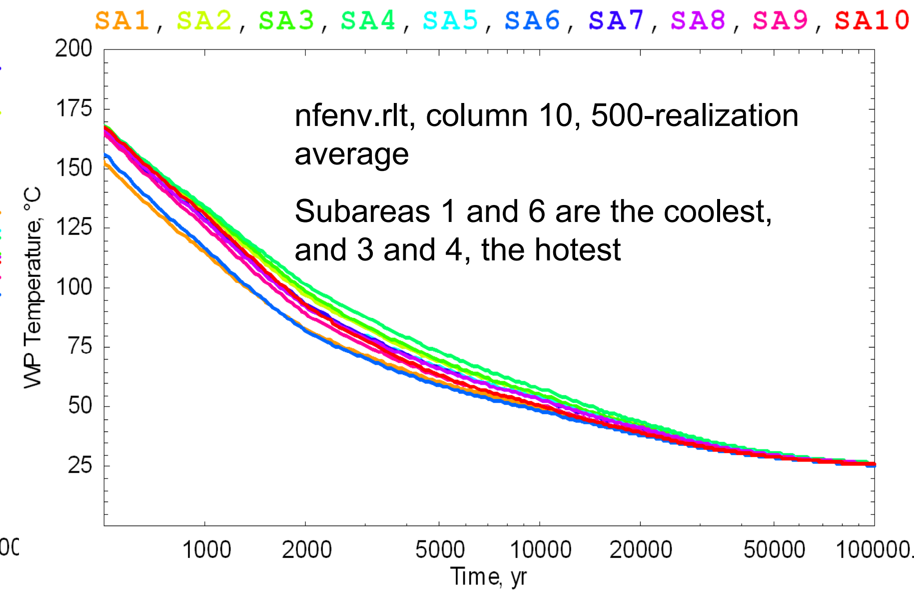


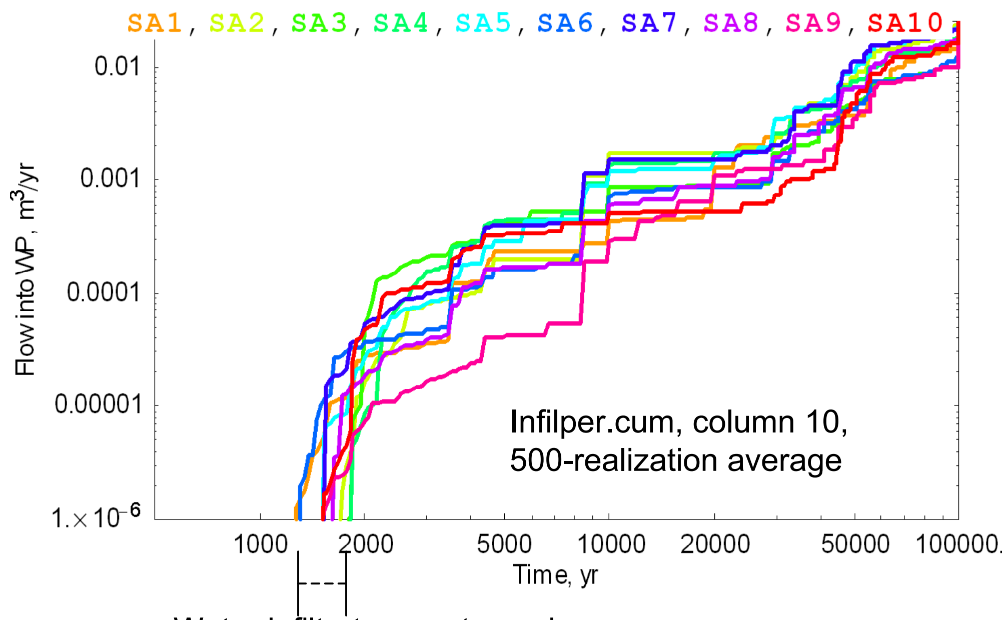


Cooler subareas start releasing at earlier times

No clear trend noted in the magnitude of normalized releases

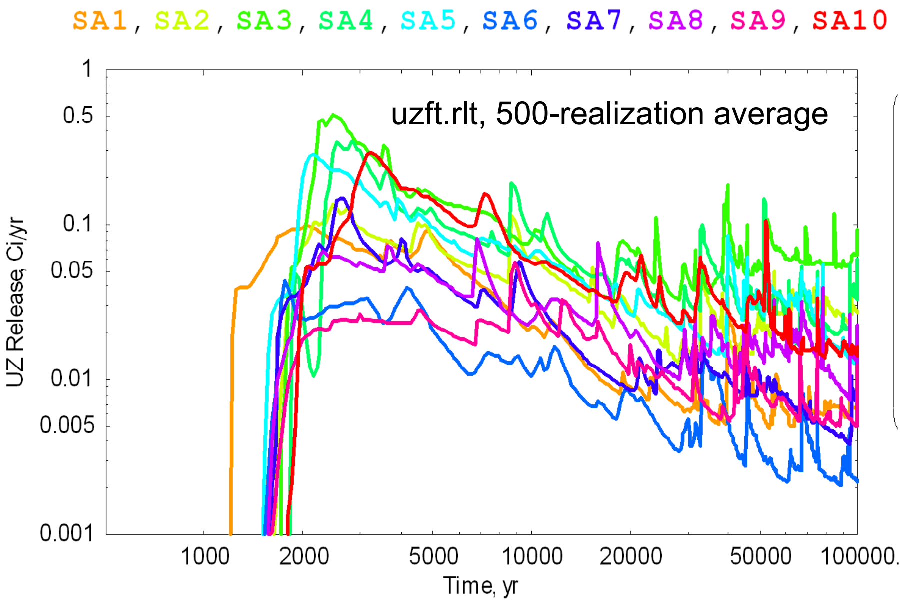




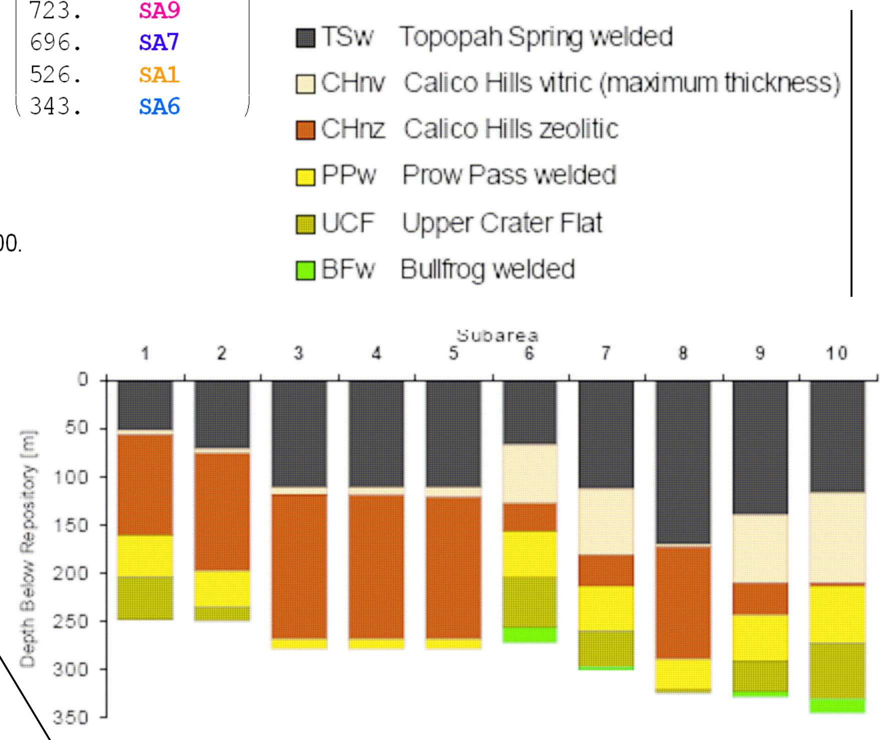


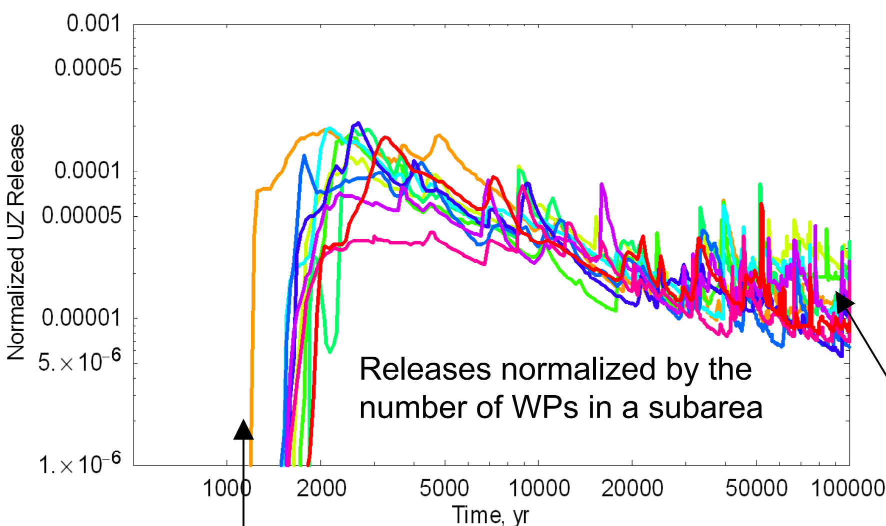
Water infiltrates waste packages sooner in cooler subareas

The difference between wetter and drier subareas (top left plot) is not significant to induce appreciable difference in EBS releases.



No WPs	Subarea
2904.	SA3
1793.	SA4
1747.	SA10
1452.	SA5
1062.	SA2
931.	SA8
723.	SA9
696.	SA7
526.	SA1
343.	SA6

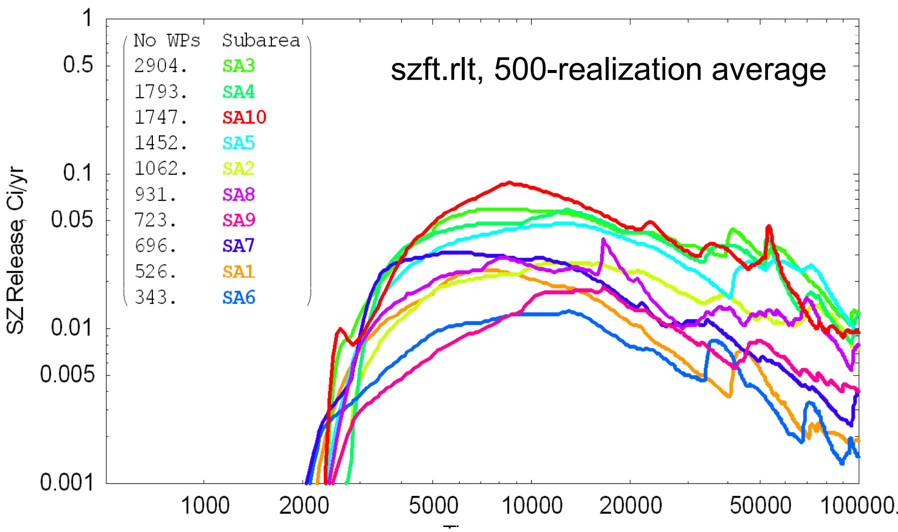


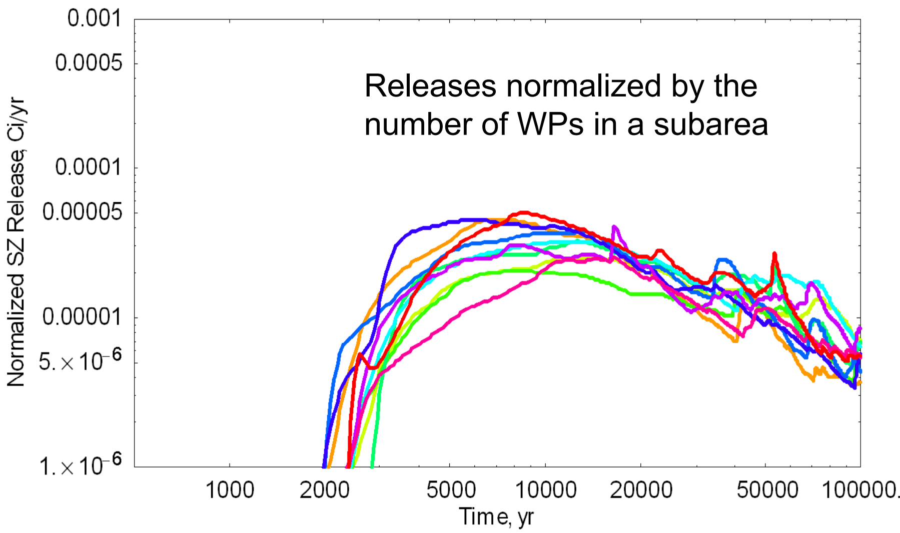


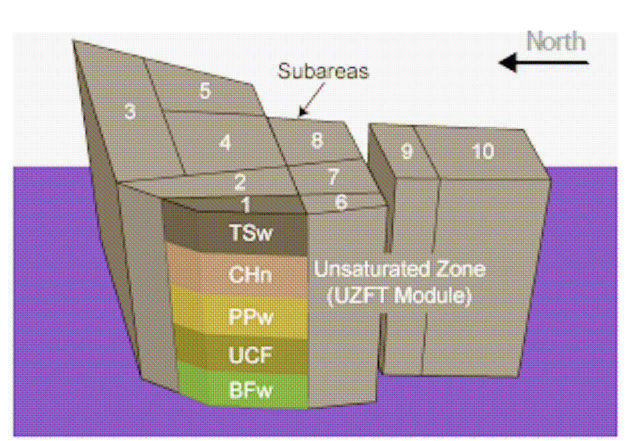
Subarea 3 shows the earliest release because: (i) earliest EBS release and (ii) low retardation in the UZ due to short CHnv thickness

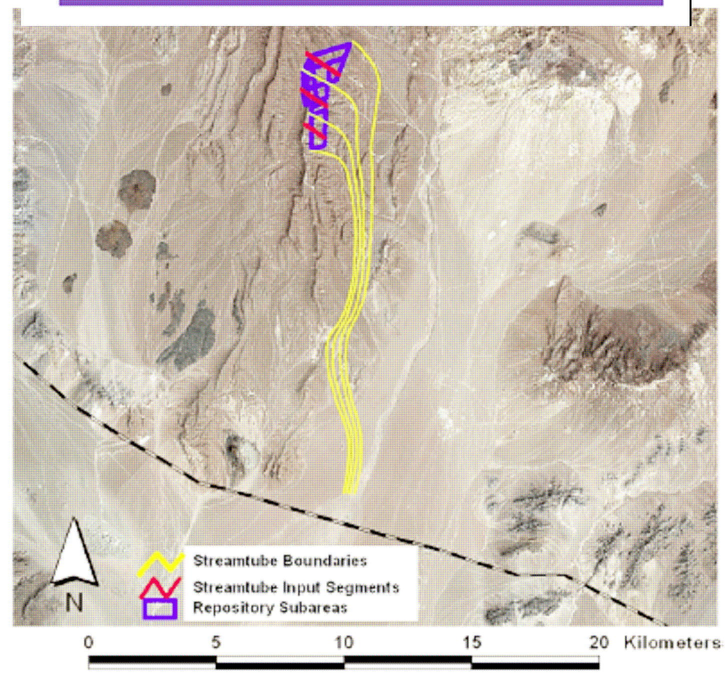
No clear trend noted in the magnitude of normalized releases

SA1, SA2, SA3, SA4, SA5, SA6, SA7, SA8, SA9, SA10







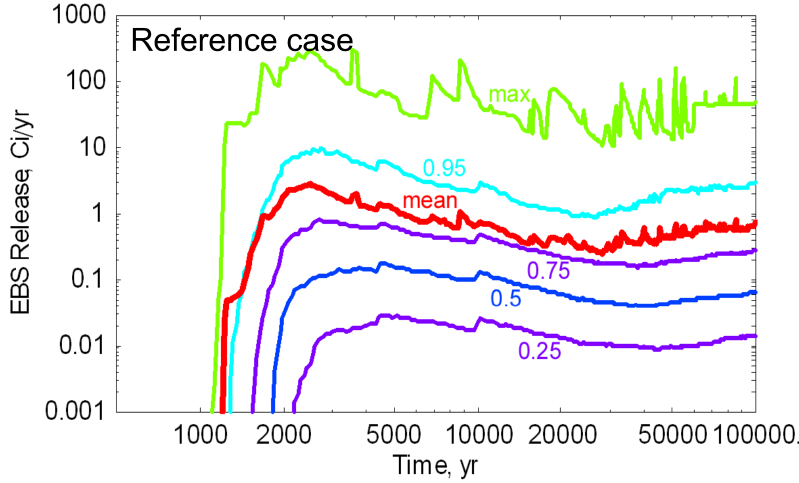


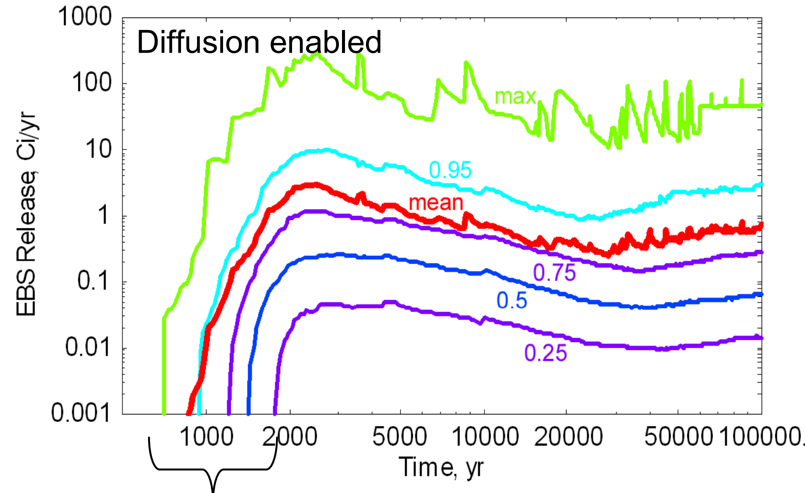
No clear trend noted in the normalized releases. It appears all subareas are equivalent. Thus, it is sufficient to run one-subarea only and scale results to estimate repository releases and doses.

Diffusive Releases

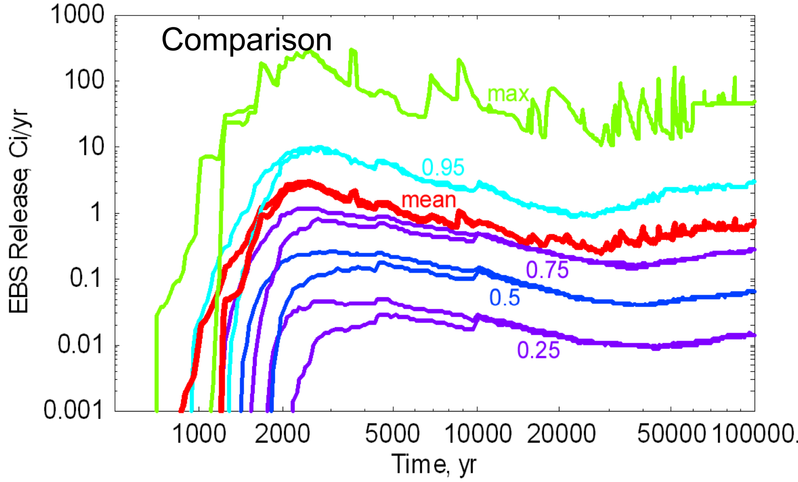
- In the reference case, diffusive releases (as defined in the TPA equations) are disregarded
- Test are needed to compare the magnitude of the TPA diffusive releases
- A 500-realization run was executed, with the following changes to enable diffusive releases:
  - WeldCrackLength[m] = 0.0
  - InternalFilmCrossSectionalArea[m^2] = 4.0e-4
  - FractionOfWPsWithDiffusionTilt[] = 0.5
- It is recognized that
  - parameters associated with dimensions of the diffusive pathway (cross sections and lengths) are highly uncertain
  - the diffusive model is only “exploratory” to do first approximation testing of the effect of diffusive releases
- Diffusive release test (Attachment A, test 5)

EBS Releases



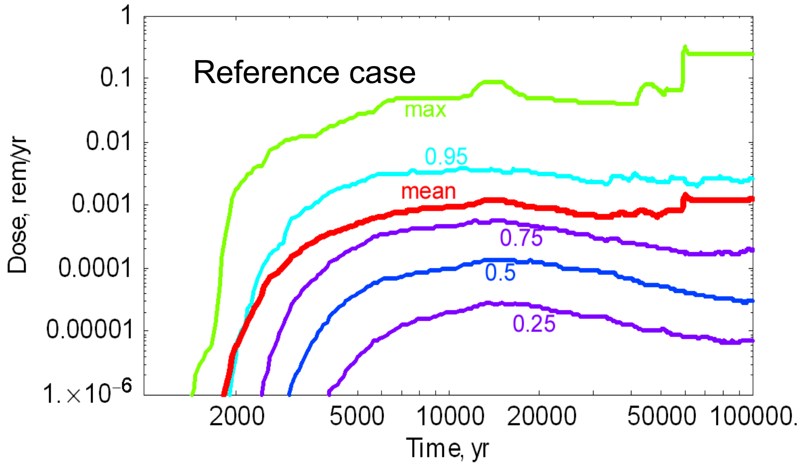


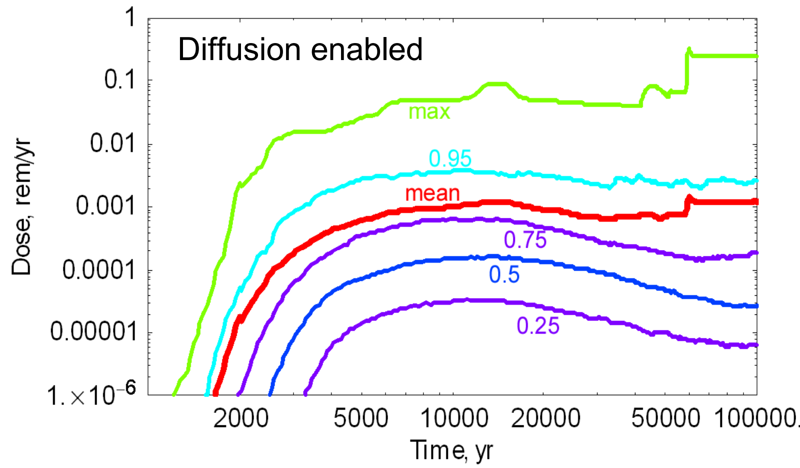
Diffusive releases tend to occur earlier than advective releases. Advective releases occur only until the temperature drops below FlowOnsetTemperature[C]

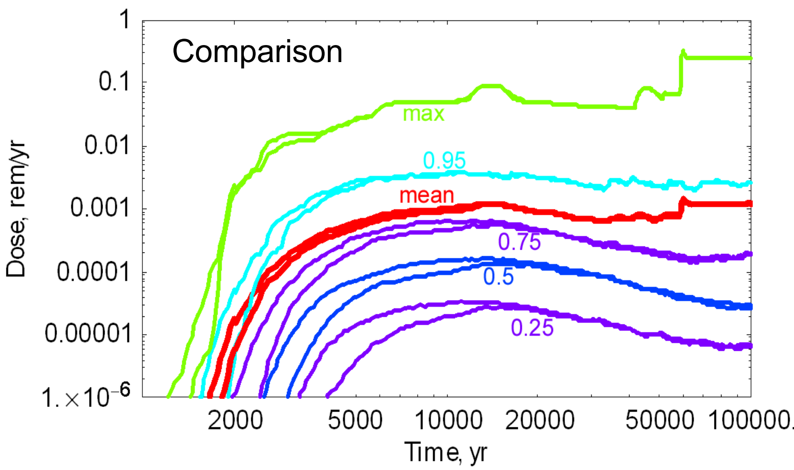


- Enabling diffusion increases the total releases from the EBS
- The average release of the diffusion enabled case is practically identical to the reference case after 2,000 years
- It can be concluded that the increase due to diffusive releases is not significant

Total Dose







- Enabling diffusion marginally increases the total mean dose
- The mean dose is practically unaffected after 3,000 yr
- Diffusive releases from the EBS are not significant compared to advective releases
- It is acknowledged that there is uncertainty in the parameters and model for EBS diffusive release

Conclusions

- EBS, UZ, and SZ releases are mutually consistent
- Doses are consistent with SZ releases
- Cooler subareas tend to release earlier
- No clear trend was noted in the magnitude of releases normalized by the number of waste packages in a subarea (all subareas "behave" similarly)
- Colloids are important for dose assessments
- Release rates from the EBS are consistent with mass balance expectations
  - Releases from high solubility radionuclides are controlled by the waste form lifetime
  - Releases from low solubility radionuclides are controlled by water flow rates
- Using the exploratory model for diffusive release from the EBS, it is concluded that diffusion marginally increases the total mean dose

SOFTWARE VALIDATION REPORT (SVR)

SVR#:	Project#: 06002.01.354	
Software Name: TPA		Versions: 5.1betaT, 5.1betaU, and 5.1betaW
Test ID: S-3	Test Series Name: Radionuclide Dose Contributions	

Test Method

- ☐ code inspection
- ☒ output inspection
- ☐ hand calculation
- ☒ spreadsheet
- ☒ graphical
- ☐ comparison with external code results

Test Objective: This task seeks to understand which radionuclides dominate dose rates to the RMEI during various time periods of interest and which processes affect dose rates.

Test Environment Setup

Hardware (platform, peripherals): Desktop PCs

Software (OS, Lahey F95 compiler, libraries, auxiliary codes or scripts): Microsoft Windows XP, R2.4.1 Language Environment, DPLOT, EXCEL

Input Data (files, data base, mode settings): See Attachment A.

Assumptions, constraints, and/or scope of test: See Attachment A.

Test Procedure: This validation task report is divided into three Subtasks. Subtask 1 evaluates the radionuclide dose contributions for the nominal case, including seismic events; Subtask 2 evaluates the same for the Faulting scenario; and Subtask 3 evaluates the dose contributions for igneous disruptive scenarios. See Attachment A for description of test procedures.

Test Results

Location: See Attached CD labeled “TPA Version 5.1 Validation Task S-3"

Test Criteria and Analysis of Results: see Attachment A.

Test Evaluation (Pass/Fail): Pass

Notes:

Tester: *Christopher Grossman (nominal)* *Tina Ghosh (faulting)* *Richard Codell (igneous)*	Date: 05/23/2007

Attachment A
TPA Version 5.1 Validation Task S-3
Description of Test Activities

Subtask 1. Identify relevant radionuclides to nominal-seismic scenario dose estimates

1.A. Test Procedures

1.A.1. Execute 500-realization simulations using the reference case input for the nominal-seismic scenario, *tpa.inp*, with append flags on for 10,000-, 100,000-, and 1,000,000-year simulation periods.

1.A.2. Calculate and plot the total dose statistics (minimum, 5th-, 25th-, 50th-, 75th-, 95th-percentiles, mean, and maximum) from the output file, *totdose.res*, for the three simulation periods. To calculate the statistics use the script, totdose.exe, provided by O. Pensado.

1.A.3. Plot the average dose per radionuclide from the output file, *rgwna.tpa*, for the three simulation periods.

1.A.4. Plot the percent of peak groundwater dose contribution of radionuclides from the output file, *rgwnr.tpa*, for the three simulation periods.

1.A.5. Plot the saturated zone releases of the most contributing radionuclides to the mean dose, from the output file, *szft.rlt*, for the three simulation periods.

1.B. Test Criteria

1.B.1. Are mean dose curves similar for the three simulation periods of the nominal scenario with seismic disruption? Differences should be rationalized.

1.B.2. Are the dominant radionuclide contributors similar for the three simulation periods? Differences should be rationalized.

1.B.3. Are dominant radionuclide doses consistent with saturated zone releases? Differences should be rationalized.

1.C. Test Results

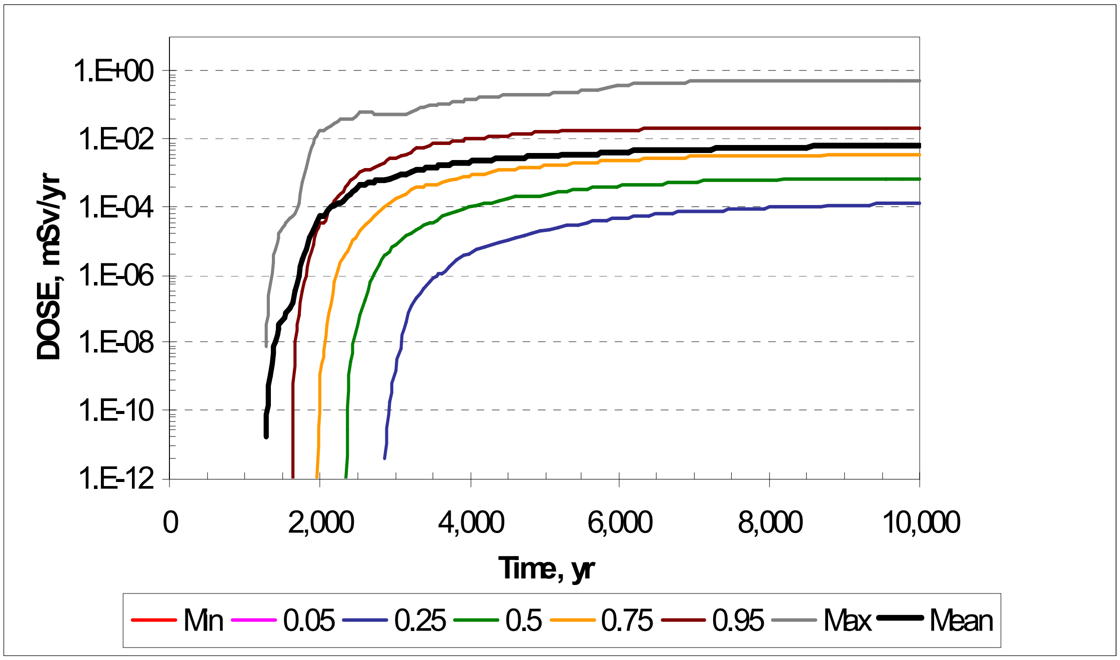


Figure 1-1. Total Dose Statistics for 10,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations. (1mSv/yr = 100mrem/yr)

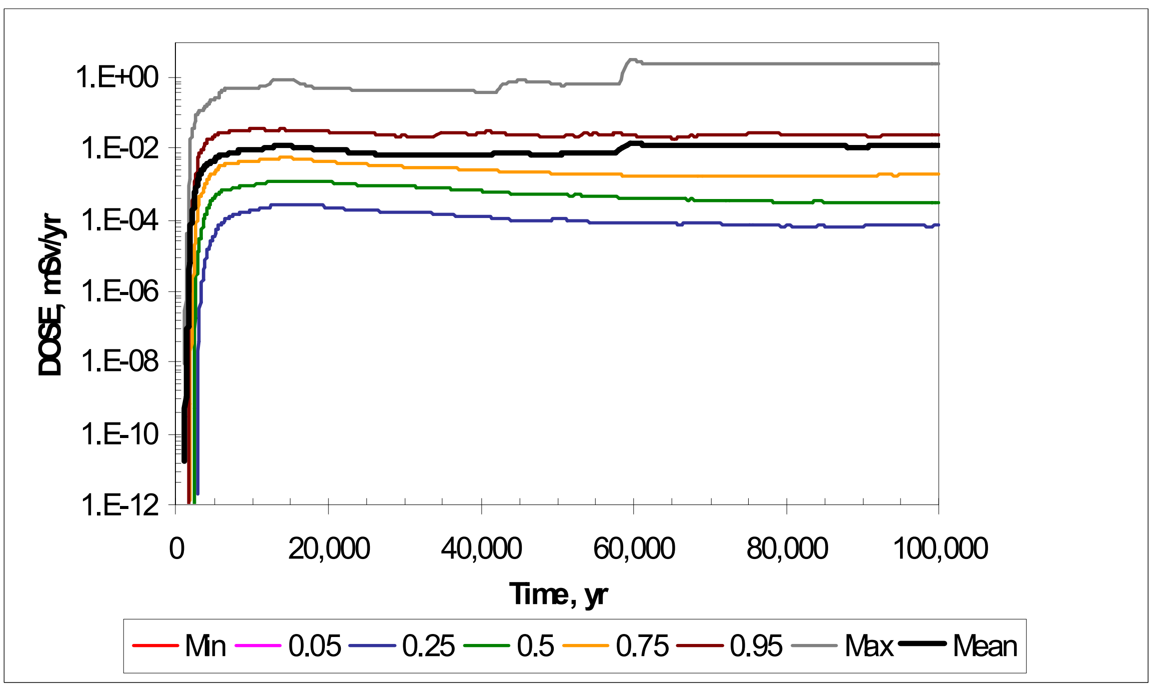


Figure 1-2. Total Dose Statistics for 100,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations. (1mSv/yr = 100mrem/yr)

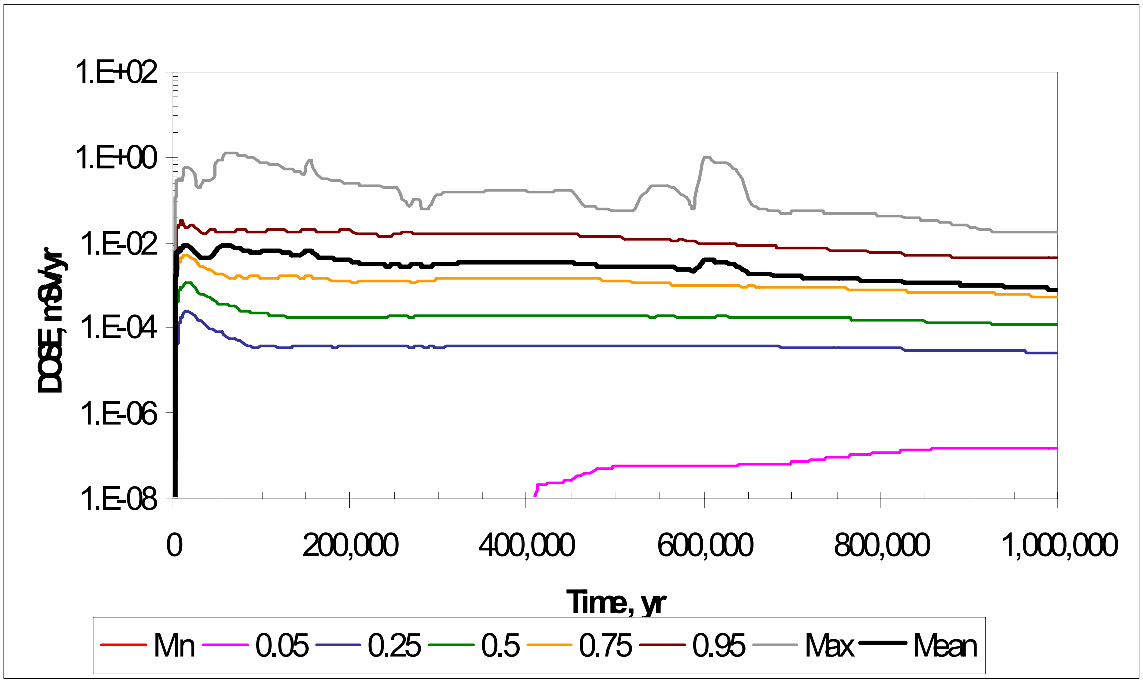


Figure 1-3. Total Dose Statistics for 1,000,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations. (1mSv/yr = 100mrem/yr)

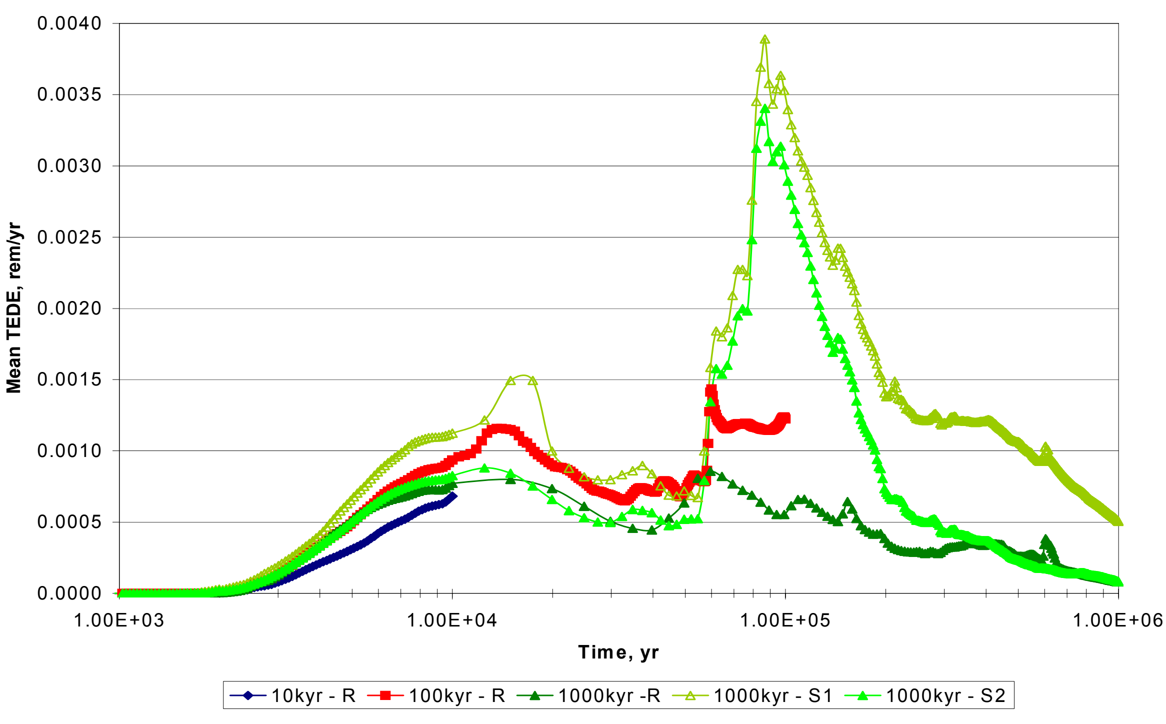


Figure 1-4. Comparison of Mean Total Dose for Three Simulation Periods of the Nominal Scenario with Seismic Disruption Reference Case and Supplemental Analyses using TPA 5.1 Beta W for 500 (350 for Supplemental Analyses) Realizations.

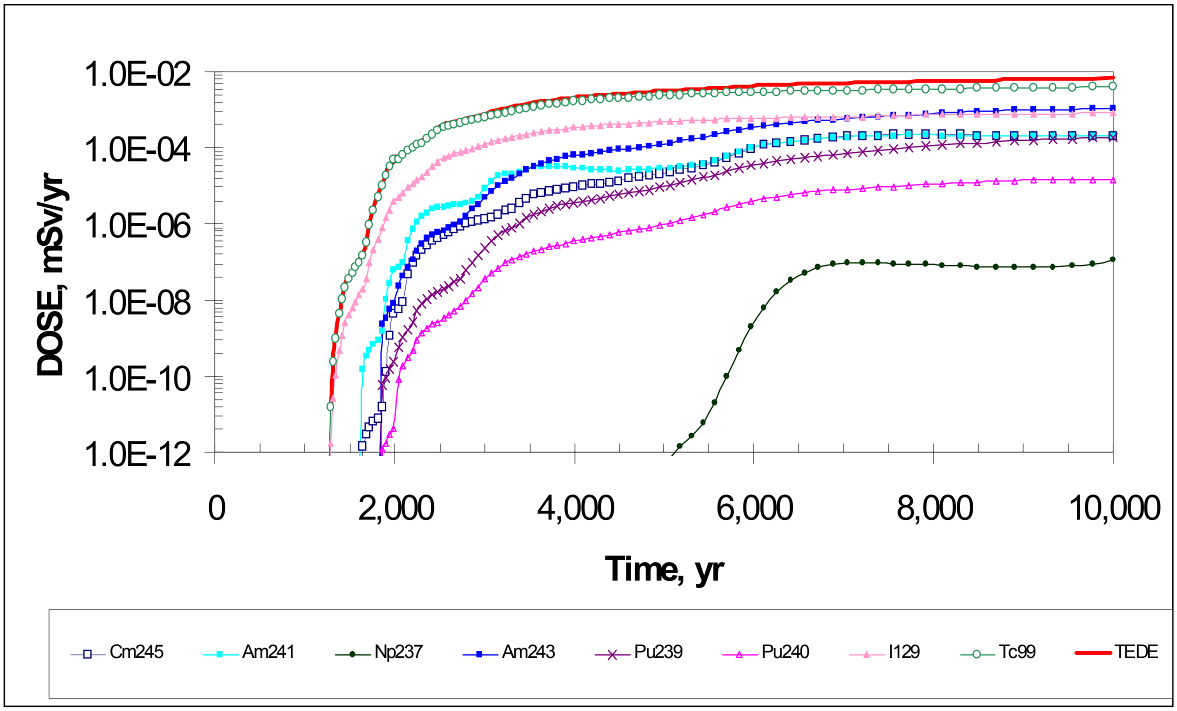


Figure 1-5. Average Radionuclide Dose for 10,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations. (1mSv/yr = 100mrem/yr)

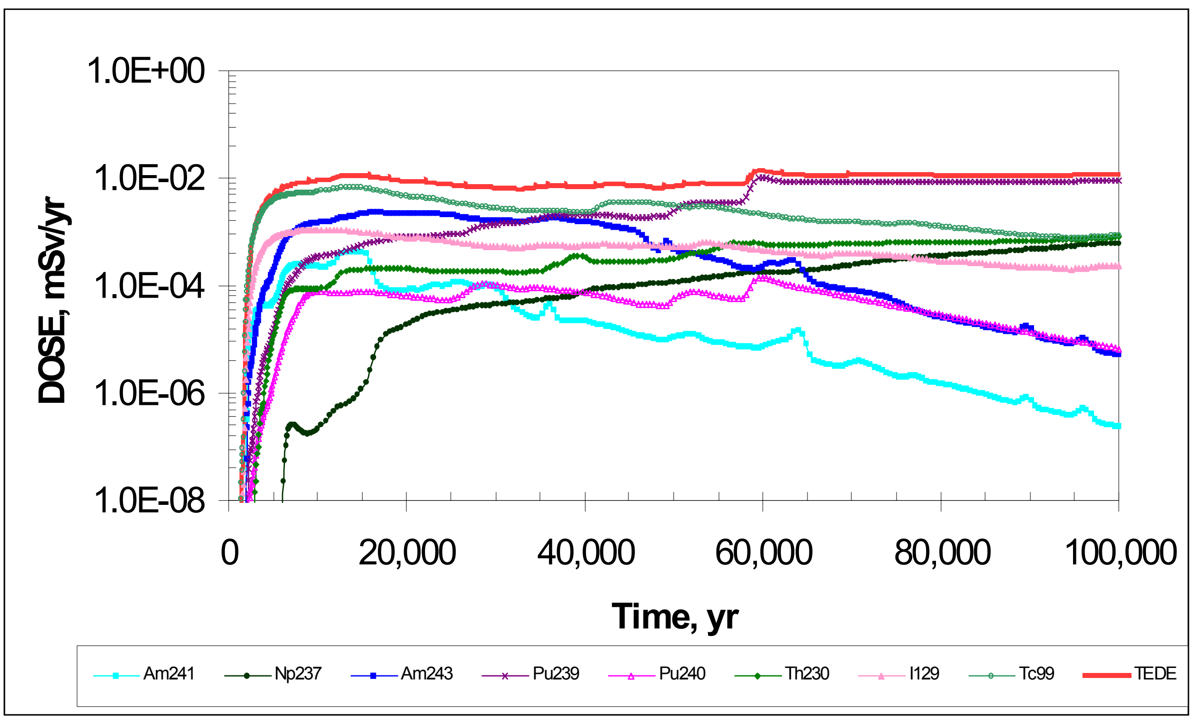


Figure 1-6. Average Radionuclide Dose for 100,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations. (1mSv/yr = 100mrem/yr)

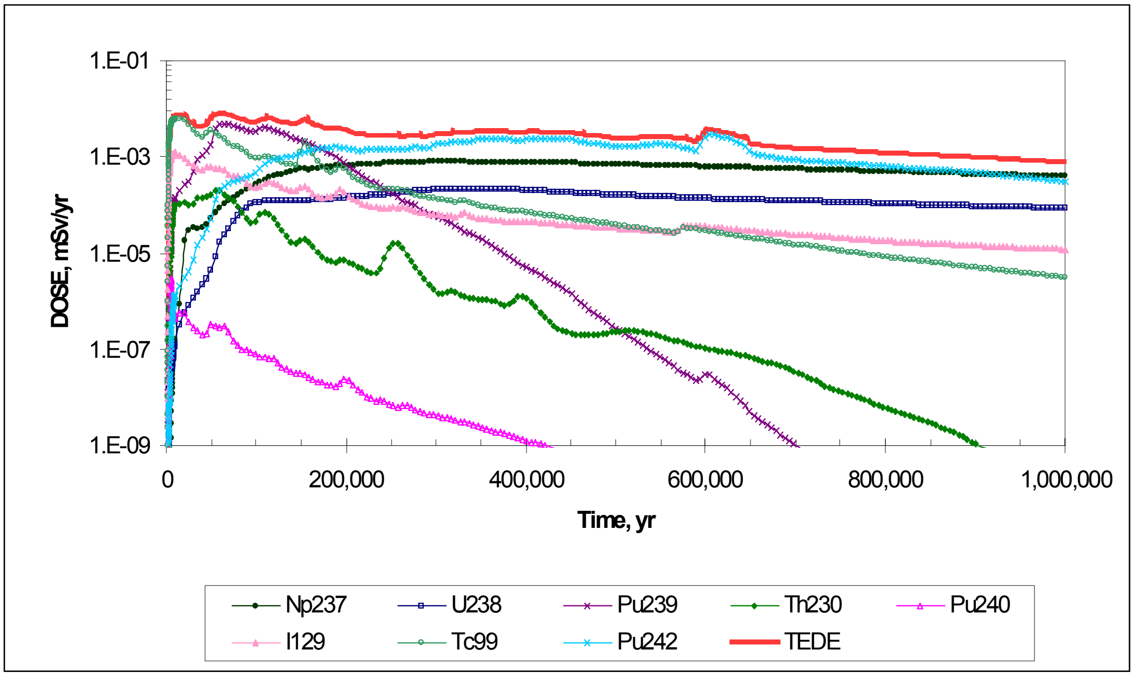


Figure 1-7. Average Radionuclide Dose for 1,000,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations. (1mSv/yr = 100mrem/yr)

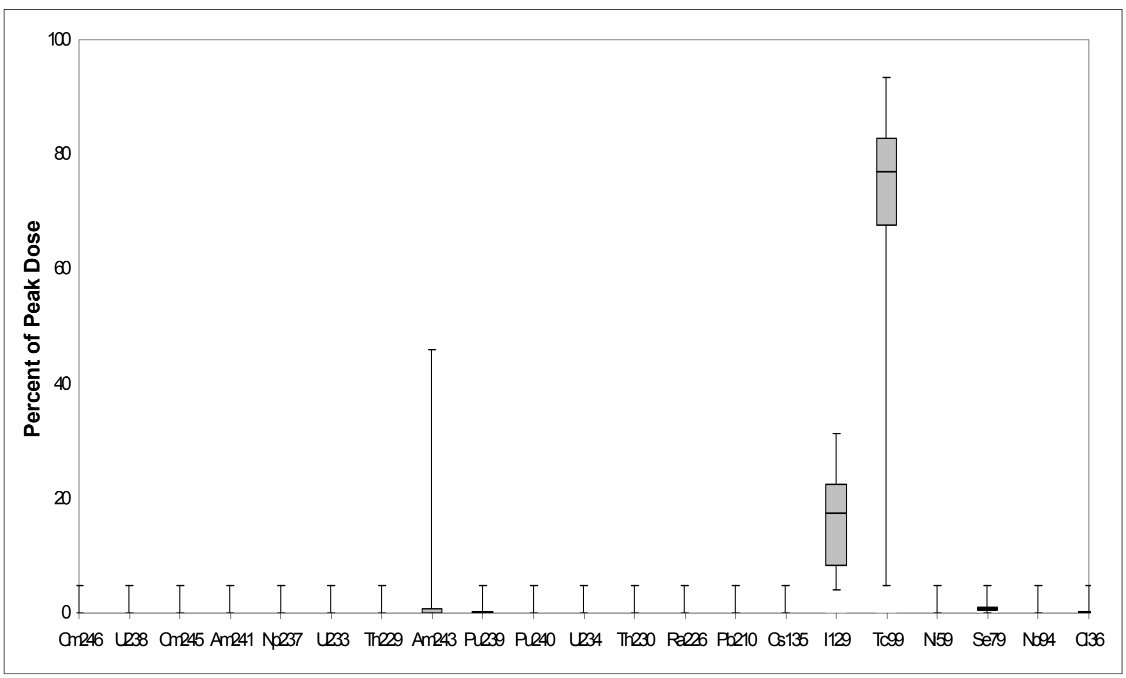


Figure 1-8. Radionuclide Contributions for 10,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations.

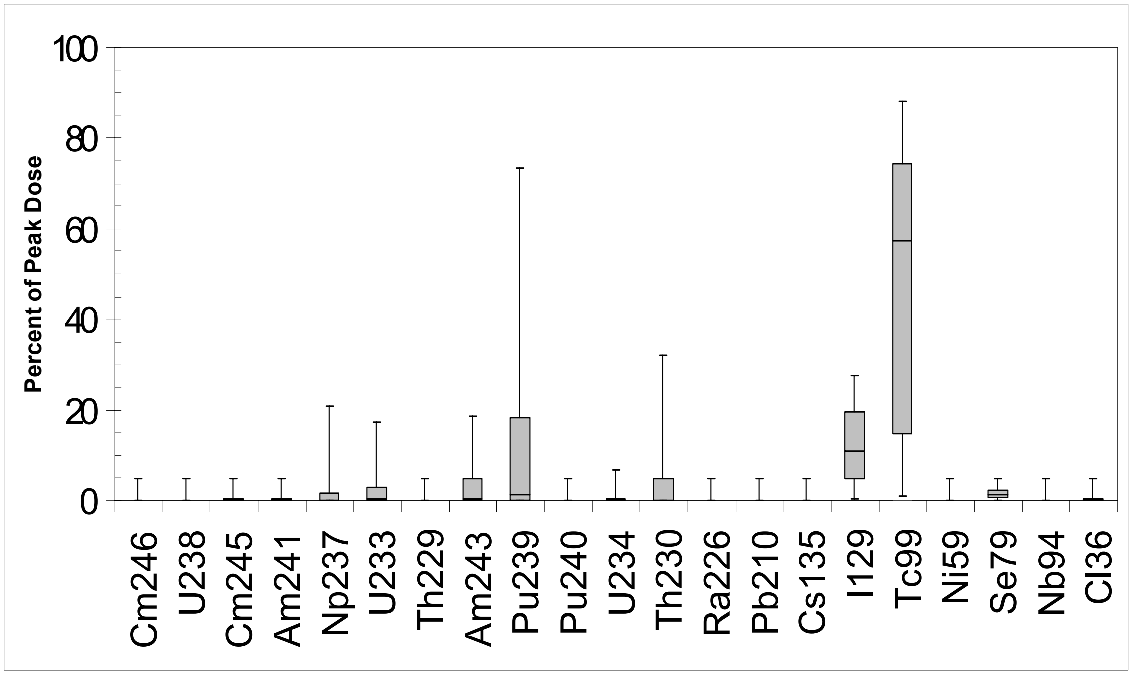


Figure 1-9. Radionuclide Contributions for 100,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations.

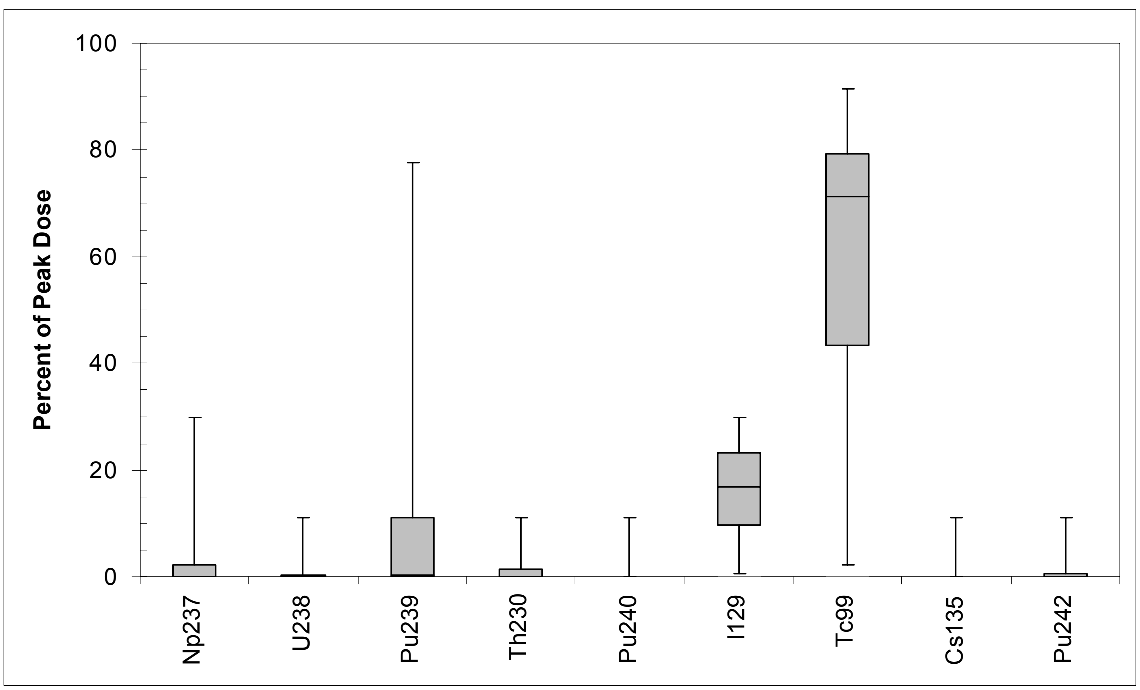
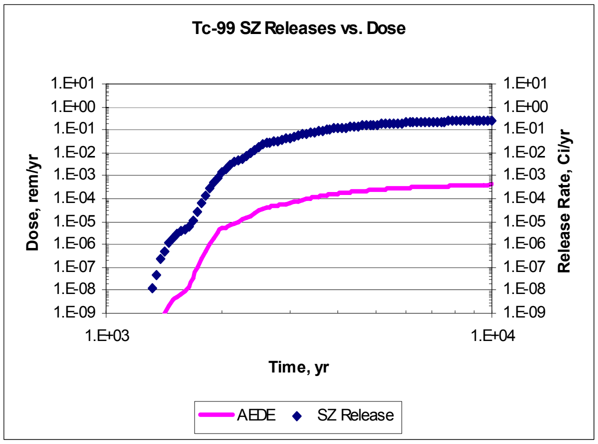
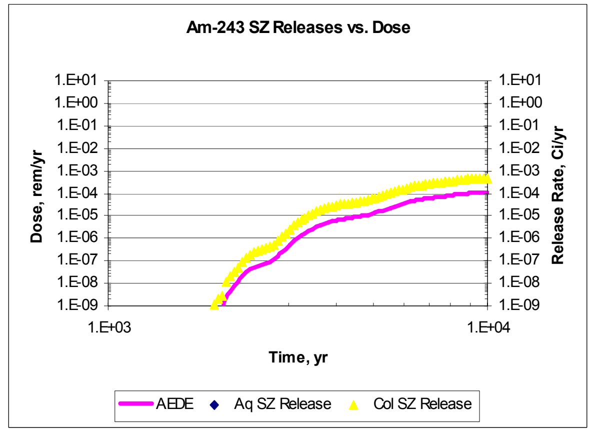


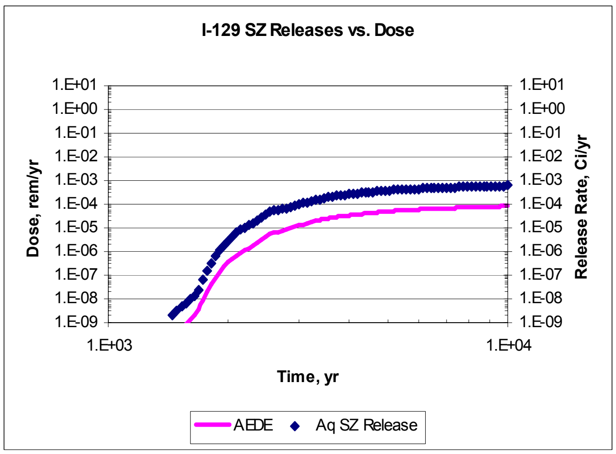
Figure 1-10. Radionuclide Contributions for 1,000,000-year Nominal Scenario with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta W for 500 Realizations.



(a)



(b)



(c)

Figure 1-11. Saturated Zone Releases (Aq SZ Release) and Resulting Doses (AEDE) of (a) Tc-99, (b) Am-243, and (c) I-129 for 10,000-year Nominal Scenario with Seismic Disruption Case Simulation using TPA 5.1 Beta W for 500 Realizations.

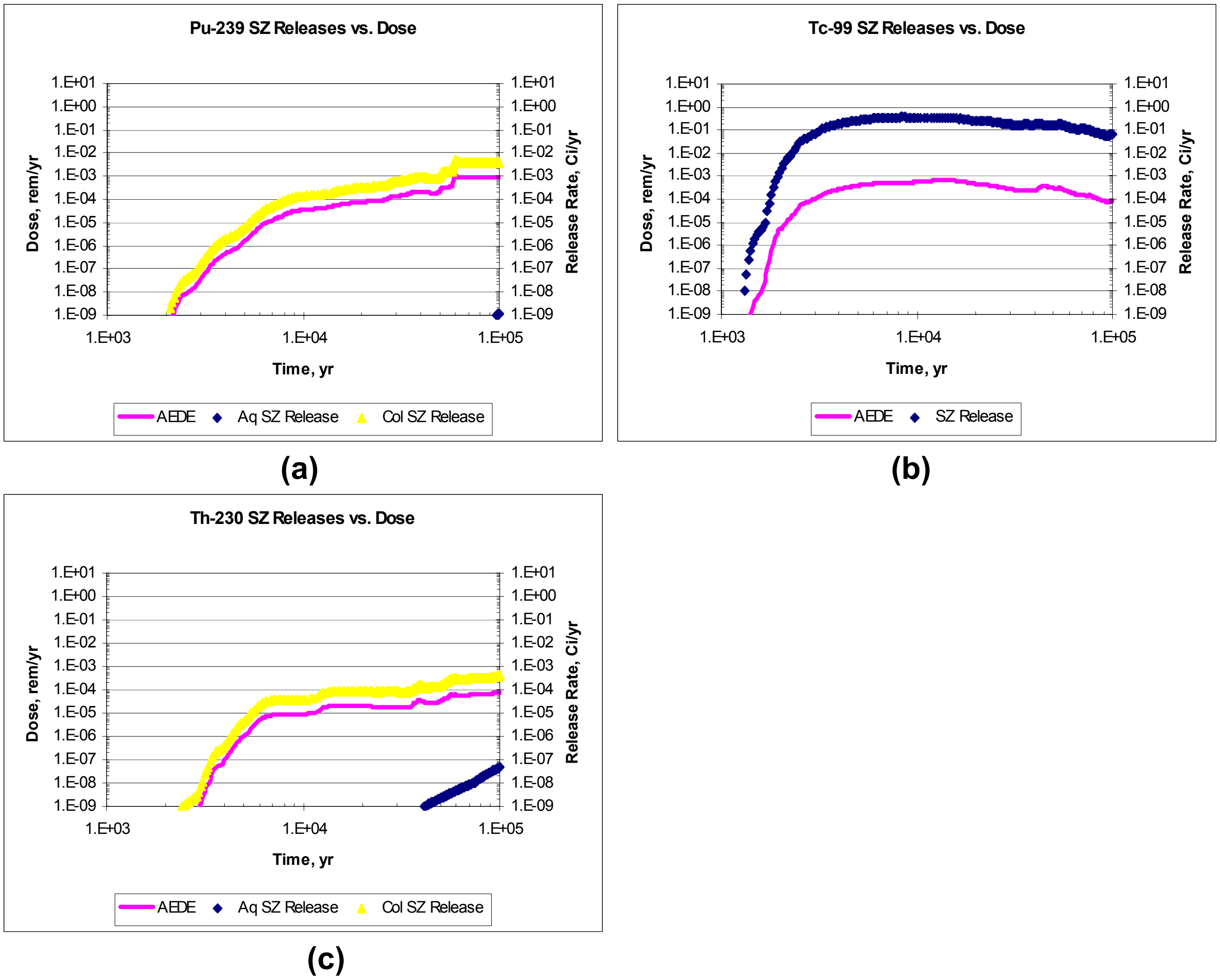
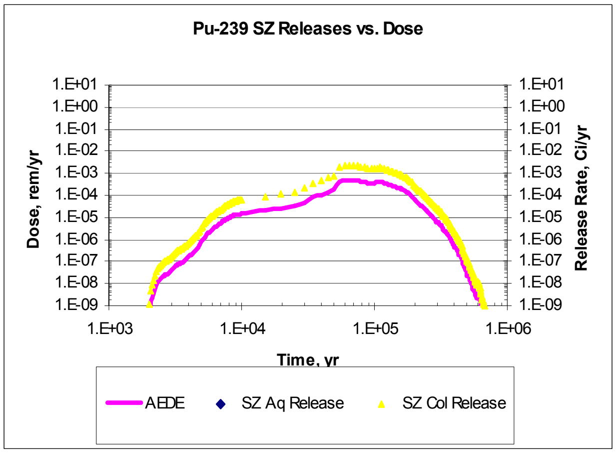
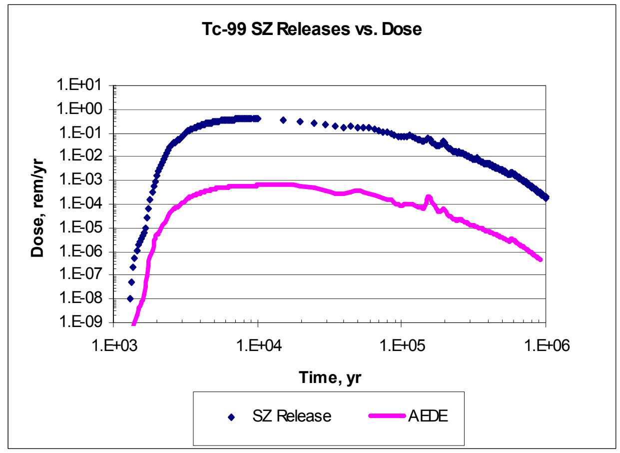


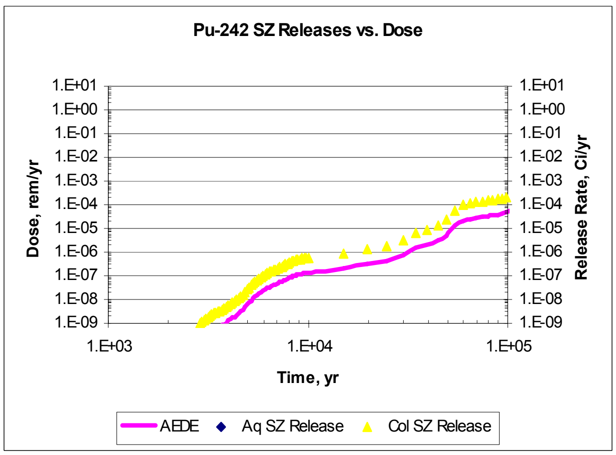
Figure 1-12. Saturated Zone Releases and Resulting Doses of (a) Pu-239, (b) Tc-99, and (c) Th-230 for 100,000-year Nominal Scenario with Seismic Disruption Case Simulation using TPA 5.1 Beta W for 500 Realizations.



(a)



(b)



(c)

Figure 1-13. Saturated Zone Releases and Resulting Doses of (a) Pu-239, (b) Tc-99, and (c) Pu-242 for 1,000,000-year Nominal Scenario with Seismic Disruption Case Simulation using TPA 5.1 Beta W for 500 Realizations.

1.D. Discussion of Results

Figures 1-1 through 1-3 above illustrate the total dose statistics for the reference case input set from the nominal scenario with seismic disruption. The peaks of the mean curve from each figure are 0.68 mrem/yr at 10,000 years, 1.4 mrem/yr at 59,500 years, and 0.86 mrem/yr at 59,500 years for the three simulation periods, respectively. The mean dose curve represents approximately the 83rd, 93rd , and 93rd percentiles for the three simulation periods, respectively.

Figure 1-4 above illustrates the differences in the dose curves for the three simulation periods. The 10,000 year dose is below the other dose curves due to post-10,000 year seismic events that fail waste packages. Whereas, the 1,000,000 year dose is less than the 100,000 year dose due to a smaller simulated inventory. Generally, the three dose curves are consistent and Test Criterion 1.B.1 is generally met, however, differences are noted and explained in subsequent paragraphs.

One notable difference is the increase in dose at a given time from the 10,000-year simulation to the 100,000-year simulation. This difference is explained by the modeling approach for treatment of seismically (i.e., mechanically) failed waste packages. First, seismic events are sampled over the simulation period. Therefore, the 10,000-year simulation does not consider the impact of seismic events that may occur beyond 10,000-years. Second, mechanically-failed waste packages in subareas with initiation of localized corrosion are assumed to begin releasing at the time of localized corrosion failures, but the number of waste packages releasing is controlled by the mechanical parameters typically resulting in more releasing waste packages than for LC alone. Thus the 100,000-year simulation shows higher releases, and thus doses, because seismic events after 10,000-years are able to release from more waste packages prior to 10,000 years than from localized corrosion alone in the 10,000-year simulation. This effect will be mitigated by treating seismic activity as a separate disruptive scenario class, thus avoiding the combination of localized corrosion failures seismically induced mechanical failures in the same realizations (see Task S-4, Attachment C for additional discussion of the seismicity as a separate scenario class).

The second notable difference is that the aforementioned increasing dose trend with simulation duration is not observed when moving from the 100,000-year to 1,000,000-year simulation duration. The explanation described before should typically hold true, however, the number of simulated radionuclide species was reduced in the 1,000,000-year simulations for computational efficiency, thus resulting in lower reported doses. It should be noted that a shortened or alternate list of radionuclides may be appropriate for 1,000,000-year simulations when analysts are interested in dose contributions at very long times; however, careful analysis will be required to determine the approriate radionuclides to consider for this long time frame. Accordingly, the reduced list used in this analysis should be considered arbitrary. The effect of this simulated inventory will be discussed in the next paragraph. Analysis of the 10,000- and 100,000-year simulations' dominant radionuclides, as summarized in Table 1-1 below and Figures 1-8 and 1-9 above, suggests that colloidal Am-243 is a key dose contributor around 10,000-years. Additionally, Am-243 is the parent of Pu-239, the dominant dose contributor at the peak of the mean dose for both the 100,000-year and 1,000,000-year simulations, as summarized in Table 1-1 below and Figures 1-9 and 1-10 above. Am-243 was a key radionuclide missing from the 1,000,000-year simulation inventory. Therefore, a supplemental analyses (S1) was performed for 1,000,000-years using almost the entire 100,000-year inventory with the addition of Pu-242 but without Ra-226, Pb-210, Cs-235, Ni-59, Se-79, and Ni-94. The latter nuclides were excluded because they were deemed insignificant in both the 10,000- and 100,000-year simulations and historically have not been considered major contributors to the overall risk. Additionally, other changes were made to the *tpa.inp* file to improve the computational efficiency of the NEFTRAN (NEFMKS) unsaturated zone transport calculations. These included exclusion of the Calico Hills non-welded vitric layers for subareas with thin deposits. Also, matrix permeabilities for units which occasionally result in two matrix layers simulated for the unsaturated zone were adjusted within their range to minimize this potential and only allow a single matrix layer to be simulated for any given subarea. Note that these changes are for validation test purposes only and results should not be taken out of this context. The results from this analysis, as depicted in Figure 1-4 above, as expected, suggests that the difference in inventory results in a noticeable difference in simulated doses. However, differences in the input for the simulation may also explain some of the differences.

A second supplemental (S2) analysis was performed to assess the impact of the UZ changes between the reference and first supplemental analyses. The second supplemental analysis retained the unsaturated zone changes from the first supplemental analysis, but reverted back to the reference analysis inventory for 1,000,000-years. Results illustrated in Figure 1-4 above indicate general consistency between the first and second supplemental analyses up to approximately 50,000-years, thereby suggesting that the selection of simulated inventory may be the main reason for the differences noted at these earlier times between the reference case and the first supplemental analyses in Figure 1-4 above. However, from about 50,000 to 200,000-years, the first and second supplemental analyses notably diverge suggesting that the unsaturated zone changes are the reason for the differences noted between the reference and first supplemental analyses. Finally, after about 200,000-years, the first and second supplemental analyses diverge again indicating that the simulated inventory was the explanation for the differences between the reference and first supplemental analyses. Inspection of this time period reveals that Th-229 is the dominant radionuclide for the first supplemental analysis, but was not considered in the reference simulation. Generally, the key radionuclides for the various simulations are consistent accounting for initial simulated inventories. Therefore, Test Criterion 1.B.2 is considered passed.

Figures 1-8 through 1-10 above illustrate the range of percent contribution of individual radionuclides to the peak dose for the ensemble of 500 realizations. The grey box represents the percent contribution to peak doses from half of the realizations. The whiskers represent the percent contribution to peak doses from 90% of the realizations. These figures are generally in agreement with the average dose curves shown in Figures 1-5 through 1-8 above, respectively, for the time of peak mean dose and Table 1-1 below. The difference is due to the fact that the average radionuclide contribution is dominated by a small fraction (approximately 7-15%) of the 500 realizations in which those radionuclides listed are dominant, whereas, the percent contribution equally weights each realization. The variability in the dominant nuclides is due to the variability in the colloidal release and transport variability from mechanically failed waste packages. When a low-probability seismic event is sampled with colloidal release and transport parameters aligned for relatively quick release and transport, the associated radionuclide (e.g., Am-243 and Pu-239) doses rise as well dominating the average dose of all realizations. Because of the limited number of samples, evaluating the representative mean dose from the seismic scenario may require separate consideration apart from the nominal scenario.

Finally, Figures 1-11 through 1-13 above illustrate that doses from key radionuclides track saturated zone releases well indicating appropriate integration between the radionuclide releases and resulting dose calculations. Therefore, Test Criterion 1.B.3 is passed.

Because the (i) suggested inventories capture the peak well for each simulation period, (ii) saturated zone releases are consistent with doses, and (iii) differences in the dose curves between the three simulation periods can be rationalized, this test is considered passed. However, the users guide should clearly describe the need to carefully consider the inventory as well as low-probability seismic events (e.g., mechanical failures) to reasonably assess the dose for various simulation durations.

Table 1-1. Comparison of Three Key Average Radionuclides at Various Times for the Three Simulation Periods using TPA 5.1 Beta W.

Simulation Period (kyrs)	10 {R}*	100 {R}*	1,000 {R}*	1,000 {S1}*	1,000 {S2}*	1,000 {S3}*
Radionuclides @ 5kyrs	Tc99 I129 Am243	Tc99 I129 Am243	Tc99 I129 Pu239	Tc99 Am243 I129	Tc99 I129 Pu239	Tc99 I129 Pu239
Radionuclides @ 10kyrs (TEDE [mrem/yr])	Tc99 Am243 I129 (0.68)	Tc99 Am243 I129 (0.94)	Tc99 I129 Pu239 (0.77)	Tc99 Am243 I129 (1.12)	Tc99 I129 Pu239 (0.83)	Tc99 I129 Pu239 (0.83)
Radionuclides @ 50kyrs	N/A	Tc99 Pu239 Am243	Tc99 Pu239 I129	Tc99 Pu239 Am243	Pu239 Tc99 I129	Pu239 Tc99 I129
Radionuclides @ 100kyrs (TEDE [mrem/yr])	N/A	Pu239 Tc99 Th230 (1.22)	Pu239 Tc99 Pu242 (0.62)	Pu239 Pu242 Th229 (3.40)	Pu239 Pu242 Np237 (2.89)	Pu239 Pu242 Np237 (2.97)
Radionuclides @ 500kyrs	N/A	N/A	Pu242 Np237 U238	Th229 Np237 Pu242	Pu242 Np237 U238	Np237 Pu242 U238
Radionuclides @ 1,000kyrs (TEDE [mrem/yr])	N/A	N/A	Np237 Pu242 U238 (0.080)	Th229 Np237 Pu242 (0.51)	Pu242 Np237 U238 (0.082)	Np237 Pu242 U238 (0.15)
Time of Peak Mean Dose [kyrs]	10	59.5	59.5	86.7	86.7	86.7
Peak Mean Dose [mrem/yr]	0.68	1.4	0.86	3.89	3.40	3.46
Radionuclides @ Time of Peak Mean Dose	Tc99 Am243 I129	Pu239 Tc99 Th230	Pu239 Tc99 Pu242	Pu239 Pu242 Th229	Pu239 Pu242 Tc99	Pu239 Pu242 Tc99

***NOTES:**
{R} - Reference case 500 realizations - see *tpa_R.inp*;
{S1} - Enlarged inventory case with altered UZFT parameters (e.g., MatrixPermeability, ChnvThickness) and 350 realizations - see *tpa_S1.inp*;
{S2} - Reference inventory case with altered UZFT parameters (e.g., MatrixPermeability, ChnvThickness) and 350 realizations - see *tpa_S2.inp*.
{S3} - S2 input with altered *nuclides.dat* inventory for Np-237 and Pu-239.

Subtask 2. Identify relevant radionuclides to faulting scenario dose estimates

2.A. Test Procedures

2.A.1. Execute 500-realization simulations using the reference case input for the faulting scenario, *tpa.inp*, with append flags on for 100,000-, and 1,000,000-year simulation periods.

2.A.2. Calculate and plot the conditional dose statistics (minimum, 5th-, 25th-, 50th-, 75th-, 95th-percentiles, mean, and maximum) from the output file, *totdose.res*, for the 100,000- and 1,000,000-year simulation periods. To calculate the statistics use the script, totdose.exe, provided by O. Pensado. Plot the mean conditional dose for 100,000-year and 1,000,000-year simulation periods from both faulting scenario and nominal scenario with seismic disruption.

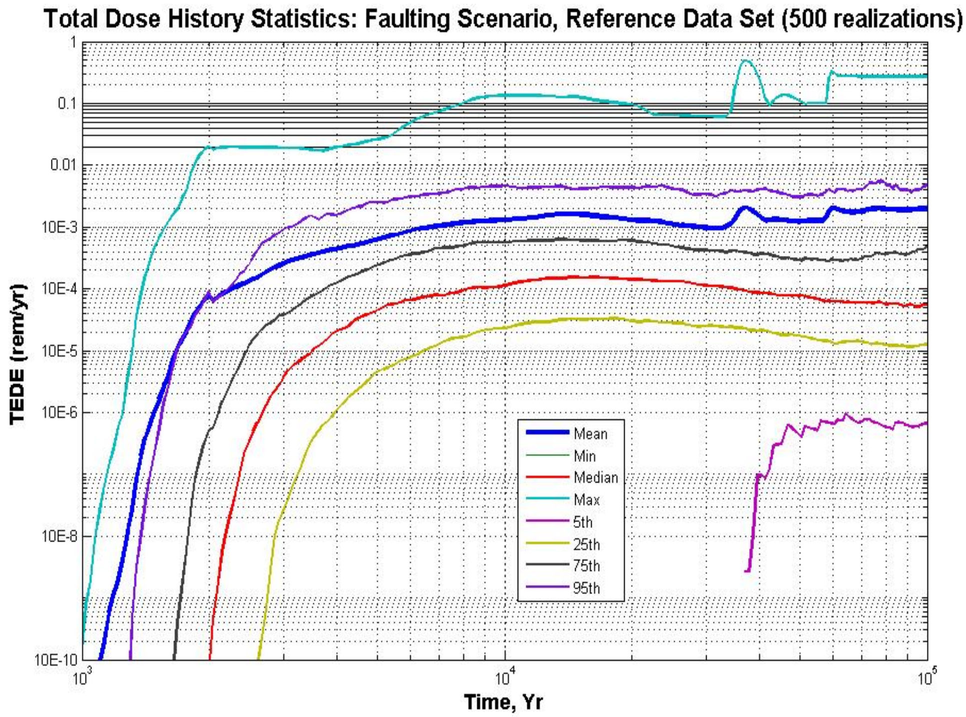
2.A.3. Plot the average conditional dose per radionuclide from the output file, *rgwna.tpa*, for the 100,000-year simulation period.

2.B. Test Criteria

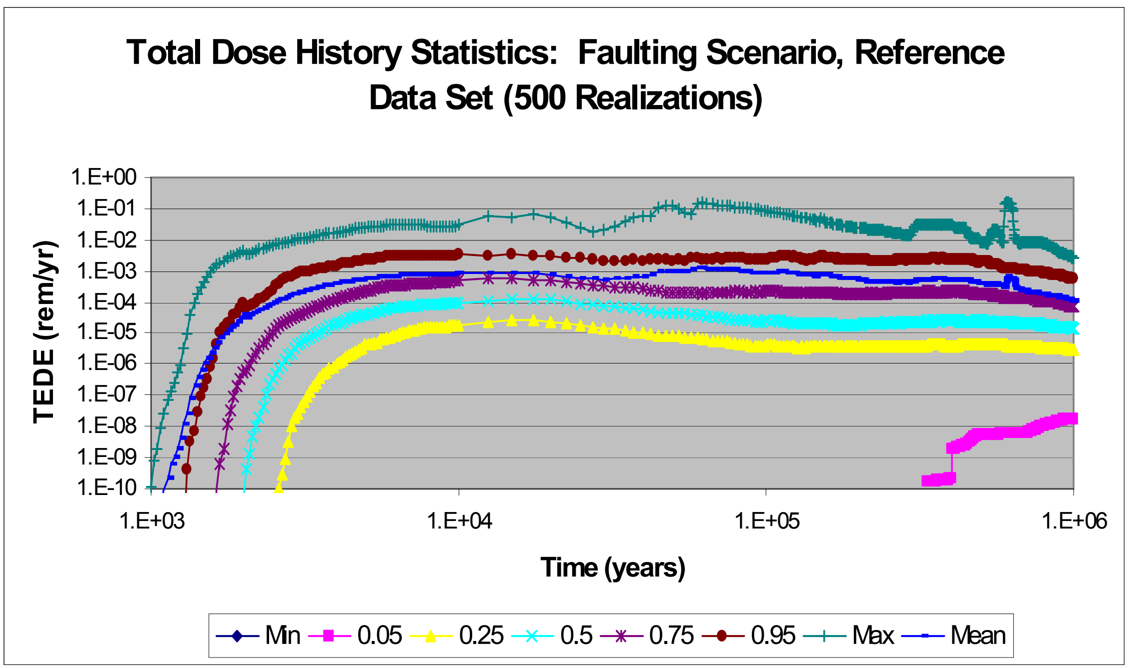
2.B.1 Is the change in conditional dose from the faulting disruptive scenario consistent with trends in the nominal scenario after accounting for faulting failed waste packages?

2.B.2. Are the dominant radionuclide contributors similar for the faulting scenario and nominal scenario with seismic disruption?

2.C. Test Results



(a)



(b)

Figure 2-1. Conditional Dose Statistics for (a) 100,000- and (b) 1,000,000- year Faulting Scenario Reference Case Simulation using TPA 5.1 Beta U for 500 Realizations.

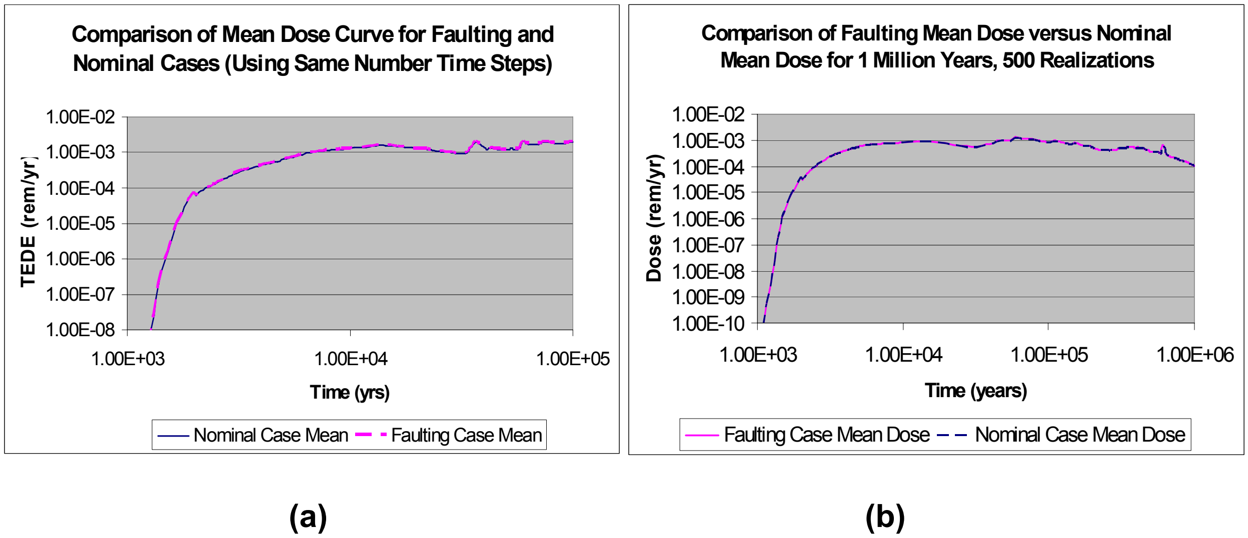


Figure 2-2. Mean Dose Curves for (a) 100,000-year and (b) 1,000,000-year Faulting Scenario and Nominal with Seismic Disruption Reference Case Simulation using TPA 5.1 Beta U for 500 Realizations.

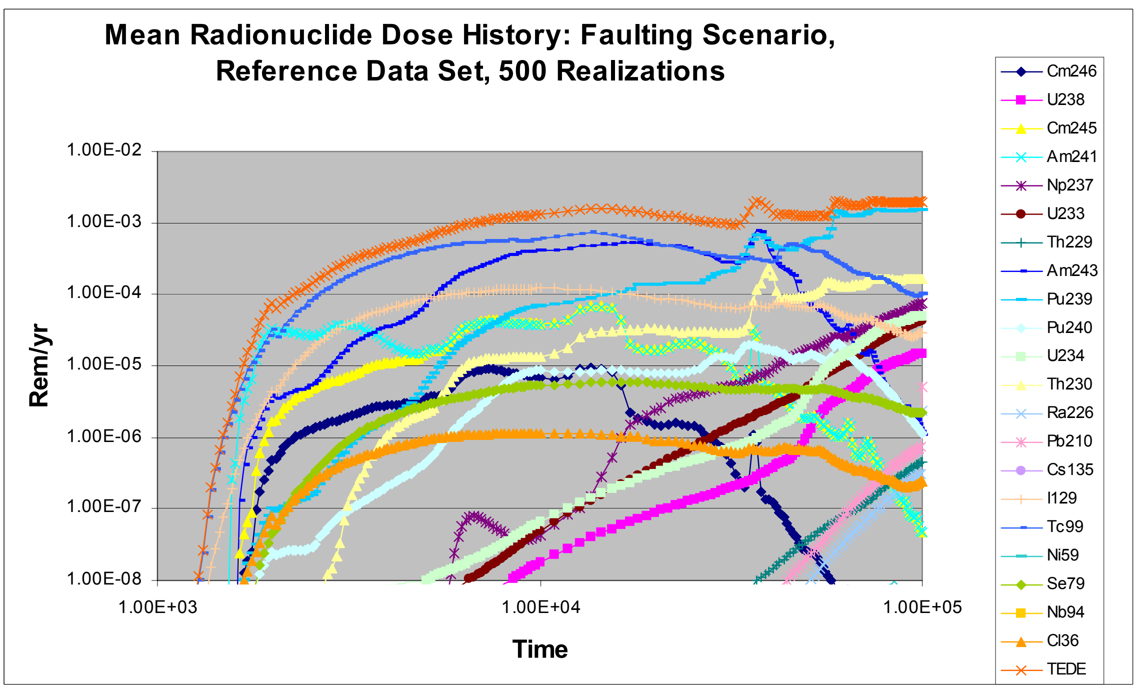


Figure 2-3. Average Radionuclide Dose for 100,000-year Faulting Scenario Reference Case Simulation using TPA 5.1 Beta U for 500 Realizations.

2.D. Discussion of Results

Figure 2-1 illustrates the conditional total dose statistics for the faulting scenario reference case input set. The peak of the mean curve is 2.12 mrem/yr at 60,000 years. This result is consistent (< 3% difference; the nominal case using the reference data set for betaU yielded a peak of the mean total dose of 2.07 mrem/yr at 60,000 years) with results reported for the nominal scenario with seismic disruption in this analysis as is illustrated in Figure 2-2 for both the 100,000-year and 1,000,000-year simulation periods. Therefore, Test Criterion 2.C.1 is considered passed.

Dominant dose contributors include Am-243 (colloidal) and Pu-239 (colloidal), Tc-99, and Th-230 as can be seen from Figure 2-3 above. At 10,000-,100,000-, 1,000,000-years and times of peak mean doses, the rank order of top contributing radionuclides do not change compared to the nominal case for this analysis. Therefore, Test Criterion 2.C.2 is considered passed.

Subtask 3. Identify radionuclides relevant to igneous scenario dose estimates for alternative ash models and igneous intrusion

3.A. Test Procedures

3.A.1 Execute 1000-realization simulation using the direct-release-only case input for the igneous scenario, *tpa.inp*, for 10,000-years and 100,000 years, using both the TEPHRA/ASHREMOB model and the ASHPLUME/ASHREMOVO/DCAGS model.

3.A.2 Plot the mean conditional ground-surface doses for the most significant radionuclides from the output files ***rgsna.tpa*** and total mean doses from output files ***rgssa.tpa*** for the four cases.

3.A.3 Present additional tabular information on mean doses for the four extrusive cases.

3.A.4 Use a 1000-realization igneous intrusion simulation for 1 million years (developed for System Level Task 4).

3A.5 Plot the mean conditional groundwater doses for the most significant radionuclides from the output file ***rgwna.tpa*** and the total mean dose from ***rgwsa.tpa.***

3.B Test Criteria

3.B.1 Are mean dose curves similar for the TEPHRA/ASHREMOB and ASHPLUME/DCAGS models for extrusive volcanism? Differences should be rationalized.

3.B.2 Are mean dose curves similar for the 10,000-year and 100,000-year simulation periods for the igneous extrusive scenario when the same ash model has been used? Differences should be rationalized.

3.B.3 Are doses from dominant radionuclides in the igneous intrusion case consistent with other disruptive cases and the nominal-seismic case?

3.C. Test Results

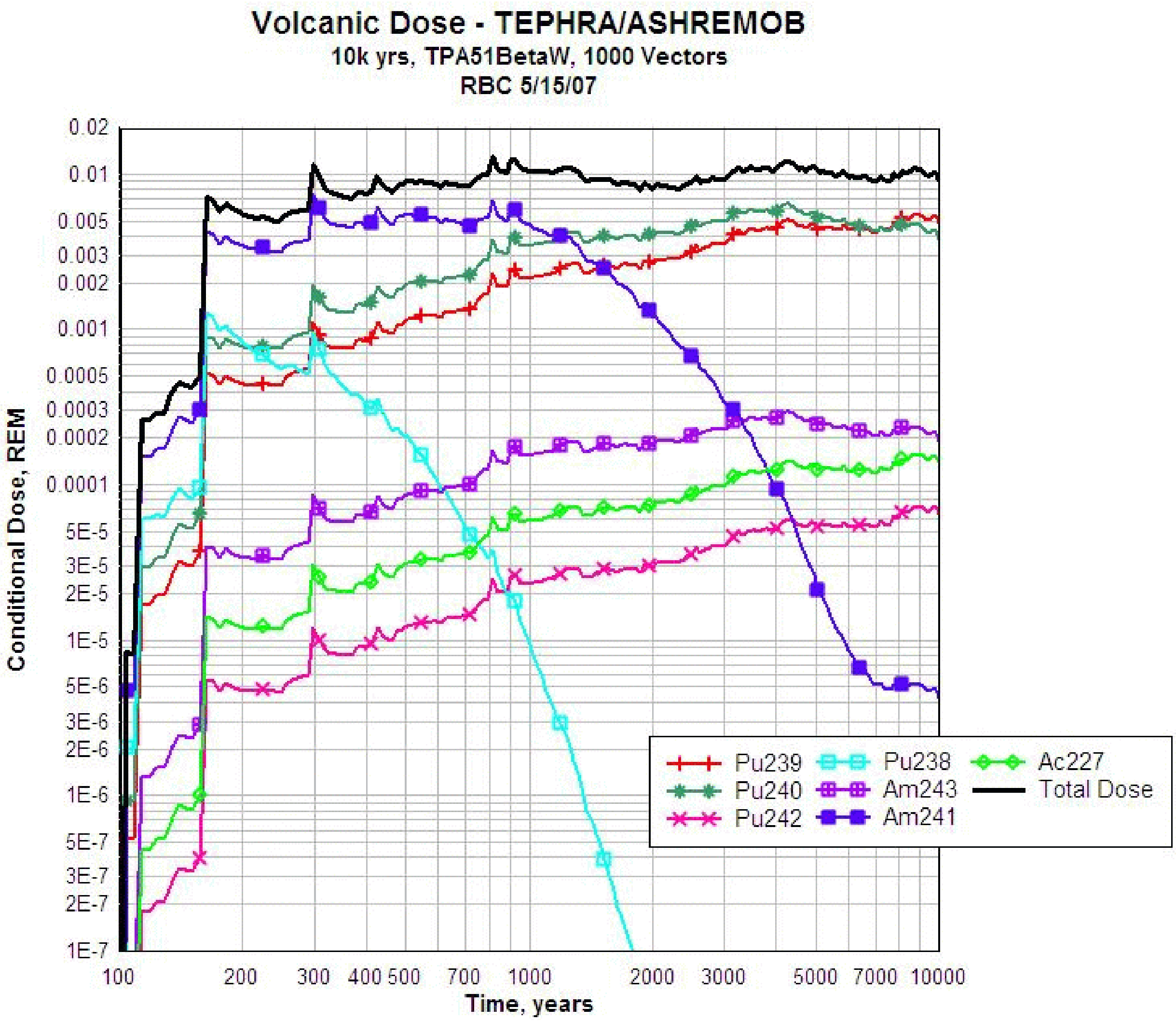


Figure 3-1. Mean Dose for Igneous Extrusion, 10,000 years, TEPHRA/ASHREMOB Model, TPA5.1betaW

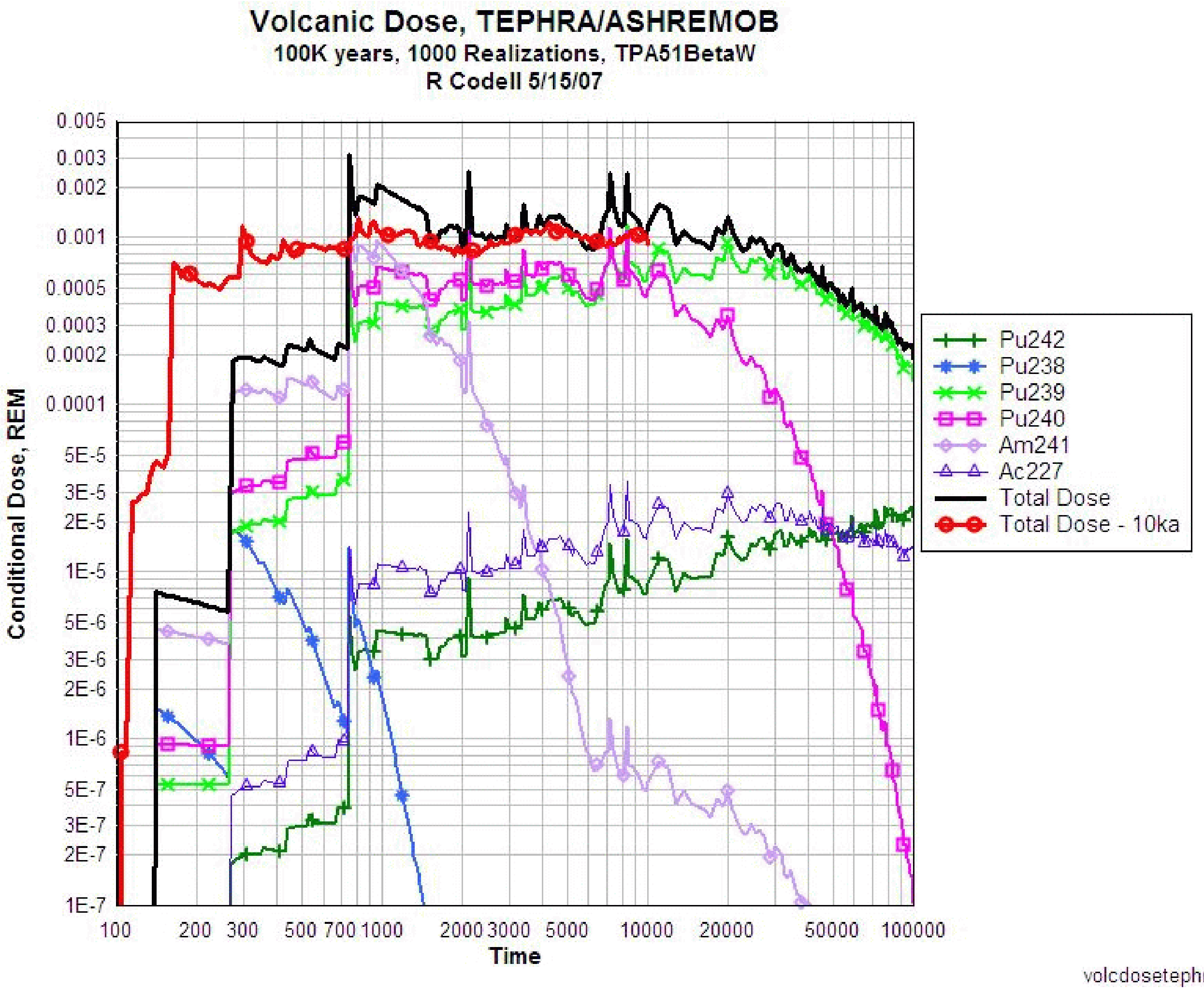


Figure 3-2. Mean Dose for Igneous Extrusion, 100,000 years, TEPHRA/ASHREMOB Model, TPA5.1betaW (with 10,000 year total conditional dose added with scaling)

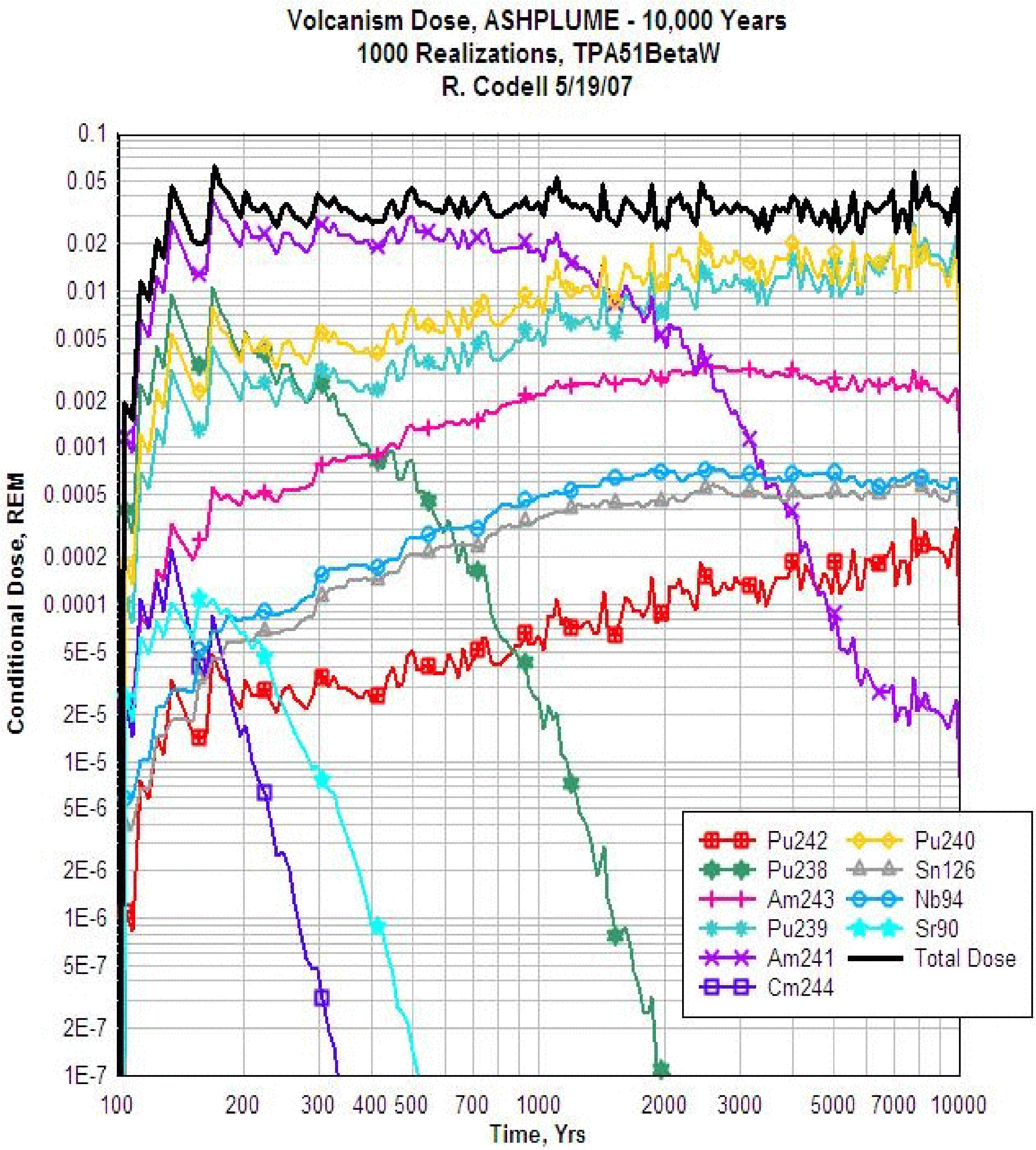


Figure 3-3. Mean Dose for Igneous Extrusion, 10,000 years, ASHPLUME/DCAGS Model, TPA5.1betaW

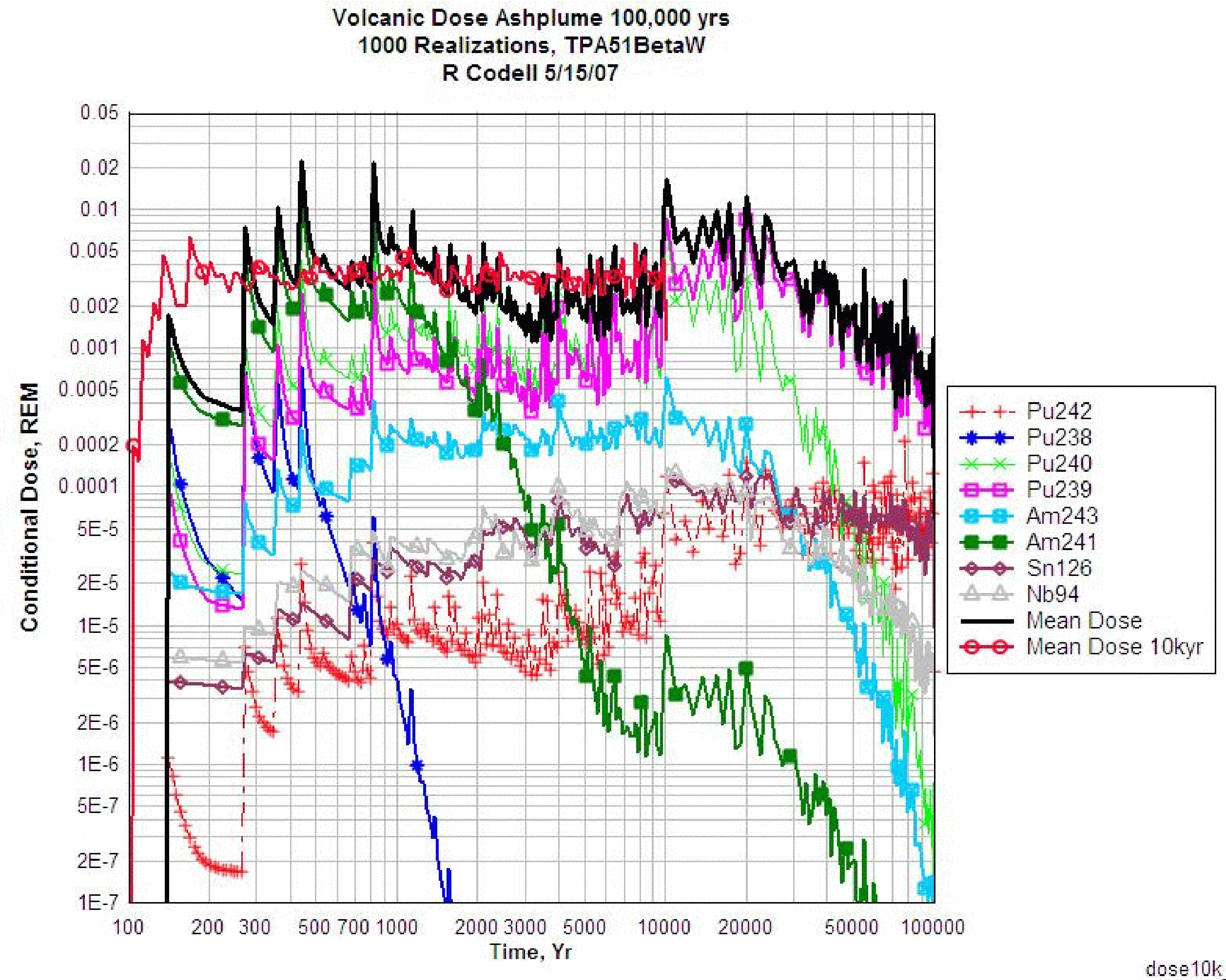


Figure 3-4. Mean Dose for Igneous Extrusion, 100,000 years, ASHPLUME/ASHREMOVO/DCAGS Model, TPA5.1betaW (with 10,000 year conditional total dose added with scaling)

Table 3-1. Fraction of Radionuclide Contribution to Dose Mean-over-time-period for Extrusive Volcanism Case

Radionuclide	TEPHRA 10KA	ASHPLUM E 10KA	TEPHRA 100KA	ASHPLUME 100KA
Pu242	0.00345	0.00285	**0.01152**	0.00059
Am242m	0.00018	0.0003	0.00004	0.00133
Pu238	**0.01651**	**0.02616**	0.0017	**0.14398**
Am243	**0.01782**	**0.05933**	0.01666	**0.02084**
Pu239	**0.29432**	**0.23311**	**0.45204**	**0.05262**
Pa231	0.00094		0.00179	
Ac227	0.0082	0.00003	0.01563	
Am241	**0.27098**	**0.34141**	**0.14453**	**0.6683**
Np237	0.00051	0.00058	0.00192	0.00021
Th229	0.00001	0.00001	0.00097	
Cm244	0.00002	0.00023		0.00222
Pu240	**0.38635**	0.**31042**	**0.35123**	**0.09251**
Cs137		0.00015		0.00275
Sn126		0.01035		0.00373
Nb94		**0.01352**		0.00563
Sr90		0.0003		0.00473

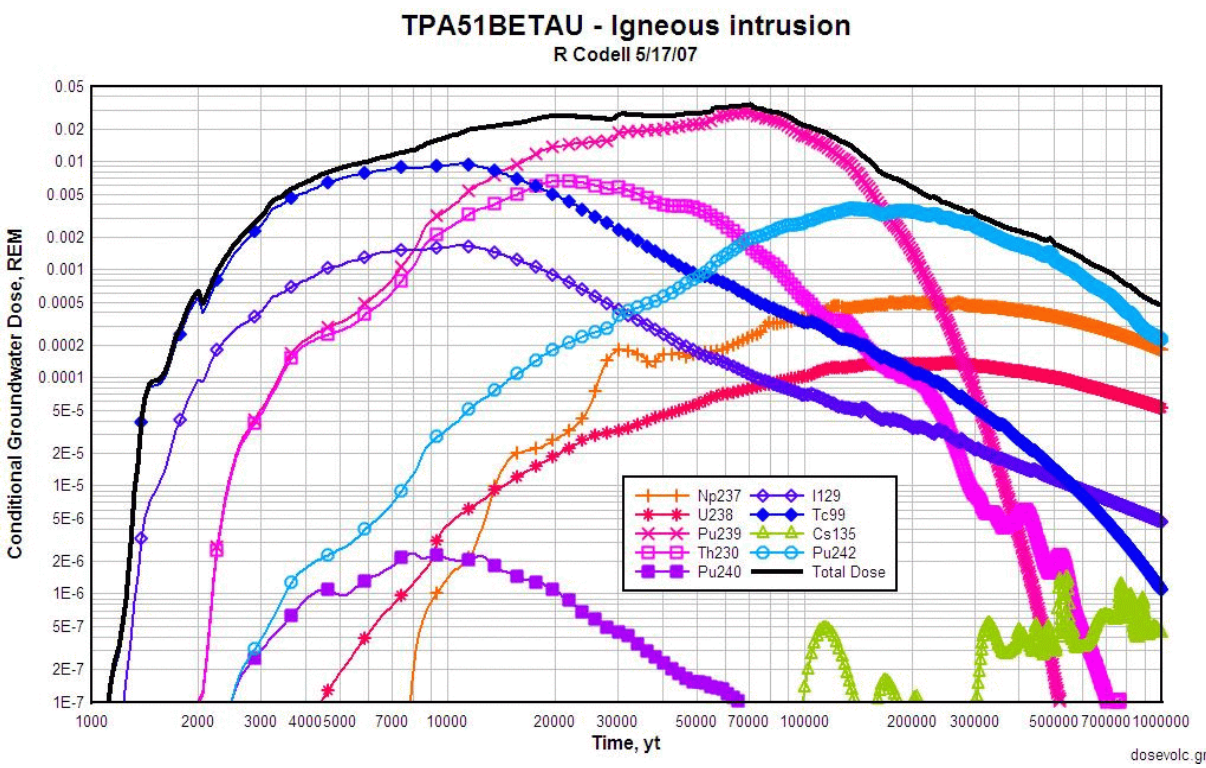


Figure 3-5. Conditional Groundwater Dose, Intrusive Volcanism Case, 1 Million Years for Volcanism between 100 and 10,000 years only, TPA5.1betaU version

3.D. Discussion of Results

3.D.1 Dose Risk

Note that the doses in all figures presented in this section are conditional, and not probability weighted for dose risk. The dose risk would be obtained from the conditional doses by multiplying the ordinate by10^{-3} for Figures 3-1 and 3-3 (i.e., 10^{-7}/year event probability by 10,000 year time period) and 10^{-2} for Figures 3-2 and 3-4 (i.e.,10^{-7}/year event probability by 100,000 year time period). Because the igneous disruption took place for only the first 10,000 years in the igneous intrusion scenario, it is not possible to calculate dose risk for the 1,000,000 year period. However, for the first 10,000 years, the conditional dose should be multiplied by 10^{-3} to calculate the dose risk.

3.D.2 Convergence of Results

Although not the focus of this exercise, the poor statistical stability or convergence of the mean dose for the igneous extrusive scenario is a factor in the interpretation of the results. Support for the conclusion that the mean dose is not well-converged can be explained by several factors, including the following:

(1) Figures 3-1 and 3-2 show the mean doses for the 10,000 and 100,000-year igneous extrusive cases, respectively using the TEPHRA/ASHREMOB model and 1000 realizations. Figure 3-2 also shows the 10,000-year total dose from Figure 3-1, corrected for probability so they could be plotted on the same figure. The apparent lack of agreement for Figure 3-1 and the first-10,000 years of Figure 3-2, is a result of different levels of convergence for the two runs. For both figures, the sampling interval for the volcanic event was the entire time period of interest, which results in a 10-times larger time interval between samples for the 100,000 year case, with consequently poorer statistical convergence of the mean dose;

(2) Results for the mean doses are less converged for Figures 3-3 and 3-4 for the 10,000 and 100,000-year igneous extrusive case, respectively using the ASHPLUME/ASHREMOVO/DCAGS approach. For this approach, the poor convergence of the mean dose is exacerbated by the shorter time constants in the model for removal of radionuclide contamination from the ground surface than with the TEPHRA/ASHREMOB approach. The longer time constant for the latter approach leads to a smoother output than the rather short-lived peaks of the former.

(3) Although a special techniques have been formulated (i.e., the convolution approach) that always result in a smooth mean-dose curve for the igneous extrusive case, this technique was not in a form easily used to determine the contribution of individual radionuclides. Therefore it was not employed in the present analysis.

Bearing in mind the narrow purposes of this exercise; i.e., to determine which radionuclides contribute most importantly to the risk from volcanism, the results presented in this section are adequate.

3.D.3 Dose Contributions by Radionuclide

The contribution to dose by individual radionuclides depends on a number of factors, including the time after repository closure and whether the model chosen was the ASHPLUME/ASHREMOVO/DCAGS approach or the TEPHRA/ASHREMOVO approach. What is obvious for all cases of extrusive volcanism is that the biggest contributors to dose are from the radionuclides Pu-238, Pu-239, Pu-240, and Am-241, with smaller contributions from Pu-242, and Am-243. Other radionuclides, presented in Tables 3-1 and 3-2 show all other radionuclides contribute substantially less to the total dose.

Table 3-1 presents the contribution to time-averaged dose over the period of interest (i.e., 0 to 10,000 years or 0 to 100,000 years) for each radionuclide, showing in a broad sense the relative importance of each radionuclide for the four cases discussed above. This table is less useful for determining the major contributors for the peak-of-the-mean dose. Table 3-2 shows the fractional contribution for the most significant radionuclides for the four cases at the time that the peak-of-the-mean dose occurs for each of the four cases.

In both tables, there are discrepancies among the contributions to dose. A large part of these discrepancies can be laid to the difference in the times for the peak-of-the-mean doses. Another contributing factor would be the difference in the time constants for the models. If the peak-of-the-mean dose occurs early, then direct deposition of the plume on the location of the RMEI dominates the dose. However, if the TEPHRA/ASHREMOB approach is used, most of the deposition will not be directly on the RMEI. This would result in the peak-of-the-mean dose occurring at a later time. Therefore, longer-term processes involved with the re-mobilization model have more influence on the results, which emphasizes the contribution of longer-lived radionuclides. Since the ASHPLUME/ASHREMOVO/DCAGS approach does not have the long time constants associated with the redistribution model of the alternative approach, the results for the ASHPLUME approach emphasize the contribution of short-lived radionuclides.
As an example of this reasoning, consider the dose for the 100,000 year case. The largest contributors to dose for the 100,000 year case with the ASHPLUME/ASHREMOVO/DCAGS approach were from the radionuclides Am-241 and Pu-238 became a significantly larger contributor to dose, despite their relatively short half-lives (432.2 and 87.7 years, respectively). This contributed to early peaks for these radionuclides since the airborne transport is instantaneous in the ASHPLUME case. The TEPHRA/ASHREMOB model has considerably longer time constants caused by re-distribution processes that bring the radioactive contamination to the RMEI after long times. Therefore, radioactive decay of the relatively short-lived Am-241 and Pu-238 places more emphasis on the longer-lived radionuclides for the TEPHR/ASHREMOB case.

Table 3-2. Fractional Dose Contributions for Extrusive Igneous Cases (greater than 0.1%) at Time of Peak-of-the-Mean Dose

	10ka-TEPHRA	100ka-TEPHRA	10ka-ASHPLUME	100ka-ASHPLUME
Radionuclide	**Fraction of Total**	**Fraction of Total**	**Fraction of Total**	**Fraction of Total**
Pu242	0.002	0.002		0.001
Am242m			0.001	0.001
Pu238	0.003	0.004	**0.166**	0.034
Am243	0.013	0.012	0.009	0.012
Pu239	**0.175**	**0.166**	**0.071**	**0.116**
Pa231	0.001			
Ac227	0.005	0.005		
Am241	**0.514**	**0.536**	**0.622**	**0.635**
Cm244			0.001	
Pu240	**0.288**	**0.274**	**0.124**	**0.198**
Cs137			0.001	
Sn126				0.001
Sn121m			0.001	
Nb94			0.001	0.001
Zr93				
Sr90			0.002	
Time of Peak, yrs	811.2	750.3	168.2	435.7

3.D.4 Intrusive Volcanism Dose

Figure 3-5 was plotted from a 1-million year run for 1000 realizations with seismic disruptive, igneous extrusive and igneous intrusive flags turned on. However, the sampling period for the volcanic event was chosen to be 10,000 years. Therefore, this run does not capture the consequences of volcanism beyond 10,000 years.

Table 3-3 shows the contribution to dose risk at the time of the peak-of-the-mean and at 10,000 years.

Table 3-3 - Contributions to Intrusive Igneous Dose Risk

Radionuclide	Contribution, 10,000 yr	Contribution - 70,020 yr (Peak-of-the-mean)
Np-237	8.5e-5	0.007
U-238	0.00026	0.002
Pu-239	0.216	0.862
Th-230	0.142	0.0049
Pu-240	0.00012	2.5e-6

I-129	0.096	0.0032
Tc-99	0.542	0.017
Cs-135	5e-14	6e-14
Pu-242	0.002	0.059

3.E Conclusions for Igneous Cases

3.E.1 Extrusive Igneous Cases

The validation studies demonstrate that there are significant differences in results between the two alternative ash models; i.e., the TEPHRA/ASHREMOB case and the ASHPLUME/ASHREMOVO/DCAGS case. These variance in results has been explained in terms of the differences in the time constants between the two models. The ASHPLUME model emphasizes direct deposition on the RMEI site and the shorter time constants for removal of contamination through the ASHREMOVO processes. The largest contributors to dose risk appear to be Pu-238, Pu-239, Pu-240 and Am-241, although the order differs depending on the model and time frame. Differences between the two alternative ash models to have been explained adequately in terms of their physical differences. Therefore, Test Criterion 3.B.1 is considered passed.

Differences between 10,000-year and 100,000-years runs of the same ash model can be explained in terms of poor convergence, even for 1000 realizations. Special techniques are routinely used to improve convergence when calculating the mean dose, but these procedures were not set up to compare results for individual radionuclide contributions. Nevertheless, the results for 10,000-year and 100,000-year runs are qualitatively similar, and Test Criterion 3.B.2 is considered passed.

3.E.2 Intrusive Igneous Case

The most significant radionuclides for the igneous intrusive case depended on the time that the peak-of-the-mean occurred. For the 10,000 year time period, the peak-of-the-mean occurred at 10,000 years. The most significant radionuclides in order of their contribution to the mean dose were Tc-99, Pu-239, Th-230, and I-129. The simulation was not designed to calculated the dose risk cannot beyond 10,000 years (i.e., to compute dose risk, the igneous sampling period should have extended to the time period of interest). Nevertheless, the peak-of-the-mean occurred at 70,200 years for the case calculated. In this case, the most significant radionuclides were Pu-239, Pu-242, Tc-99 and Th-230. The igneous intrusive case follows the other groundwater scenarios closely in terms of the importance of particular radionuclides. Therefore Test Criterion 3.B.3 is considered passed.

SOFTWARE VALIDATION REPORT (SVR)

SVTR#:	Project#: 20.06002.01.352
Software Name: TPA	Versions: 5.1betaT, 5.1betaU, 5.1betaW, 5.1betaY
Test ID: **S-4**	Test Series Name: Numerical Stability

Test Method

- ☐ code inspection
- x output inspection
- ☐ hand calculation
- x spreadsheet
- x graphical
- ☐ comparison with external code results

Test Objective: Verify the stability of the mean dose results for: (1) the nominal scenario for various time periods of interest and number of realizations; (2) the igneous and faulting cases of the disruptive scenario for various time periods of interest and number of realizations; and (3) time step size.

Test Environment Setup

Hardware (platform, peripherals): Desktop computers

Software (OS, compiler, libraries, auxiliary codes or scripts): XP

Input Data (files, data base, mode settings): In the *tpa.inp* file, modify the number of realizations, LHS and seismic seeds, simulation times, disruptive scenario flags (faulting and igneous), and time steps as required by any test.

Assumptions, constraints, and/or scope of test: See Attachments A, B, and C

Test Procedure: See Attachments A, B, and C.

Attachment A describes procedures used to evaluate overall numerical stability of the code for various simulation time periods, disruptive flag settings (including seismic, faulting, and igneous), and time step settings.
Attachment B provides supplemental analyses to further probe numerical stability convergence of the Igneous Extrusive Model scenario.
Attachment C provides a supplemental analysis to evaluate the potential effects on convergence from seismic induced waste package mechanical failures.

Test Results

Location: See the attached DVDs labeled “TPA Version 5.1 Validation Task S-4.”.

Test Criterion and Analysis of Results: The software should exhibit reasonable statistical stability in the main results for a variety of simulation time periods of interest. The following system-level tests should be conducted.

See Attachments A, B, and C for analysis of results.

Test Evaluation (Pass/Fail): **PASS** (See Attachments A, B, C)

Notes:

Tester: R. Rice / R. Codell / J. Mancillas	Date: 6/7/07

Attachment A
TPA Version 5.1 Validation Task S-4
Numerical Stability

TEST DESCRIPTION

Task Title: "Numerical Stability" - Verify the stability of the mean dose results for: (1) the nominal scenario for various time periods of interest and number of realizations; (2) the igneous disruptive scenario for various time periods of interest and number of realizations; and (3) time step size.

Task Lead: R. Rice

Other team member(s): C. Grossman, D. Codell

Files to be modified: Listed below for each test.

Output files: See attached DVDs labeled "TPA Version 5.1 Validation Task S-4, Attachment A"

TEST PROCEDURE

1. Execute the reference TPA code for 10kyr and 100kyr for a set of realizations (e.g., 401, 450, 500, 600, 700, 800, 900, and 1,000 realizations) with 5 LHS seeds and the reference seismic seed. Repeat above with 5 seismic seeds and the reference LHS seed. For the 10kyr and 100kyr runs, use 201 and 401 time steps, respectively. For the 1000kyr execution time, use 5001 time steps and repeat the above tests except for a subset of the above realizations (e.g., 401, 600, and 1,000 realizations for 3 LHS seeds and 3 seismic seeds).
2. For the igneous and faulting cases of the disruptive scenarios, in separate TPA code executions, activate either the igneous or faulting flag. Use 10kyr and 100kyr runs for a set of realizations (e.g., 401, 450, 500, 600, 700, 800, 900, and 1,000 realizations) with 201 and 401 time steps, respectively. For the 1000kyr execution time, use 5001 time steps and repeat the above test except for a subset of the realizations (e.g., 401, 600, and 1,000 realizations).
3. Execute the basecase TPA code for 10kyr, 100kyr, and 1000kyr in a multiple realization run (e.g., 401 realizations) for 201 and 101 time steps (10kyr), for 401, 201, and 101 time steps (100kyr) and for 5001, 2501, 1001, 501, and 201 time steps (1000kyr).

For all of these tests, the results in *pkmndose.res* will be examined to determine whether any single realization (or a few realizations) have a disproportionately high contribution to the peak mean dos; for these realizations, the TPA code outputs will be analyzed to determine the reasons for its disproportionately high contribution to the peak mean dose.
For each type of test, the results will be plotted.

TEST RESULTS

An outline of the S-4 test results included in this attachment is provided below. Each item in this outline consists of either plots or descriptive text. Following the outline below, are a series of plots and tables that illustrate the results obtained. A discussion of these results begins on page S4 A-59.

<u>**Item**</u>	<u>**Description**</u>
1.	S-4 Test Matrix.
2.	Plots Showing Basecase Peak Mean Dose for Multiple Realization TPA Code Runs with 10,000, 100,000, and 1,000,000 yrs and Using LHS and SEISMIC Seeds.
3.	Tables Showing Basecase Peak Mean Dose for Multiple Realization TPA Code Runs with 10,000, 100,000, and 1,000,000 yrs and Using LHS and SEISMIC Seeds.
4.	Plots Showing Faulting and Igneous (GW, GS, and GWGS) Peak Mean Dose for Multiple Realization TPA Code Runs with 10,000, 100,000, and 1,000,000 yrs.
5.	Tables Showing Faulting and Igneous (GW, GS, and GWGS) Peak Mean Dose for Multiple Realization TPA Code Runs with 10,000, 100,000, and 1,000,000 yrs.
6.	Plots of Expected Dose Showing Different Time Steps for 10,000, 100,000, and 1,000,000 yr.
7.	Plots of Expected Dose Comparing TPA51betaT and TPA51betaW for 401 Realizations and 10,000 yr to show effects on stability of several software changes made during the validation process.
8.	Plots of Expected Dose Comparing TPA51betaT and TPA51betaW for 500 Realizations and the Impact of Simulation Time on Results to show effects on stability of several software changes made during the validation process.
9.	Plots of Expected Dose (GW, GS, and GWGS) Using TPA51betaT for 10,000, 100,000, and 1,000,000 yr With and Without Volcanism.
10.	Plots of Expected Dose From Multiple Realizations Using TPA51betaT for 10,000, and 100,000 yr With the Reference Seed.
11.	Plots of Expected Dose Comparing the Impact of Simulation Time From Multiple Realizations Using TPA51betaT for 10,000, and 100,000 yr With the Reference Seed.
12.	Plots of Expected Dose For the Reference Case and Faulting Case From Multiple Realizations Using TPA51betaT for 10,000 yr With the Reference Seed.
13.	Plots of Expected Dose For the Reference Case and Faulting Case From Multiple Realizations Using TPA51betaT for 100,000 yr With the Reference Seed.
14.	Plots of Expected Dose (GW and GS) From Multiple Realizations Using TPA51betaT for 10,000 yr With and Without Volcanism.
15.	Plots of Expected Dose (GW and GS) From Multiple Realizations Using TPA51betaT for 100,000 yr With and Without Volcanism.

16. Screenprint Showing Peak Mean Dose of 8.6 mrem/yr Versus 820 mrem/yr for Realization 343 of 450 Using TPA51betaT for 100,000 yr Without and With Faulting, Respectively.

17. Differences Between Sampled Parameters in the *lhs.inp* Files for TPA51betaT and TPA51betaY.

18. Plots of Expected Dose from 500 Realizations Using TPA51betaT and TPA51betaY and LHS Seeds for 10,000 yr.

19. Plots of Expected Dose from 500 Realizations Using TPA51betaT and TPA51betaY and LHS Seeds for 100,000 yr.

20. Explanation for Differences in the GW, GS, and GWGS Expected Dose From TPA4.1j and TPA5.1betaT.

21. Plot of Expected Dose (GW, GS, and GWGS) From 401 Realizations Using TPA51betaT and Maximum Time for the Igneous Event of 10,000, and 100,000 yr and 100 yr (Constant).

22. Plots of Expected Dose From 500 Realizations Using TPA51betaY and LHS Seeds With and Without Seismicity For 10,000 yr.

23. Plots of Expected Dose From 500 Realizations Using TPA51betaY and LHS Seeds With and Without Seismicity For 100,000 yr.

24. Plot of Mean Dose from 401 Realizations Using TPA51betaT and LHS Seeds for 10,000 yr.

25. Plot of Mean Dose from 401 Realizations Using TPA51betaT and LHS Seeds for 100,000 yr.

26. Plot of Fraction Contribution to Peak Mean Dose by Realization from 401 Realizations Using TPA51betaT and LHS Seeds for 10,000 yr.

27. Plot of Fraction Contribution to Peak Mean Dose by Realization from 500 Realizations Using TPA51betaT and LHS Seeds for 10,000 yr.

28. Understanding Results Using TPA5.1betaT from Realization 165 of 500 and LHS Seed1 for 10,000 yr.

29. More Understanding Results Using TPA5.1betaT from Realization 165 of 500 and LHS Seed1 for 10,000 yr.

1. S-4 Test Matrix. The matrix lists TPA Version 5.1betaT code settings used in the S-4 testing. These tests are consistent with the Description of Tests presented in the Test Procedure section of this attachment. All of the proposed tests in this table were completed and the results are summarized in the Discussion of Results section. Note that, in the table below, the Reference case contains the LHS seed value from the Reference case input file, and LHS Seed 1 through Seed 4 contain four different modified values. Hence, this analysis considers is a total of five different LHS seed values.

10,000 yr

		LHS Seeds				SEISMIC Seeds				Faulting	Igneous
Realizations	**Reference**	**Seed 1**	**Seed 2**	**Seed 3**	**Seed 4**	**Seed 1**	**Seed 2**	**Seed 3**	**Seed 4**	**Reference**	**Reference**
401	v	v	v	v	v	v	**v**	v	v	v	v
450	v	v	v	v	v	v	**v**	v	v	v	v
500	v	v	v	v	v	v	**v**	v	v	v	v
600	v	v	v	v	v	v	**v**	v	v	v	v
700	v	v	v	v	v	v	**v**	v	v	v	v
800	v	v	v	v	v	v	**v**	v	v	**v**	**v**
900	v	v	v	v	v	v	**v**	v	v	**v**	**v**
1000	v	v	v	v	v	v	**v**	v	v	**v**	**v**

100,000 yr

		LHS Seeds				SEISMIC Seeds				Faulting	Igneous
Realizations	**Reference**	**Seed 1**	**Seed 2**	**Seed 3**	**Seed 4**	**Seed 1**	**Seed 2**	**Seed 3**	**Seed 4**	**Reference**	**Reference**
401	v	v	v	v	v	v	**v**	v	v	v	v
450	v	v	v	v	v	**v**	**v**	**v**	**v**	v	**v**
500	v	**v**	**v**	**v**	**v**	**v**	**v**	**v**	**v**	v	v
600	v	v	v	v	v	v	**v**	v	v	v	**v**
700	v	v	v	v	v	**v**	**v**	**v**	**v**	v	**v**
800	v	v	v	v	v	v	v	v	v	**v**	v
900	v	**v**	v	**v**	v	**v**	**v**	**v**	**v**	**v**	**v**
1000	v	v	v	v	v	v	**v**	v	v	**v**	**v**

1,000,000 yr

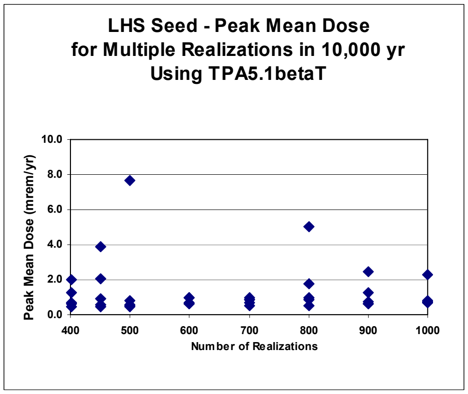
		LHS Seeds			SEISMIC Seeds			Faulting	Igneous
Realizations	**Reference**	**Seed 1**	**Seed 2**	**Seed 3**	**Seed 1**	**Seed 2**	**Seed 3**	**Reference**	**Reference**
401	v	v	v	v	v	v	**v**	v	v
600	v	v	v	v	v	v	**v**	v	v
1000	v	v	v	v	v	v	**v**	v	v

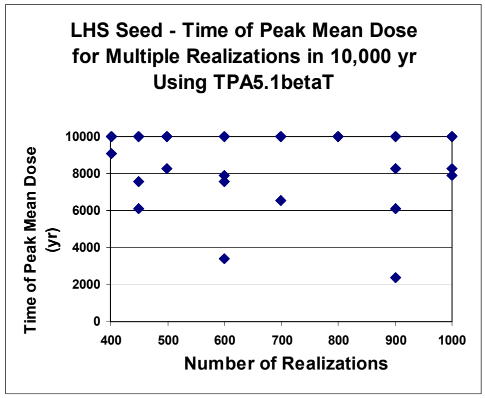
v	finished

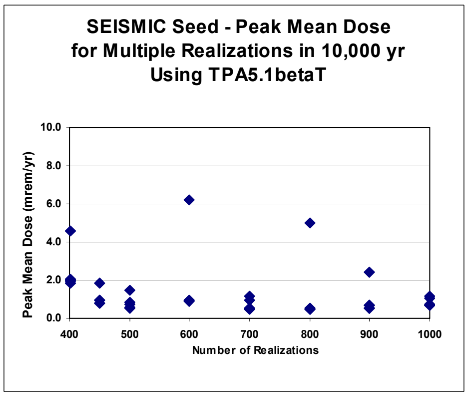
Simulation Time	**Number of Time steps (Reference - 401 Realizations)**				
10,000 yr	401 v	**201 v**	101 v	-	-
100,000 yr	801 v	**401 v**	201 v	101 v	-
1,000,000 yr	**5001 v**	2501 v	1001 v	501 v	201 v

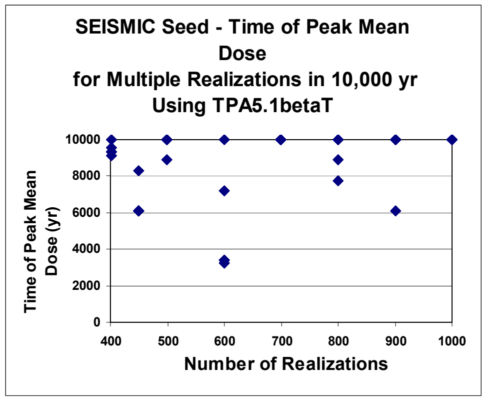
bold = reference number of time steps

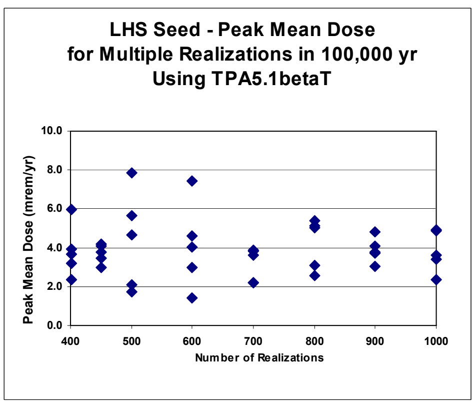
2. Plots Showing Basecase Peak Mean Dose for Multiple Realization TPA Code Runs with 10,000, 100,000, and 1,000,000 yrs and Using LHS and SEISMIC Seeds.

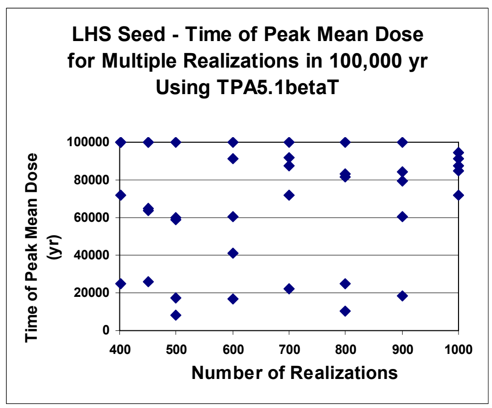


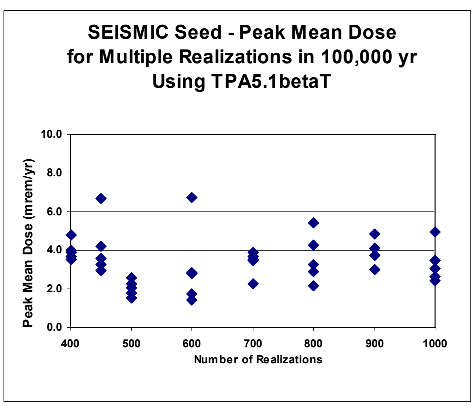


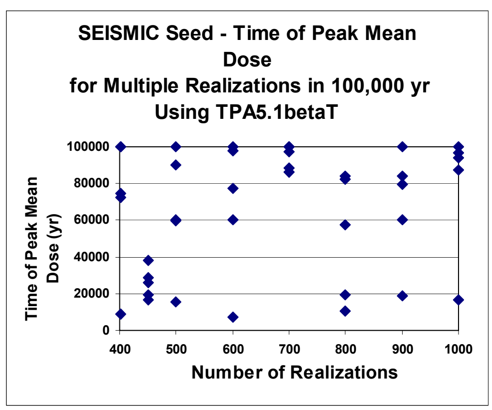


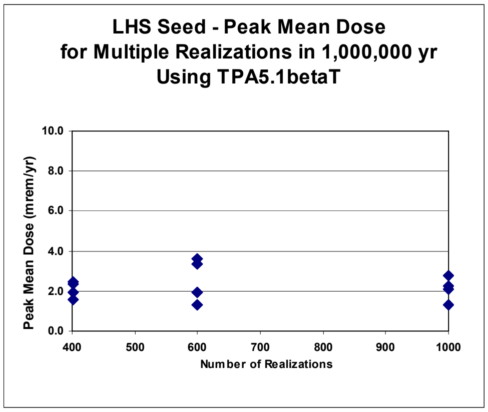


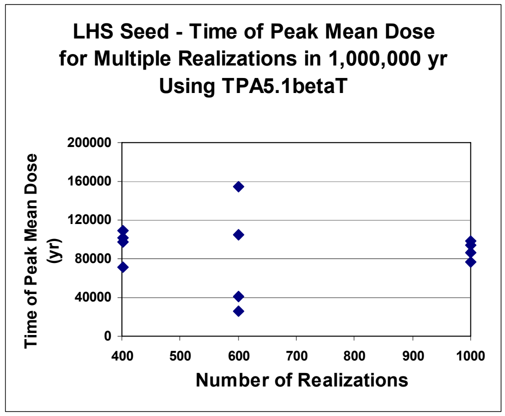


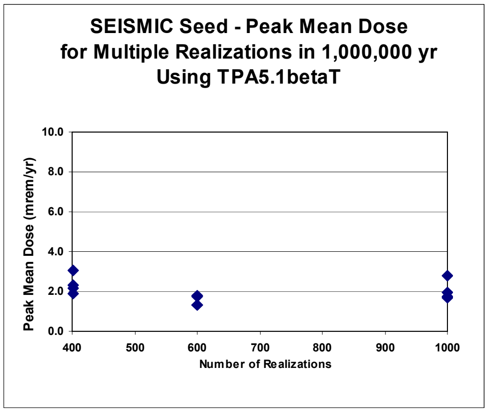


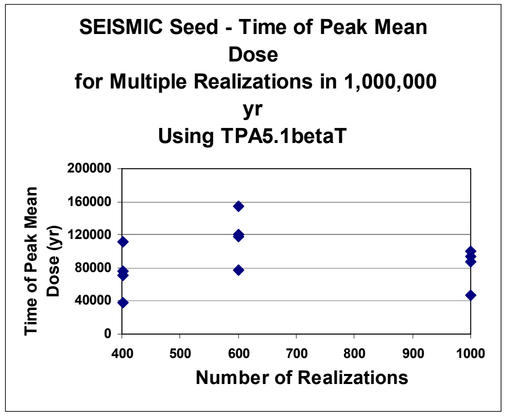





LHS Seed - Peak Mean Dose
for Multiple Realizations in 1,000,000 yr
Using TPA5.1betaT
Peak Mean Dose (mrem/yr)
10.0
8.0
6.0
4.0
2.0
0.0
400
500
600
700
800
900
1000
Number of Realizations


LHS Seed - Time of Peak Mean Dose
for Multiple Realizations in 1,000,000 yr
Using TPA5.1betaT
Time of Peak Mean Dose (yr)
200000
160000
120000
80000
40000
0
400
500
600
700
800
900
1000
Number of Realizations


SEISMIC Seed - Peak Mean Dose
for Multiple Realizations in 1,000,000 yr
Using TPA5.1betaT
Peak Mean Dose (mrem/yr)
10.0
8.0
6.0
4.0
2.0
0.0
400
500
600
700
800
900
1000
Number of Realizations


SEISMIC Seed - Time of Peak Mean Dose
for Multiple Realizations in 1,000,000 yr
Using TPA5.1betaT
Time of Peak Mean Dose (yr)
200000
160000
120000
80000
40000
0
400
500
600
700
800
900
1000
Number of Realizations

3. Tables Showing Basecase Peak Mean Dose for Multiple Realization TPA Code Runs with 10,000, 100,000, and 1,000,000 yrs and Using LHS and SEISMIC Seeds.

TPA Version 5.1betaT - LHS Seed

Maximum Time = 10,000 yr

	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
Reference	401	2.00	10,000
Seed 1	401	0.66	10,000
Seed 2	401	0.60	10,000
Seed 3	401	1.25	10,000
Seed 4	401	0.47	9,107
Reference	450	0.92	6,113
Seed 1	450	0.49	10,000
Seed 2	450	3.87	7,551
Seed 3	450	2.04	10,000
Seed 4	450	0.56	10,000
Reference	500	0.82	10,000
Seed 1	500	7.66	8,293
Seed 2	500	0.45	10,000
Seed 3	500	0.50	10,000
Seed 4	500	0.54	10,000
Reference	600	0.94	3,384
Seed 1	600	0.65	10,000
Seed 2	600	0.68	7,551
Seed 3	600	0.63	10,000
Seed 4	600	0.97	7,914
Reference	700	0.53	10,000
Seed 1	700	0.70	10,000
Seed 2	700	0.99	6,560
Seed 3	700	0.87	10,000
Seed 4	700	0.83	10,000
Reference	800	5.01	10,000
Seed 1	800	1.78	10,000
Seed 2	800	0.83	10,000
Seed 3	800	1.00	10,000
Seed 4	800	0.51	10,000
Reference	900	2.44	6,113
Seed 1	900	0.74	2,363
Seed 2	900	0.64	10,000
Seed 3	900	0.62	8,293
Seed 4	900	1.26	10,000
Reference	1000	0.68	10,000
Seed 1	1000	0.67	7,914
Seed 2	1000	2.28	10,000
Seed 3	1000	0.80	8,293
Seed 4	1000	0.74	10,000

TPA Version 5.1betaT - SEISMIC Seed

Maximum Time = 10,000 yr

	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
Reference	401	2.00	10,000
Seed 1	401	4.59	9,107
Seed 2	401	2.06	9,323
Seed 3	401	1.84	9,323
Seed 4	401	1.96	9,543
Reference	450	0.92	6,113
Seed 1	450	0.80	6,113
Seed 2	450	1.86	8,293
Seed 3	450	0.77	6,113
Seed 4	450	0.95	6,113
Reference	500	0.82	10,000
Seed 1	500	0.76	8,897
Seed 2	500	1.46	10,000
Seed 3	500	0.53	10,000
Seed 4	500	0.59	10,000
Reference	600	0.94	3,384
Seed 1	600	0.90	3,384
Seed 2	600	0.94	10,000
Seed 3	600	0.89	3,227
Seed 4	600	6.20	7,205
Reference	700	0.53	10,000
Seed 1	700	1.15	10,000
Seed 2	700	0.52	10,000
Seed 3	700	0.93	10,000
Seed 4	700	0.46	10,000
Reference	800	5.01	10,000
Seed 1	800	0.47	7,730
Seed 2	800	0.48	8,897
Seed 3	800	0.50	10,000
Seed 4	800	0.55	10,000
Reference	900	2.44	6,113
Seed 1	900	0.53	10,000
Seed 2	900	0.69	10,000
Seed 3	900	0.54	10,000
Seed 4	900	0.69	10,000
Reference	1000	0.68	10,000
Seed 1	1000	0.68	10,000
Seed 2	1000	1.15	10,000
Seed 3	1000	0.73	10,000
Seed 4	1000	1.04	10,000

TPA Version 5.1betaT - LHS Seed

Maximum Time = 100,000 yr

	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
Reference	401	3.91	72,100
Seed 1	401	3.67	24,850
Seed 2	401	5.99	100,000
Seed 3	401	3.18	100,000
Seed 4	401	2.34	100,000
Reference	450	2.97	26,200
Seed 1	450	3.48	100,000
Seed 2	450	4.19	64,900
Seed 3	450	3.76	63,550
Seed 4	450	4.10	100,000
Reference	500	2.07	59,950
Seed 1	500	7.87	8,293
Seed 2	500	5.65	17,200
Seed 3	500	1.73	100,000
Seed 4	500	4.66	59,050
Reference	600	1.40	60,400
Seed 1	600	7.43	100,000
Seed 2	600	4.05	16,750
Seed 3	600	4.62	41,050
Seed 4	600	3.00	91,450
Reference	700	3.88	100,000
Seed 1	700	2.21	87,400
Seed 2	700	3.60	91,900
Seed 3	700	2.20	71,650
Seed 4	700	3.81	22,150
Reference	800	5.41	10,450
Seed 1	800	5.04	83,350
Seed 2	800	2.57	24,850
Seed 3	800	3.09	100,000
Seed 4	800	5.13	81,550
Reference	900	4.83	84,250
Seed 1	900	3.72	18,550
Seed 2	900	3.75	100,000
Seed 3	900	3.02	60,400
Seed 4	900	4.11	79,300
Reference	1000	4.93	87,400
Seed 1	1000	2.36	94,600
Seed 2	1000	4.88	84,700
Seed 3	1000	3.40	91,450
Seed 4	1000	3.64	71,650

TPA Version 5.1betaT - SEISMIC Seed

Maximum Time = 100,000 yr

	Realizations	**Peak Mean Dose (mrem/yr)**	**Time of Peak Mean Dose (yr)**
Reference	401	3.91	72,100
Seed 1	401	4.79	9,107
Seed 2	401	3.70	100,000
Seed 3	401	4.01	100,000
Seed 4	401	3.51	74,350
Reference	450	2.97	26,200
Seed 1	450	3.58	16,300
Seed 2	450	3.25	19,450
Seed 3	450	6.66	38,350
Seed 4	450	4.21	28,900
Reference	500	2.07	59,950
Seed 1	500	1.77	59,500
Seed 2	500	2.58	15,400
Seed 3	500	1.51	90,100
Seed 4	500	2.24	100,000
Reference	600	1.40	60,400
Seed 1	600	1.72	100,000
Seed 2	600	2.82	77,500
Seed 3	600	2.77	97,750
Seed 4	600	6.73	7,376
Reference	700	3.88	100,000
Seed 1	700	2.26	97,300
Seed 2	700	3.45	86,050
Seed 3	700	3.70	88,300
Seed 4	700	3.53	100,000
Reference	800	5.41	10,450
Seed 1	800	2.91	83,800
Seed 2	800	3.27	57,250
Seed 3	800	2.16	82,450
Seed 4	800	4.24	19,450
Reference	900	4.83	84,250
Seed 1	900	3.72	18,550
Seed 2	900	3.75	100,000
Seed 3	900	3.02	60,400
Seed 4	900	4.11	79,300
Reference	1000	4.93	87,400
Seed 1	1000	2.63	93,700
Seed 2	1000	3.50	100,000
Seed 3	1000	3.05	96,850
Seed 4	1000	2.41	16,300

TPA Version 5.1betaT - LHS Seed

Maximum Time = 1,000,000 yr

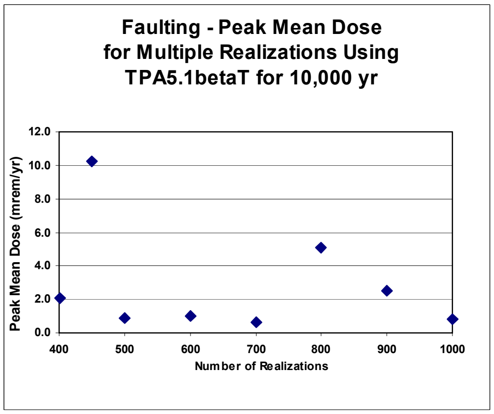
	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
Reference	401	2.34	71,460
Seed 1	401	1.57	109,400
Seed 2	401	2.47	97,040
Seed 3	401	1.95	101,600
Reference	600	1.30	154,200
Seed 1	600	3.60	105,300
Seed 2	600	1.94	25,880
Seed 3	600	3.33	40,940
Reference	1000	2.78	86,720
Seed 1	1000	1.29	93,940
Seed 2	1000	2.09	98,070
Seed 3	1000	2.28	76,820

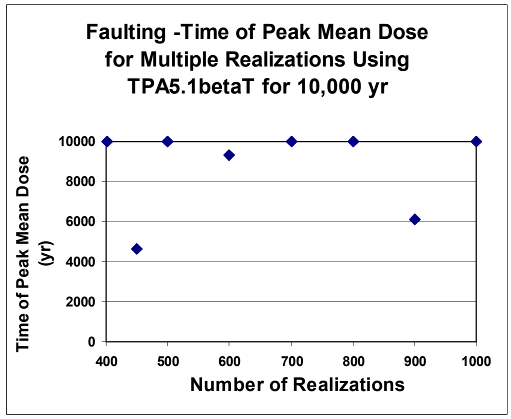
TPA Version 5.1betaT - SEISMIC Seed

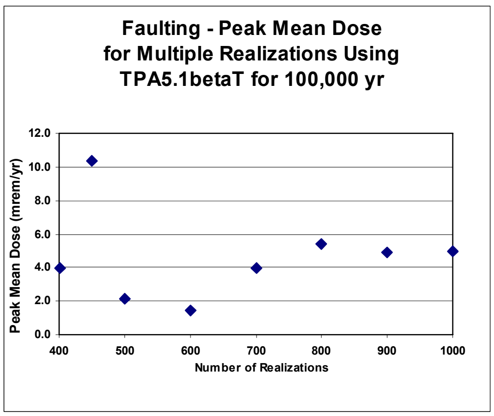
Maximum Time = 1,000,000 yr

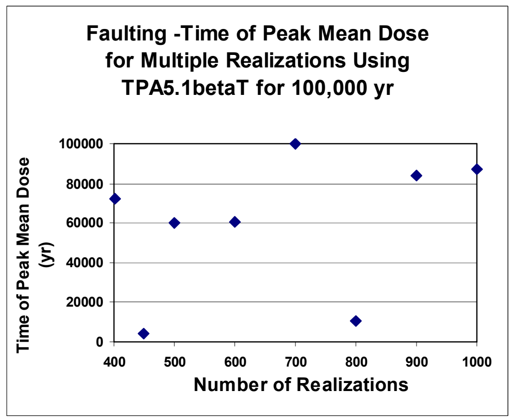
	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
Reference	401	2.34	71,460
Seed 1	401	3.03	38,460
Seed 2	401	1.90	111,700
Seed 3	401	2.15	76,410
Reference	600	1.30	154,200
Seed 1	600	1.30	120,300
Seed 2	600	1.73	77,650
Seed 3	600	1.77	117,200
Reference	1000	2.78	86,720
Seed 1	1000	1.92	46,300
Seed 2	1000	1.67	99,510
Seed 3	1000	1.72	93,740

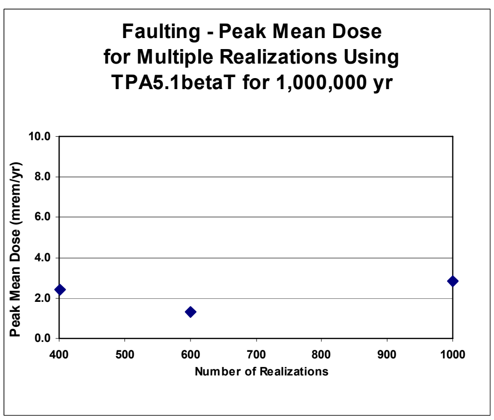
4. Plots Showing Faulting and Igneous (GW, GS, and GWGS) Peak Mean Dose for Multiple Realization TPA Code Runs with 10,000, 100,000, and 1,000,000 yrs.

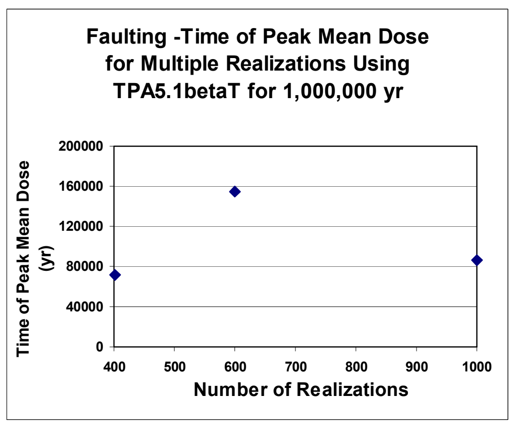


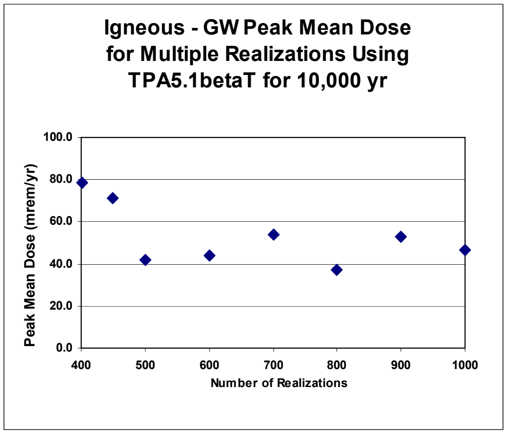


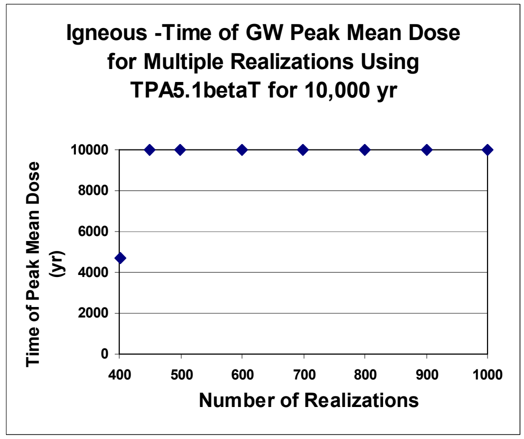


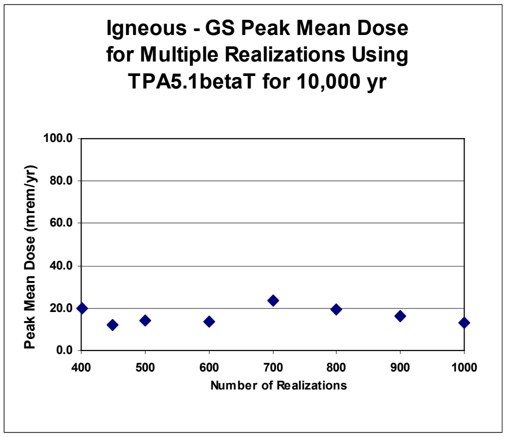


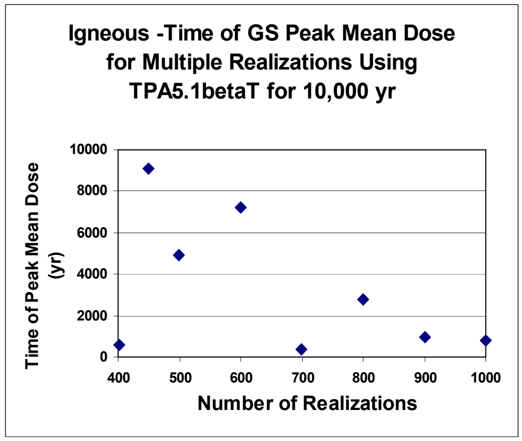


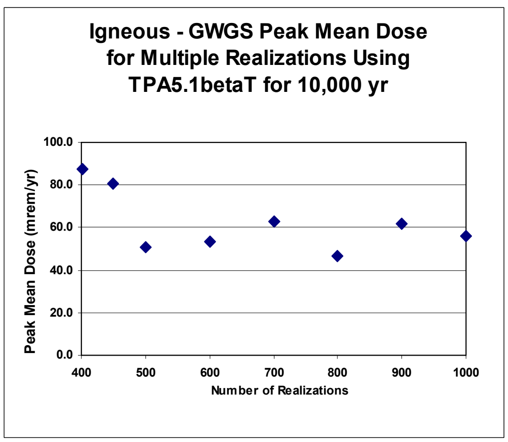


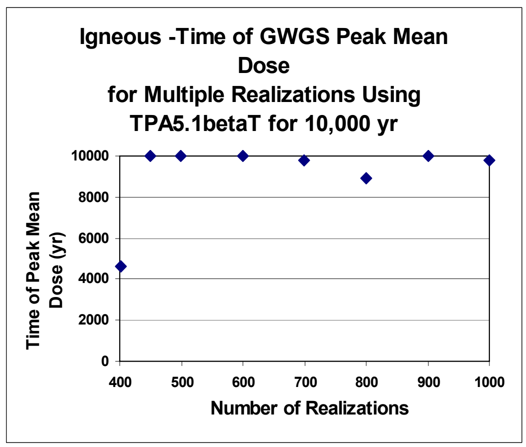

Igneous - GW Peak Mean Dose for Multiple Realizations Using TPA5.1betaT for 10,000 yr
Peak Mean Dose (mrem/yr)
Number of Realizations

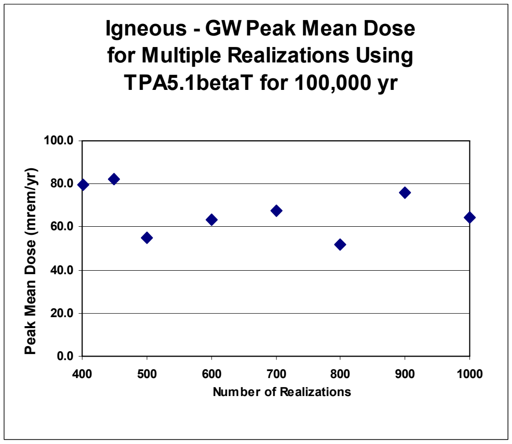

Igneous -Time of GW Peak Mean Dose for Multiple Realizations Using TPA5.1betaT for 10,000 yr
Time of Peak Mean Dose (yr)
Number of Realizations


Igneous - GS Peak Mean Dose for Multiple Realizations Using TPA5.1betaT for 10,000 yr
Peak Mean Dose (mrem/yr)
Number of Realizations

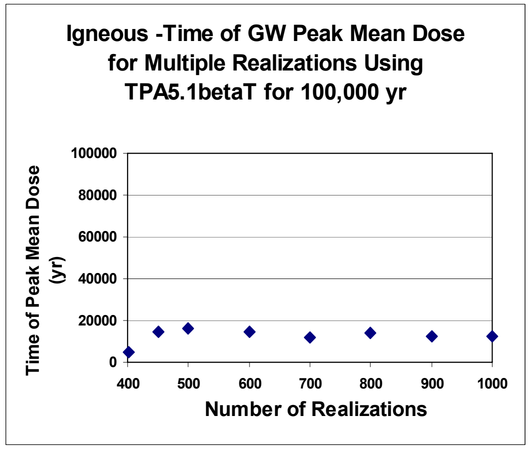

Igneous -Time of GS Peak Mean Dose for Multiple Realizations Using TPA5.1betaT for 10,000 yr
Time of Peak Mean Dose (yr)
Number of Realizations


Igneous - GWGS Peak Mean Dose for Multiple Realizations Using TPA5.1betaT for 10,000 yr
Peak Mean Dose (mrem/yr)
Number of Realizations

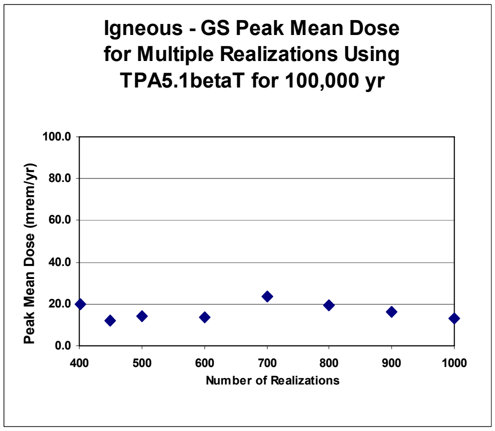

Igneous -Time of GWGS Peak Mean Dose for Multiple Realizations Using TPA5.1betaT for 10,000 yr
Time of Peak Mean Dose (yr)
Number of Realizations



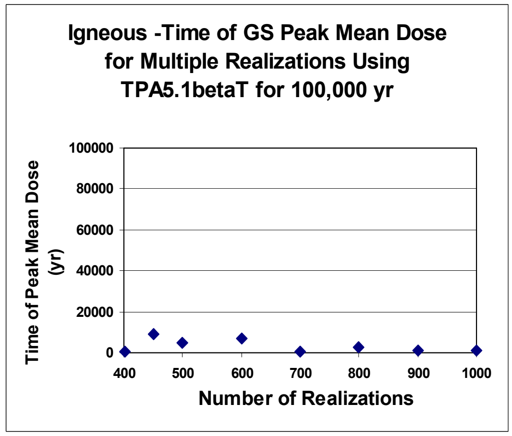
Igneous - GW Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 100,000 yr
Peak Mean Dose (mrem/yr)
100.0
80.0
60.0
40.0
20.0
0.0
400
500
600
700
800
900
1000
Number of Realizations



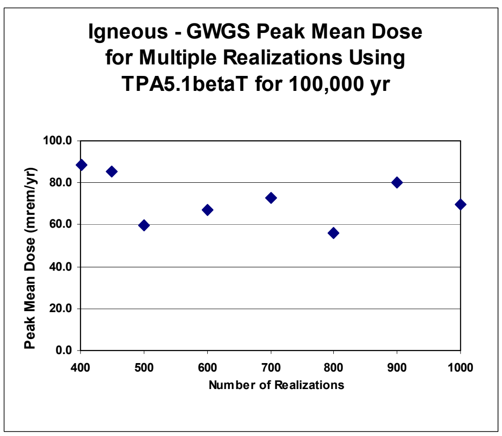
Igneous -Time of GW Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 100,000 yr
Time of Peak Mean Dose (yr)
100000
80000
60000
40000
20000
0
400
500
600
700
800
900
1000
Number of Realizations



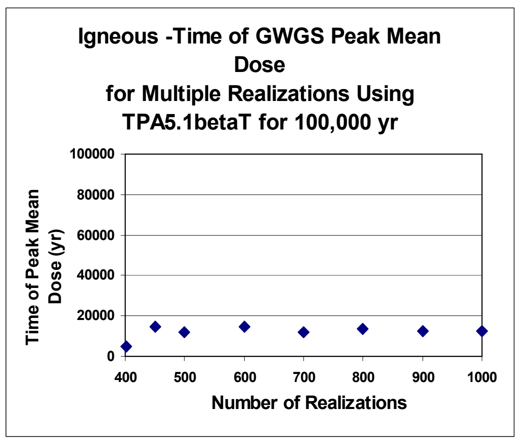
Igneous - GS Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 100,000 yr
Peak Mean Dose (mrem/yr)
100.0
80.0
60.0
40.0
20.0
0.0
400
500
600
700
800
900
1000
Number of Realizations



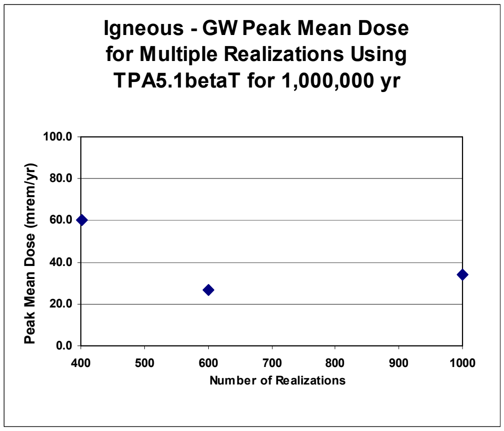
Igneous -Time of GS Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 100,000 yr
Time of Peak Mean Dose (yr)
100000
80000
60000
40000
20000
0
400
500
600
700
800
900
1000
Number of Realizations

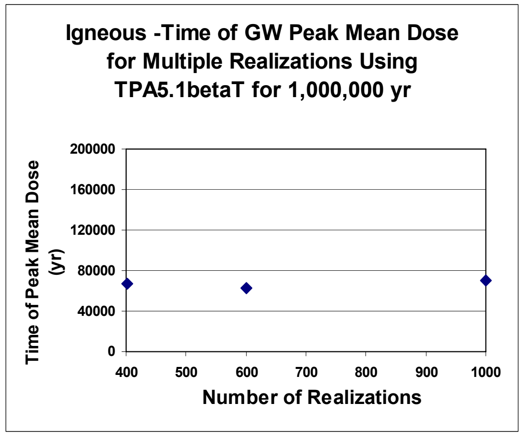


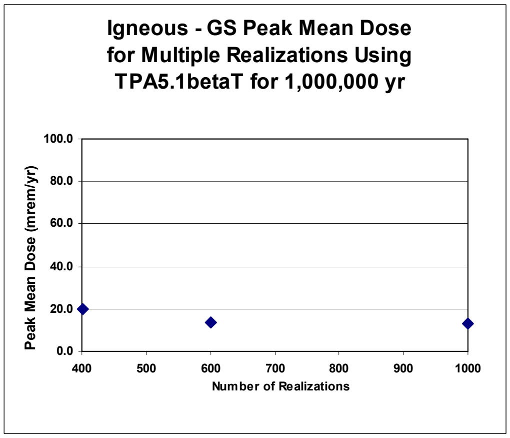
Igneous - GWGS Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 100,000 yr
Peak Mean Dose (mrem/yr)
100.0
80.0
60.0
40.0
20.0
0.0
400
500
600
700
800
900
1000
Number of Realizations

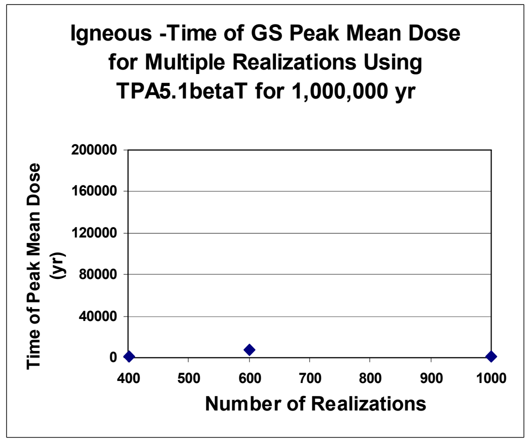


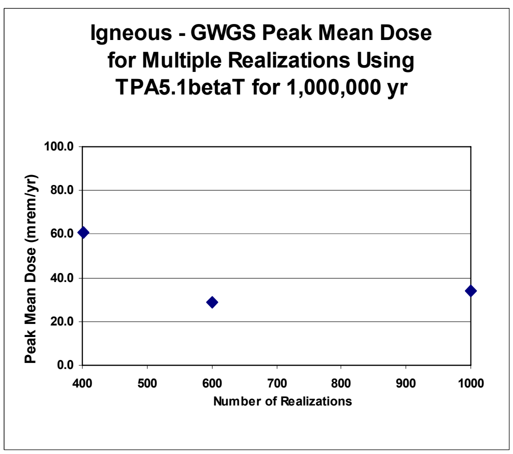
Igneous -Time of GWGS Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 100,000 yr
Time of Peak Mean Dose (yr)
100000
80000
60000
40000
20000
0
400
500
600
700
800
900
1000
Number of Realizations

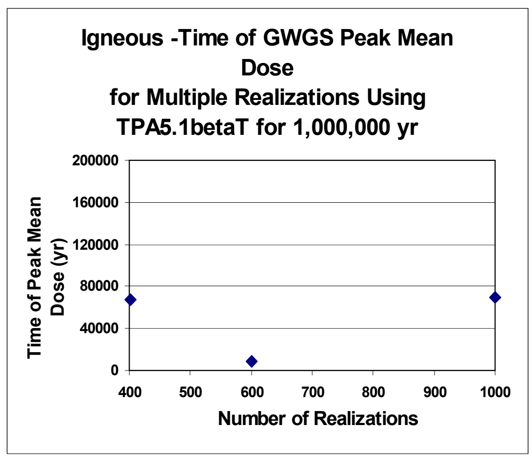

Igneous - GW Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 1,000,000 yr
Peak Mean Dose (mrem/yr)
Number of Realizations


Igneous -Time of GW Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 1,000,000 yr
Time of Peak Mean Dose (yr)
Number of Realizations


Igneous - GS Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 1,000,000 yr
Peak Mean Dose (mrem/yr)
Number of Realizations


Igneous -Time of GS Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 1,000,000 yr
Time of Peak Mean Dose (yr)
Number of Realizations


Igneous - GWGS Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 1,000,000 yr
Peak Mean Dose (mrem/yr)
Number of Realizations


Igneous -Time of GWGS Peak Mean Dose
for Multiple Realizations Using
TPA5.1betaT for 1,000,000 yr
Time of Peak Mean Dose (yr)
Number of Realizations

5. Tables Showing Faulting and Igneous (GW, GS, and GWGS) Peak Mean Dose for Multiple Realization TPA Code Runs with 10,000, 100,000, and 1,000,000 yrs.

TPA Version 5.1betaT - Faulting

	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
10,000	401	2.08	10,000
100,000	401	3.99	72,100
1,000,000	401	2.39	71,460
10,000	450	10.27	4,607
100,000	450	10.34	4,499
10,000	500	0.87	10,000
100,000	500	2.12	59,950
10,000	600	1.03	9,323
100,000	600	1.44	60,400
1,000,000	600	1.31	154,400
10,000	700	0.62	10,000
100,000	700	3.94	100,000
10,000	800	5.12	10,000
100,000	800	5.43	10,450
10,000	900	2.48	6,113
100,000	900	4.87	84,250
10,000	1000	0.81	10,000
100,000	1000	4.99	87,400
1,000,000	1000	2.81	86,720

TPA Version 5.1betaT - Igneous (Groundwater Dose Only)

	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
10,000	401	78.28	4,717
100,000	401	79.84	4,717
1,000,000	401	60.27	67,540
10,000	450	71.19	10,000
100,000	450	82.22	14,500
10,000	500	42.07	10,000
100,000	500	54.88	16,300
10,000	600	44.17	10,000
100,000	600	63.38	14,500
1,000,000	600	26.69	63,210
10,000	700	53.76	10,000
100,000	700	67.43	11,800
10,000	800	37.28	10,000
100,000	800	52.07	14,050
10,000	900	52.93	10,000
100,000	900	75.75	12,700
10,000	1000	46.59	10,000
100,000	1000	64.51	12,250
1,000,000	1000	33.96	70,020

TPA Version 5.1betaT - Igneous (Groundsurface Dose Only)

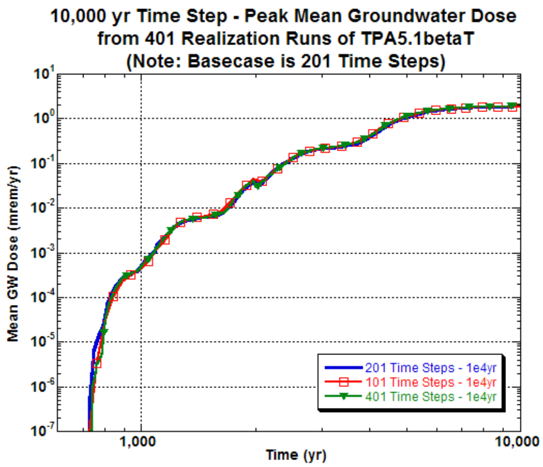
	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
10,000	401	19.89	575
100,000	401	19.89	575
1,000,000	401	19.89	575
10,000	450	11.80	9,107
100,000	450	11.80	9,107
10,000	500	14.25	4,945
100,000	500	14.25	4,945
10,000	600	13.51	7,205
100,000	600	13.51	7,205
1,000,000	600	13.51	7,205
10,000	700	23.61	377
100,000	700	23.61	377
10,000	800	19.41	2,796
100,000	800	19.41	2,796
10,000	900	16.36	947
100,000	900	16.36	947
10,000	1000	13.23	811
100,000	1000	13.23	811
1,000,000	1000	13.23	811

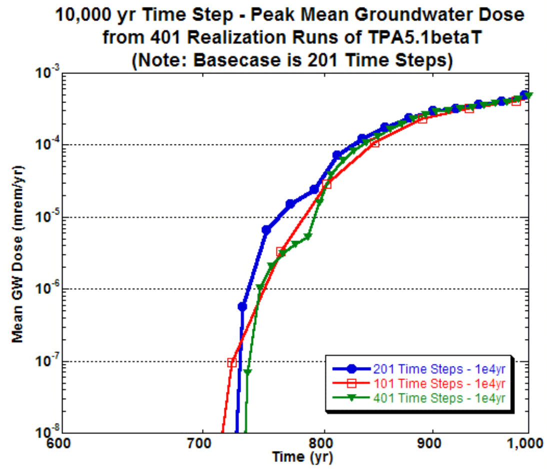
TPA Version 5.1betaT - Igneous (Groundwater & Groundsurface Dose)

	Realizations	Peak Mean Dose (mrem/yr)	Time of Peak Mean Dose (yr)
10,000	401	87.18	4,607
100,000	401	88.46	4,717
1,000,000	401	60.58	67,540
10,000	450	80.40	10,000
100,000	450	85.60	14,500
10,000	500	50.64	10,000
100,000	500	59.78	11,800
10,000	600	53.45	10,000
100,000	600	66.79	14,500
1,000,000	600	28.72	8,293
10,000	700	63.07	9,769
100,000	700	72.89	11,800
10,000	800	46.82	8,897
100,000	800	55.86	13,600
10,000	900	61.77	10,000
100,000	900	80.25	12,700
10,000	1000	56.12	9,769
100,000	1000	69.43	12,250
1,000,000	1000	34.26	70,020

6. Plots of Expected Dose Showing Different Time Steps for 10,000, 100,000, and 1,000,000 yr.

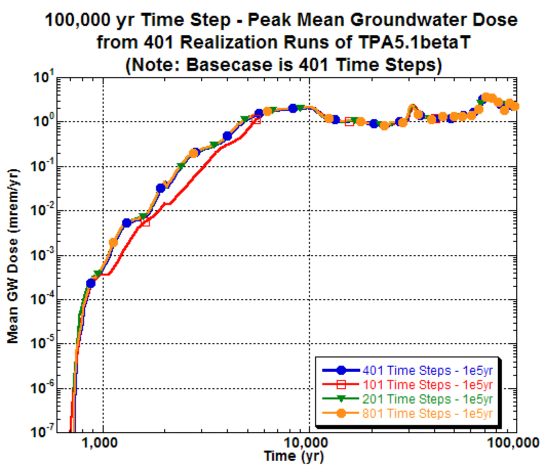
<u>Time Step – 10,000 yr</u>

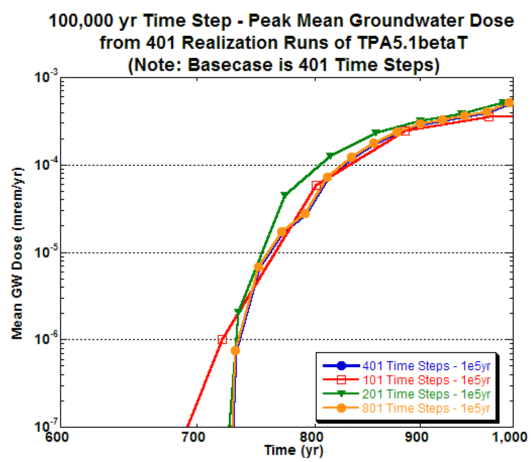




<u>Time Step – 100,000 yr</u>

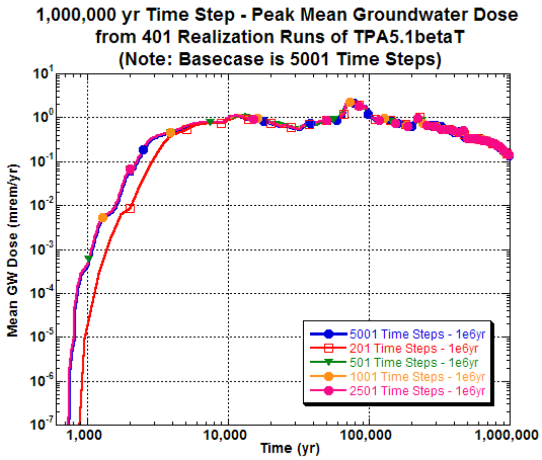
(note: 201 time steps were used in the 10,000 yr compliance period for the 401 and 801 cases)

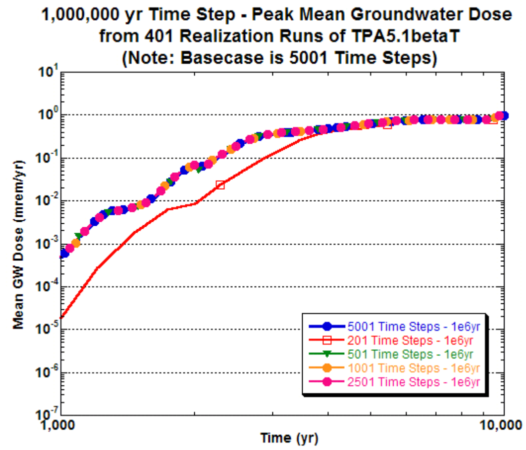


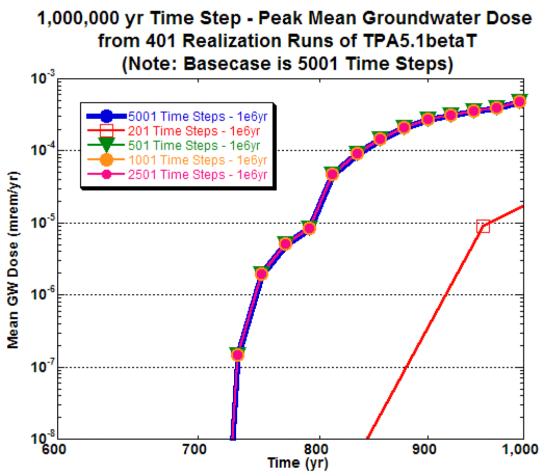


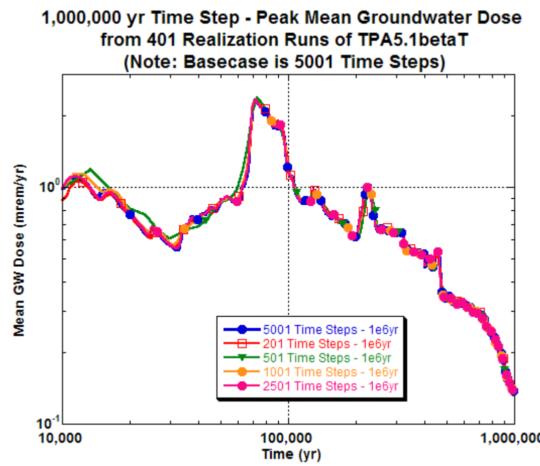
Time Step – 1,000,000 yr

(note: 201 time steps were used in the 10,000 yr compliance period for all cases except 201)



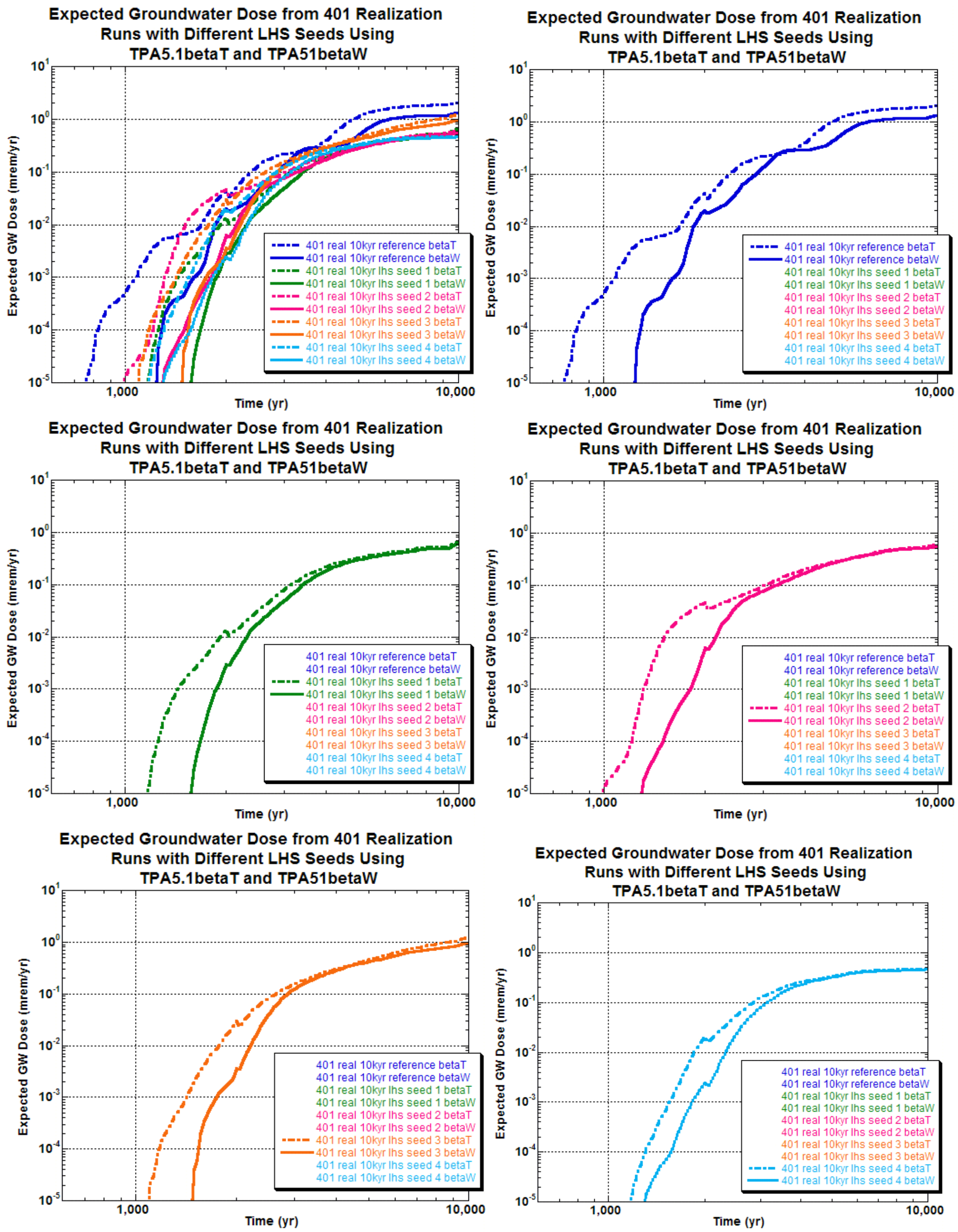






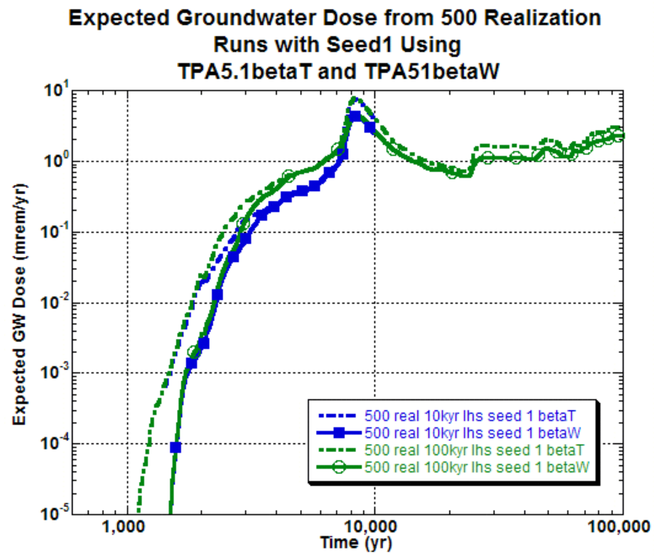
7. Plots of Expected Dose Comparing TPA51betaT and TPA51betaW for 401 Realizations and 10,000 yr to show effects on stability of several software changes made during the validation process.

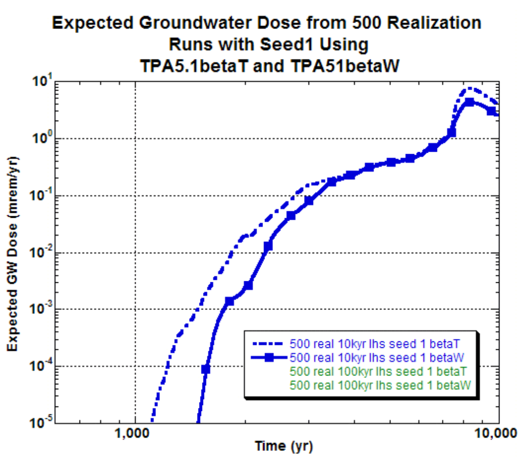
<u>Differences between Results from TPA51betaT and TPA51betaW</u>

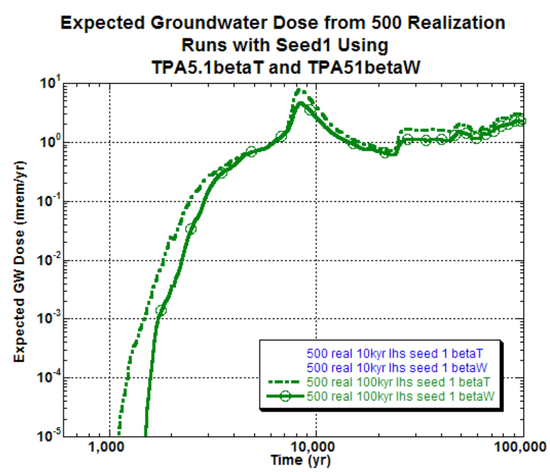


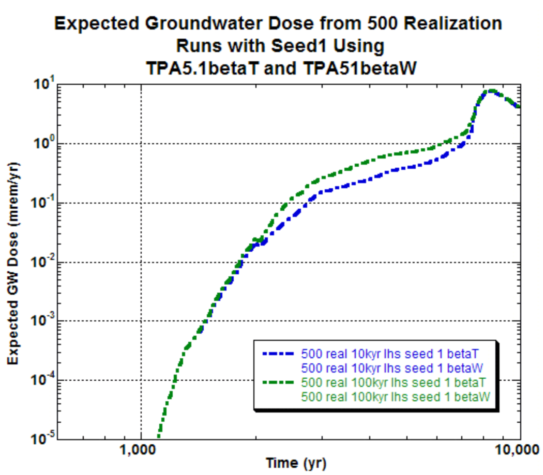
8. Plots of Expected Dose Comparing TPA51betaT and TPA51betaW for 500 Realizations and the Impact of Simulation Time on Results to show effects on stability of several software changes made during the validation process.

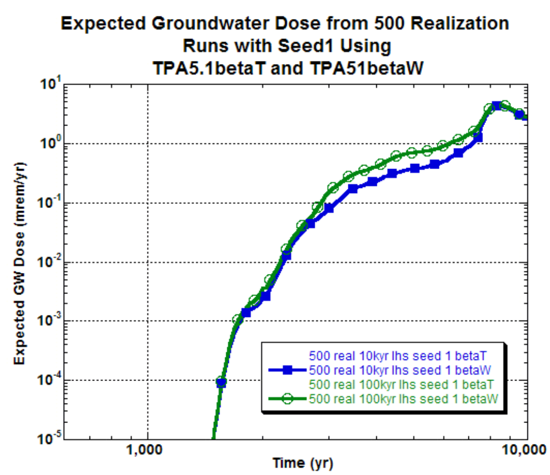
<u>All results (top); differences between results from TPA51betaT and TPA51betaW (middle); and impact of simulation time on results (bottom)</u>





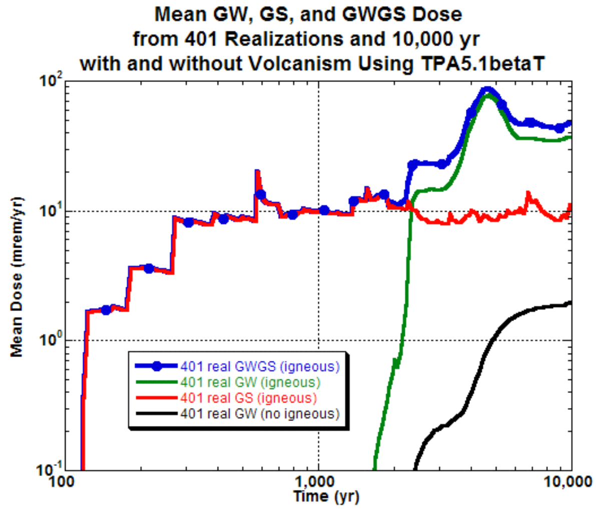


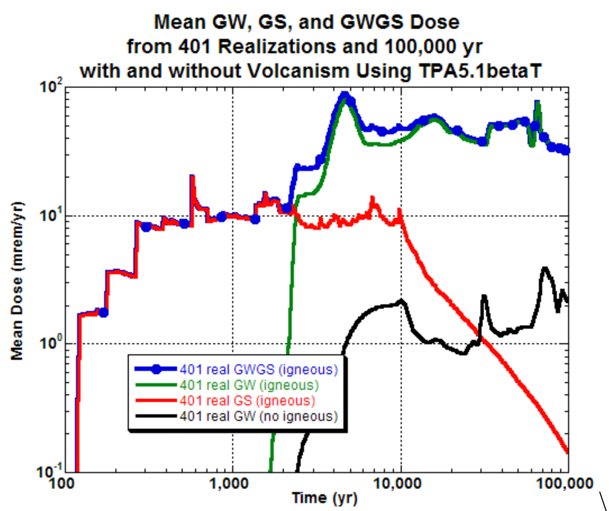


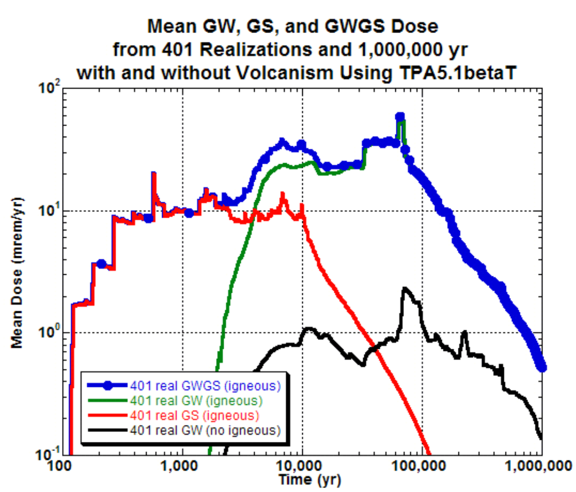


9. Plots of Expected Dose (GW, GS, and GWGS) Using TPA51betaT for 10,000, 100,000, and 1,000,000 yr With and Without Volcanism.

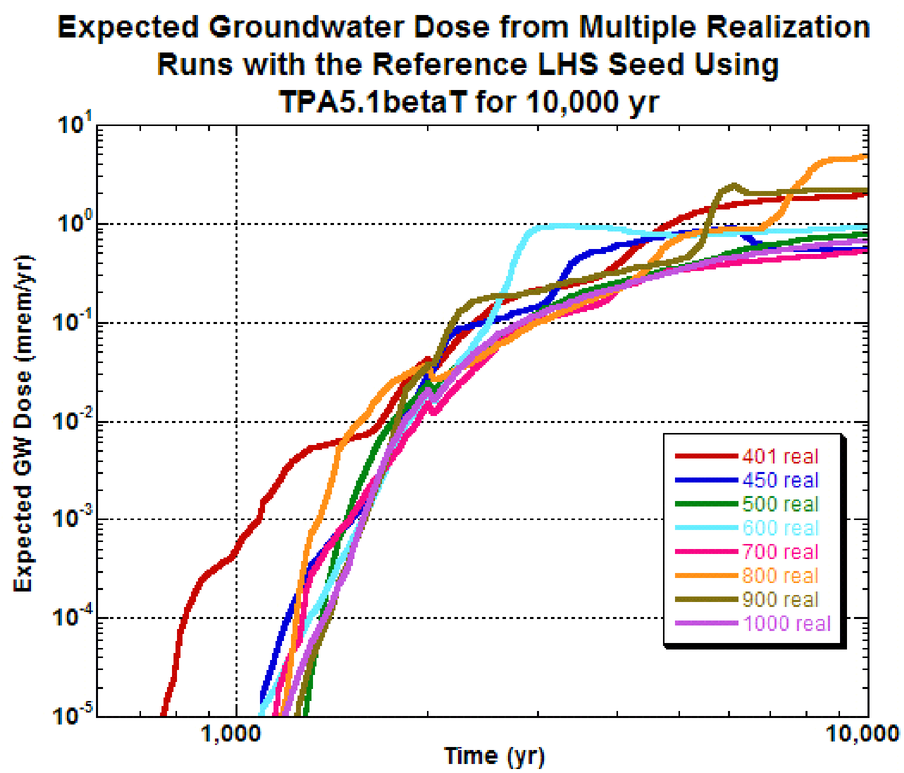
<u>GW, GS, and GWGS doses with and without volcanism (1e4yr, 1e5yr, and 1e6yr)</u>

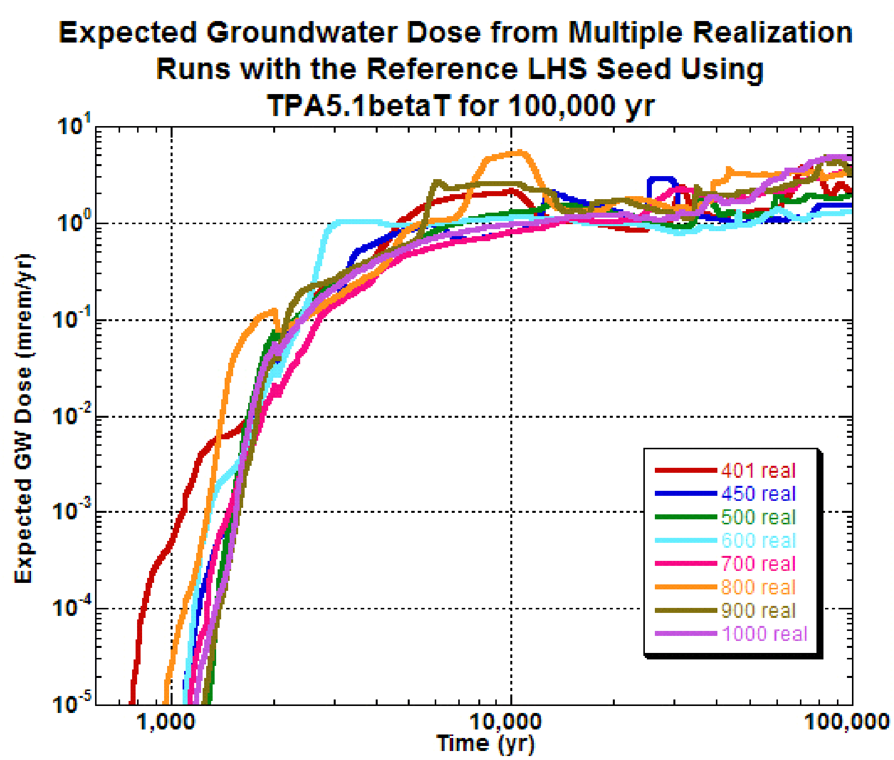




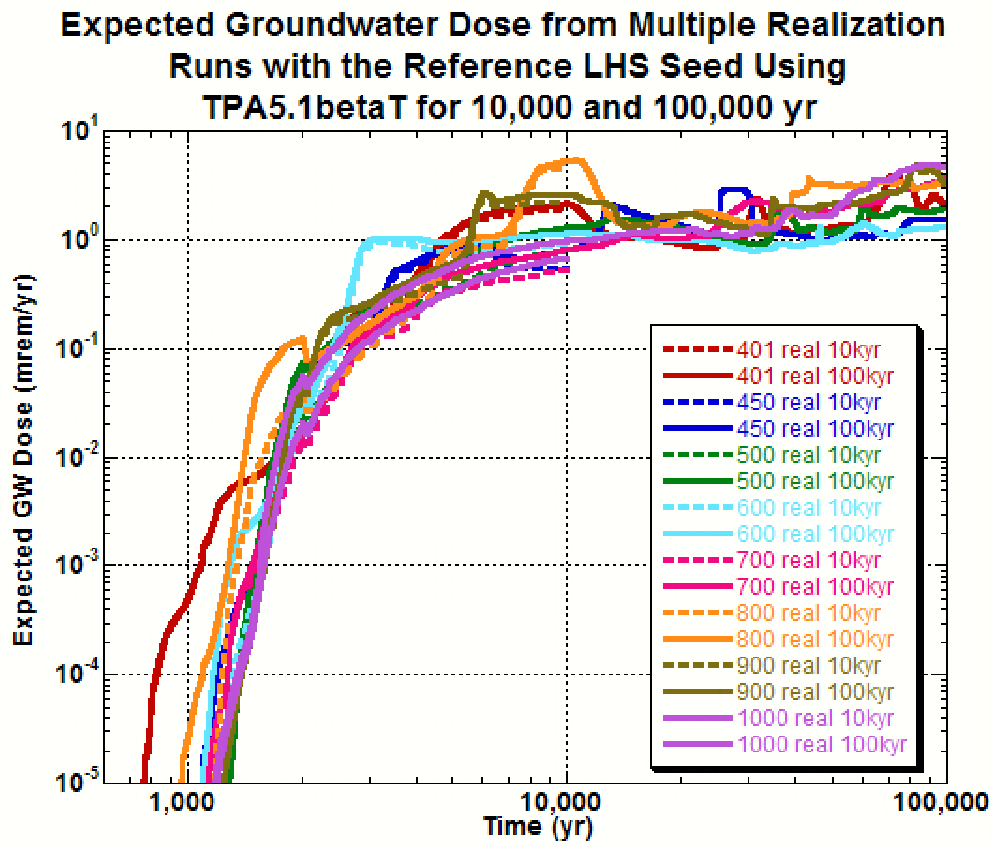


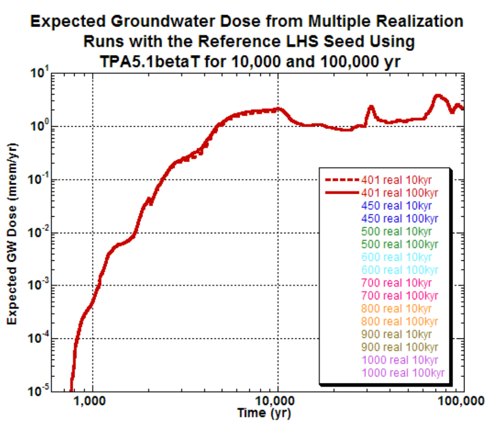
10. Plots of Expected Dose From Multiple Realizations Using TPA51betaT for 10,000, and 100,000 yr With the Reference Seed.

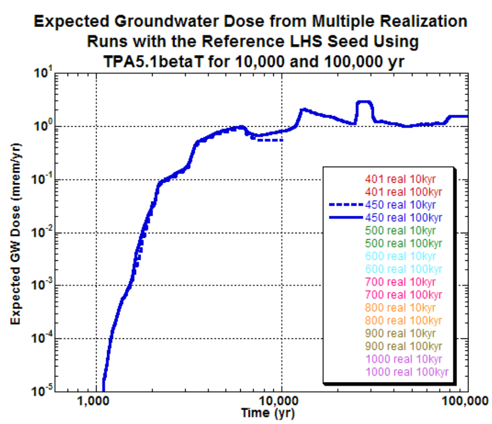


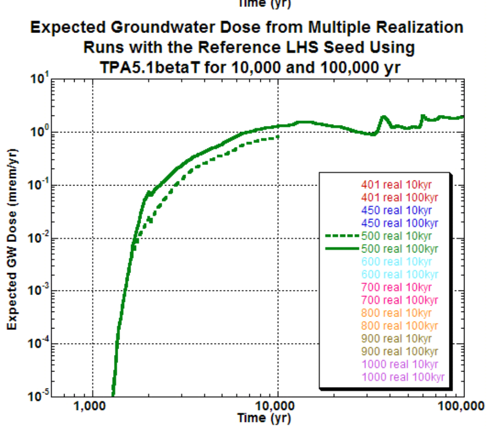


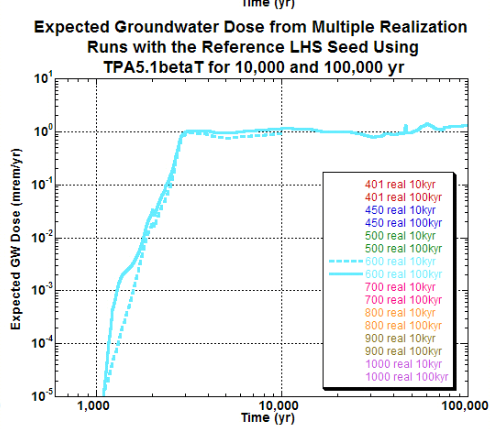
11. Plots of Expected Dose Comparing the Impact of Simulation Time From Multiple Realizations Using TPA51betaT for 10,000, and 100,000 yr With the Reference Seed.

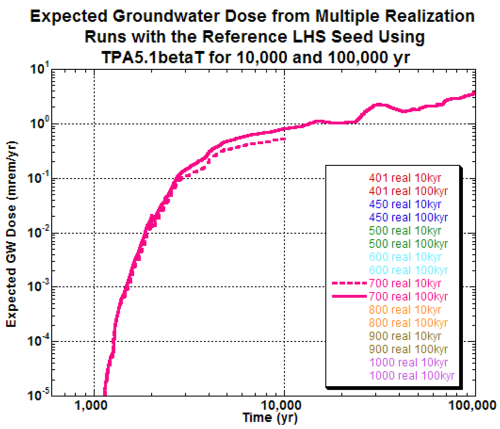


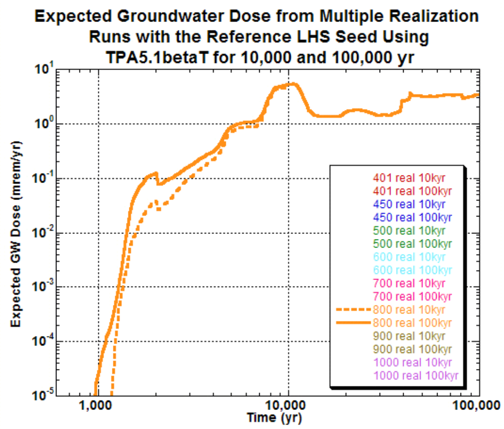









Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed Using TPA5.1betaT for 10,000 and 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
401 real 10kyr
401 real 100kyr
450 real 10kyr
450 real 100kyr
500 real 10kyr
500 real 100kyr
600 real 10kyr
600 real 100kyr
700 real 10kyr
700 real 100kyr
800 real 10kyr
800 real 100kyr
900 real 10kyr
900 real 100kyr
1000 real 10kyr
1000 real 100kyr


Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed Using TPA5.1betaT for 10,000 and 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
401 real 10kyr
401 real 100kyr
450 real 10kyr
450 real 100kyr
500 real 10kyr
500 real 100kyr
600 real 10kyr
600 real 100kyr
700 real 10kyr
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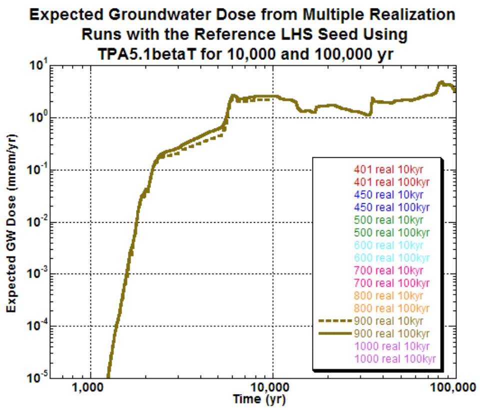
1000 real 10kyr
1000 real 100kyr


Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed Using TPA5.1betaT for 10,000 and 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
401 real 10kyr
401 real 100kyr
450 real 10kyr
450 real 100kyr
500 real 10kyr
500 real 100kyr
600 real 10kyr
600 real 100kyr
700 real 10kyr
700 real 100kyr
800 real 10kyr
800 real 100kyr
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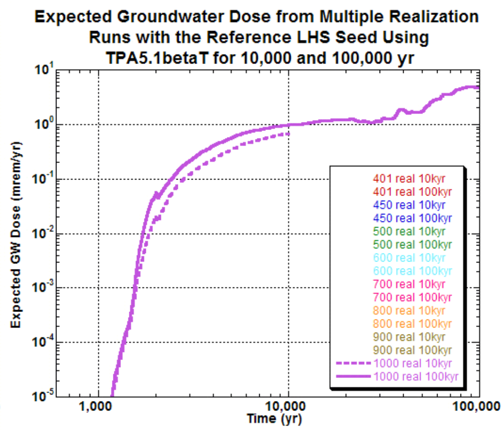
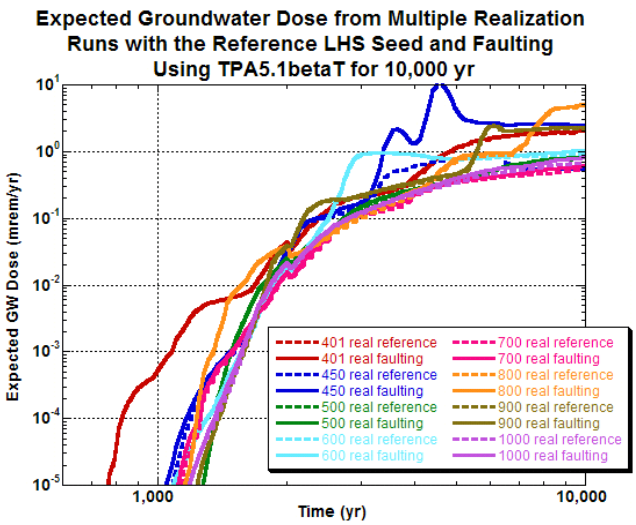
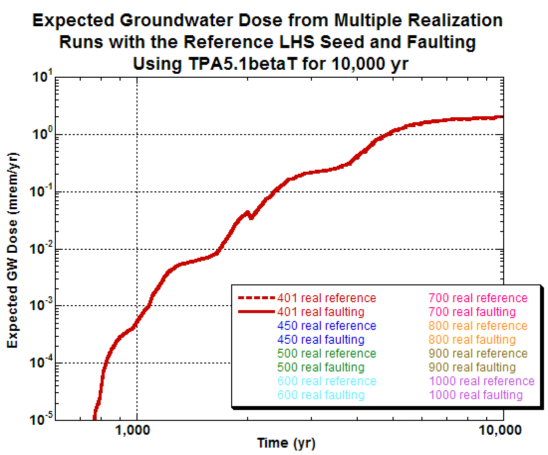
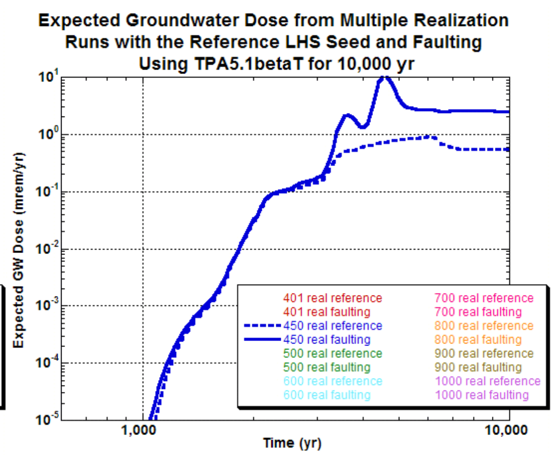
900 real 100kyr
1000 real 10kyr
1000 real 100kyr

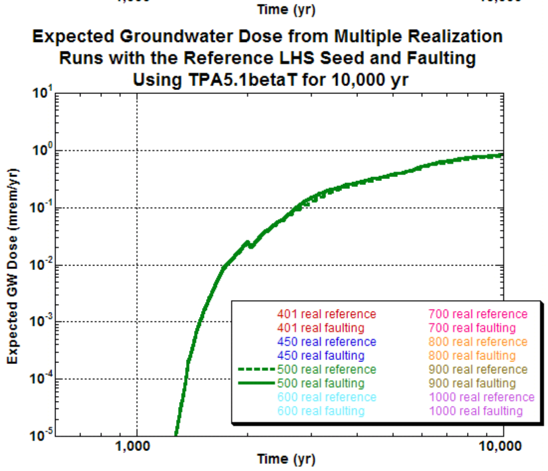

Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed Using TPA5.1betaT for 10,000 and 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
401 real 10kyr
401 real 100kyr
450 real 10kyr
450 real 100kyr
500 real 10kyr
500 real 100kyr
600 real 10kyr
600 real 100kyr
700 real 10kyr
700 real 100kyr
800 real 10kyr
800 real 100kyr
900 real 10kyr
900 real 100kyr
1000 real 10kyr
1000 real 100kyr

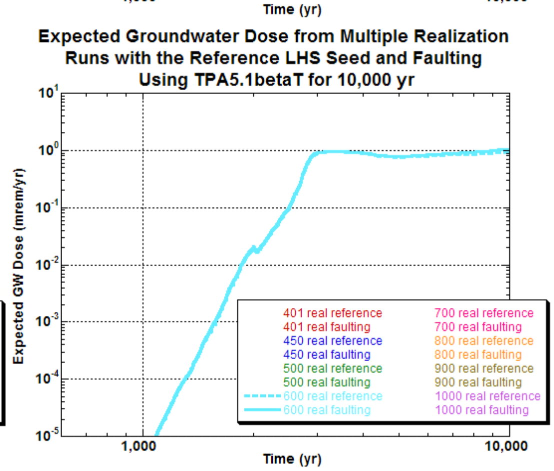
12. Plots of Expected Dose For the Reference Case and Faulting Case From Multiple Realizations Using TPA51betaT for 10,000 yr With the Reference Seed.



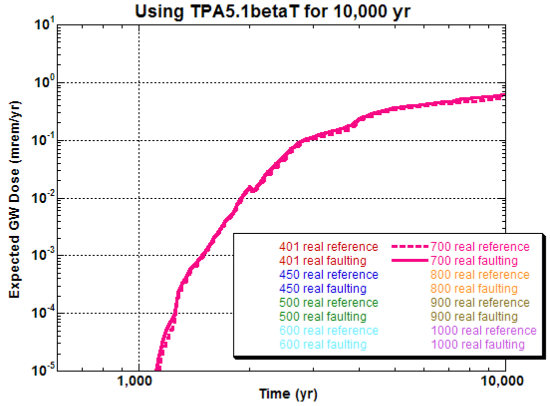




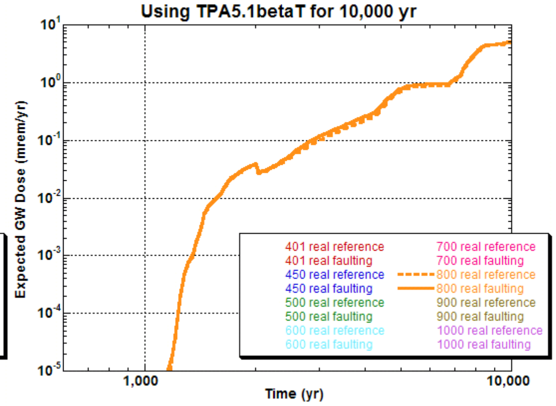




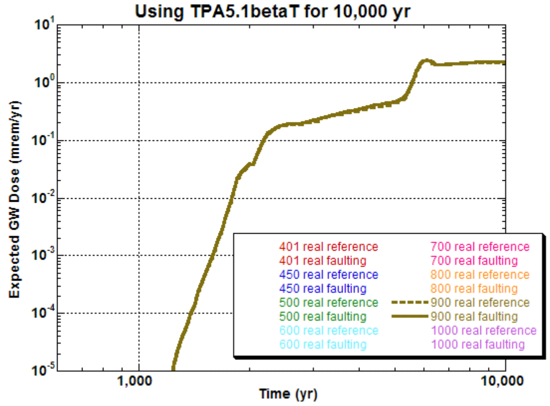
Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed and Faulting Using TPA5.1betaT for 10,000 yr



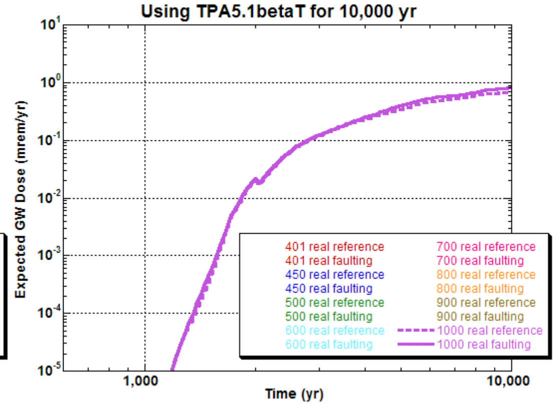
Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed and Faulting Using TPA5.1betaT for 10,000 yr



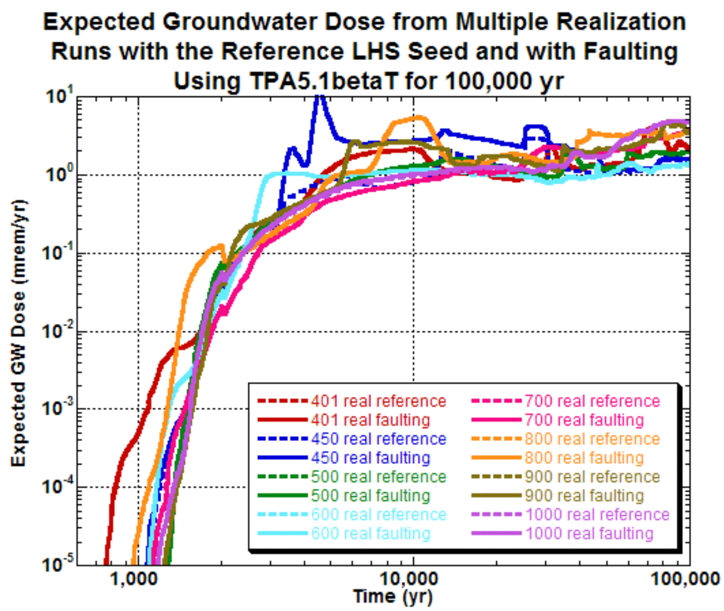
Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed and Faulting Using TPA5.1betaT for 10,000 yr

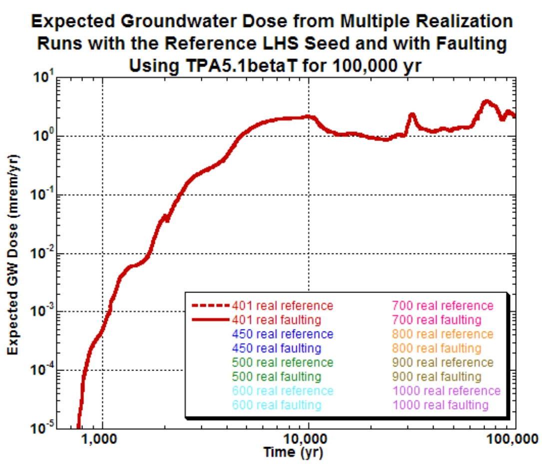


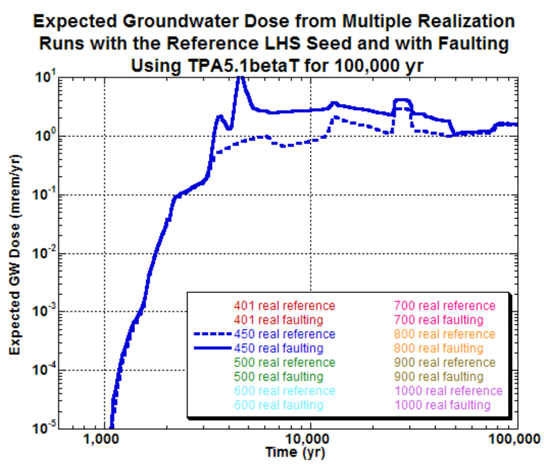
Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed and Faulting Using TPA5.1betaT for 10,000 yr

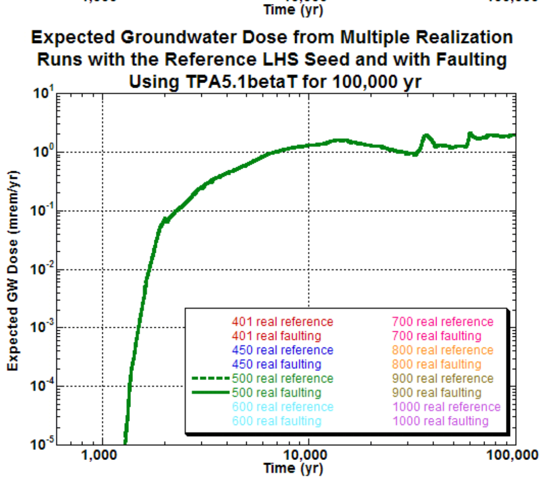


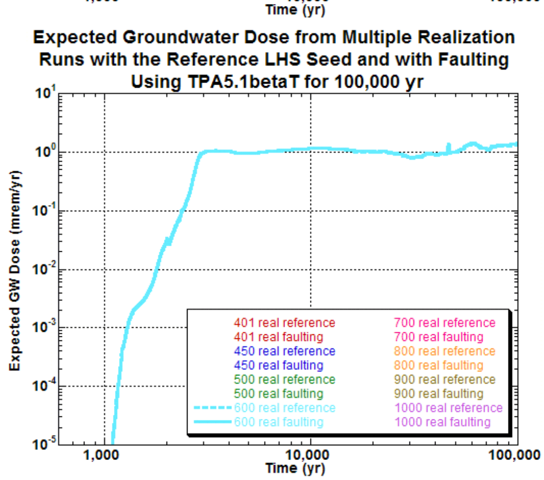
13. Plots of Expected Dose For the Reference Case and Faulting Case From Multiple Realizations Using TPA51betaT for 100,000 yr With the Reference Seed.

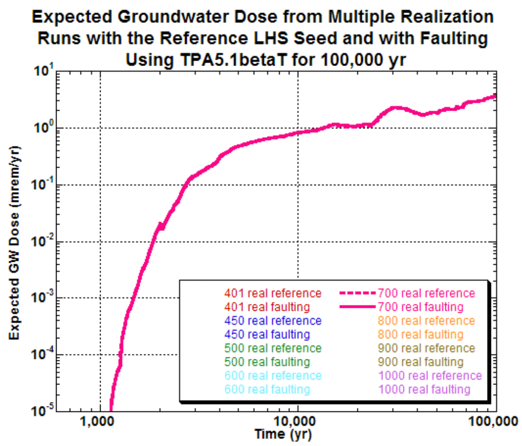


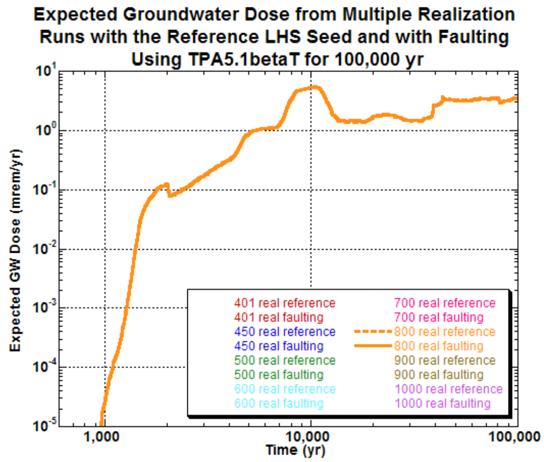


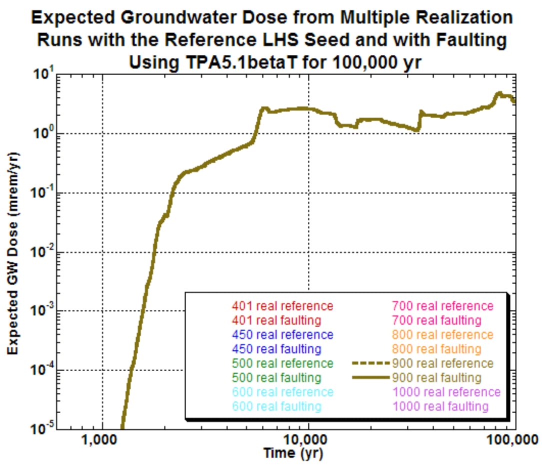


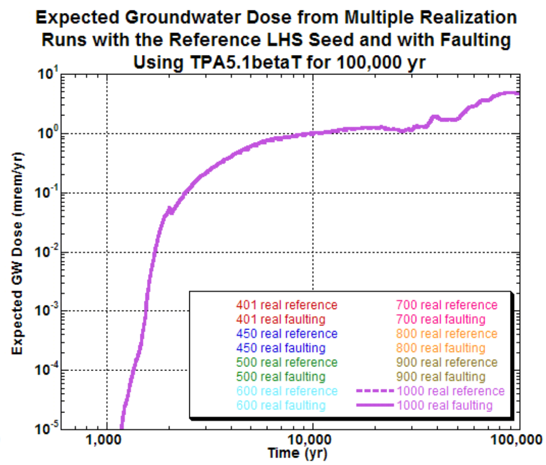




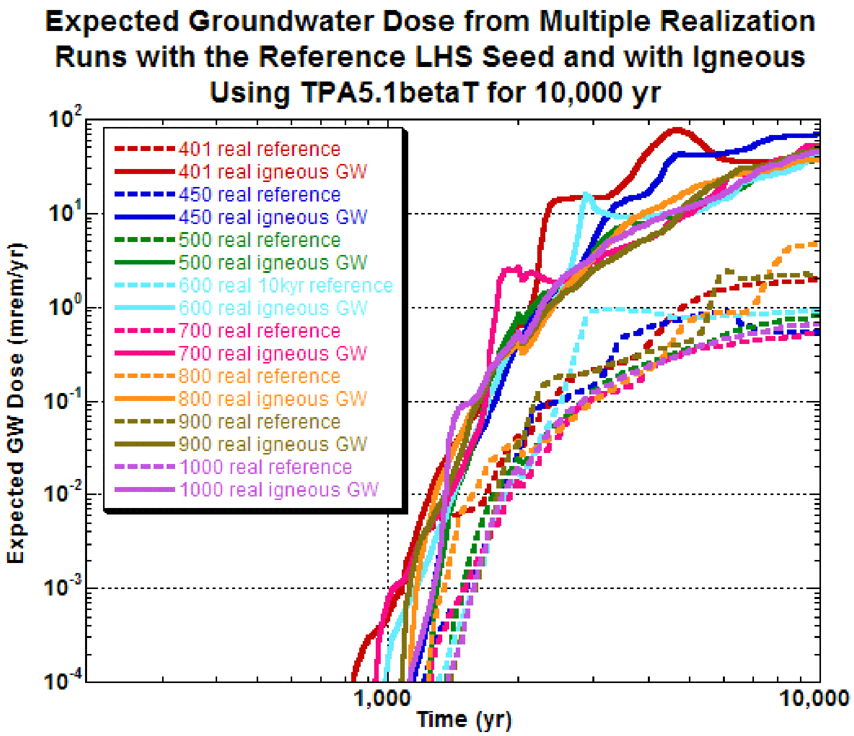

Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed and with Faulting Using TPA5.1betaT for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
401 real reference
401 real faulting
450 real reference
450 real faulting
500 real reference
500 real faulting
600 real reference
600 real faulting
700 real reference
700 real faulting
800 real reference
800 real faulting
900 real reference
900 real faulting
1000 real reference
1000 real faulting

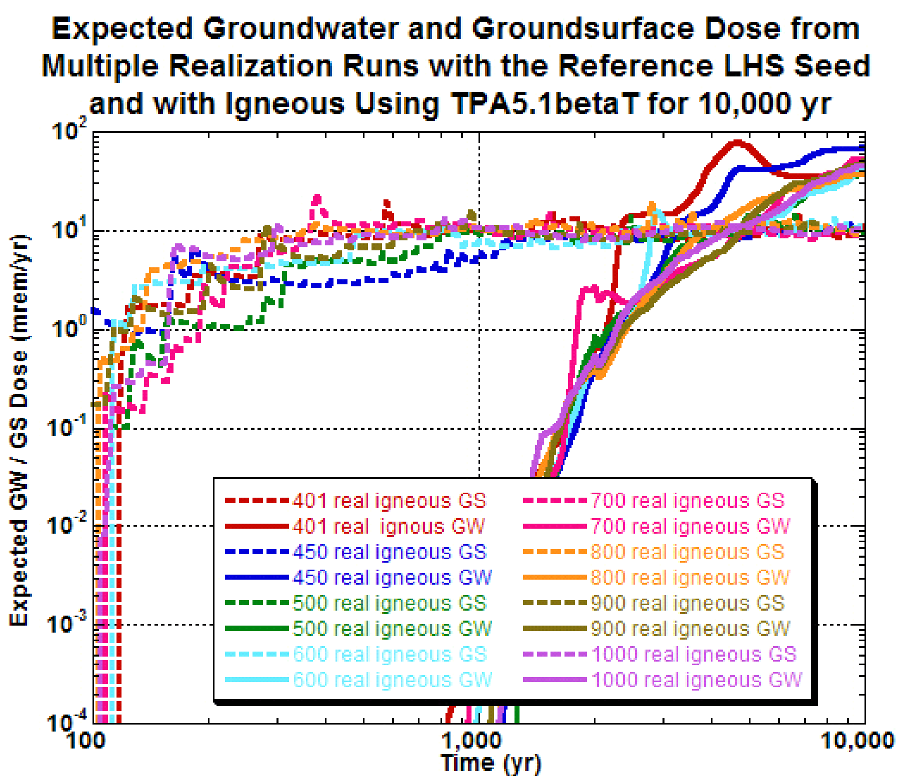

Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed and with Faulting Using TPA5.1betaT for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
401 real reference
401 real faulting
450 real reference
450 real faulting
500 real reference
500 real faulting
600 real reference
600 real faulting
700 real reference
700 real faulting
800 real reference
800 real faulting
900 real reference
900 real faulting
1000 real reference
1000 real faulting


Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed and with Faulting Using TPA5.1betaT for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
401 real reference
401 real faulting
450 real reference
450 real faulting
500 real reference
500 real faulting
600 real reference
600 real faulting
700 real reference
700 real faulting
800 real reference
800 real faulting
900 real reference
900 real faulting
1000 real reference
1000 real faulting

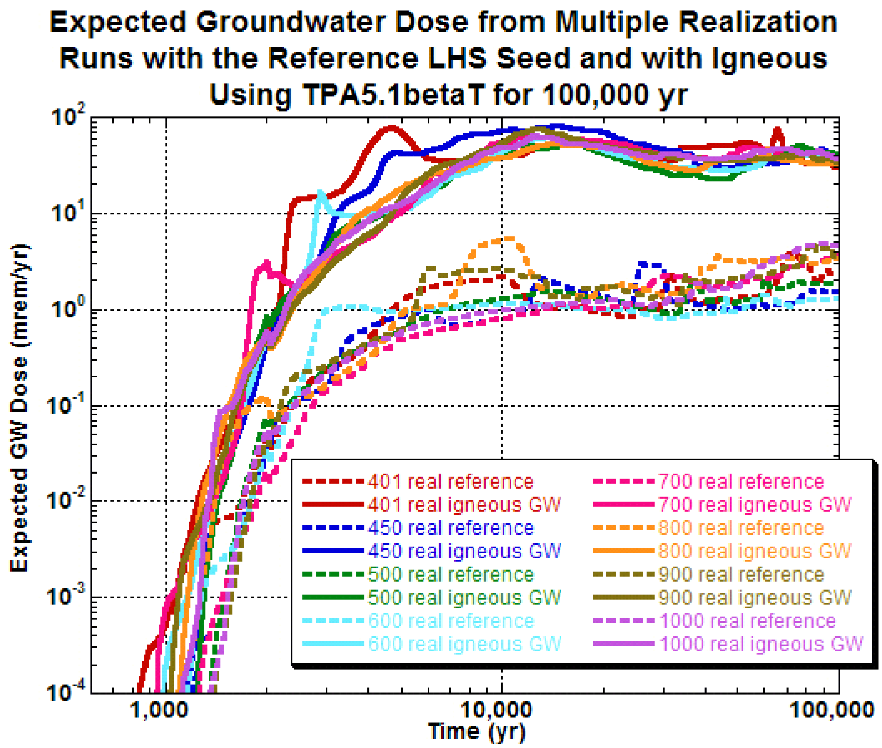

Expected Groundwater Dose from Multiple Realization Runs with the Reference LHS Seed and with Faulting Using TPA5.1betaT for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
401 real reference
401 real faulting
450 real reference
450 real faulting
500 real reference
500 real faulting
600 real reference
600 real faulting
700 real reference
700 real faulting
800 real reference
800 real faulting
900 real reference
900 real faulting
1000 real reference
1000 real faulting

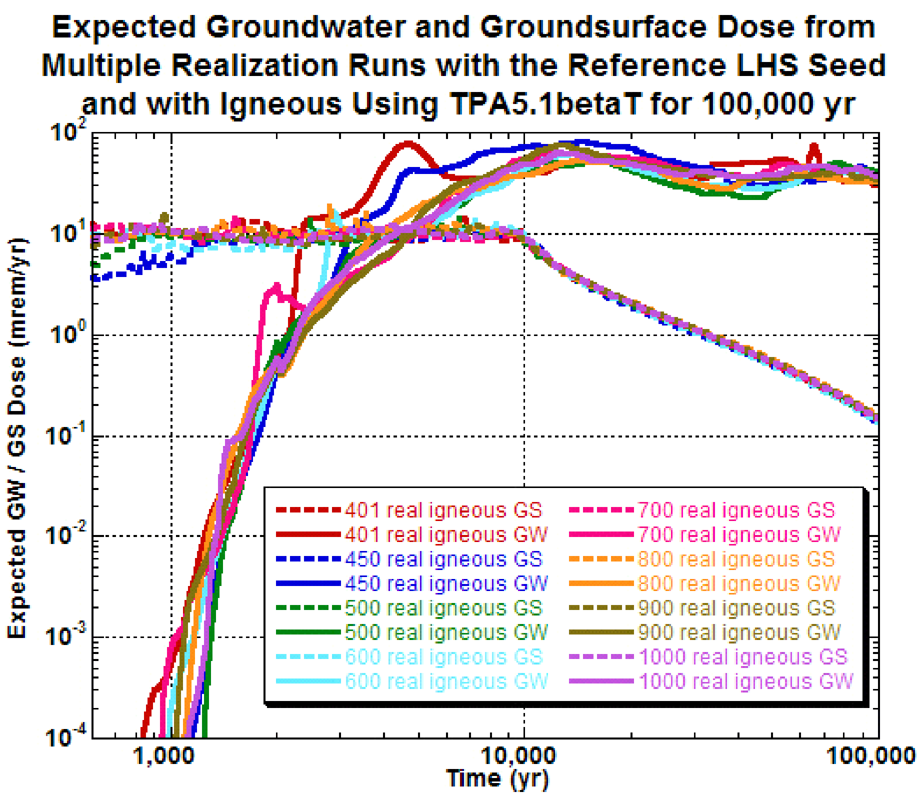
14. Plots of Expected Dose (GW and GS) From Multiple Realizations Using TPA51betaT for 10,000 yr With and Without Volcanism.





15. Plots of Expected Dose (GW and GS) From Multiple Realizations Using TPA51betaT for 100,000 yr With and Without Volcanism.





16. Screenprint Showing Peak Mean Dose of 8.6 mrem/yr Versus 820 mrem/yr for Realization 343 of 450 Using TPA51betaT for 100,000 yr Without and With Faulting, Respectively.

BASECASE (FAULTING OFF)

```
--------------------------------------------------------------------
   subarea   1 of  10          realization  343 of  450
--------------------------------------------------------------------
                  There is no SZ release
--------------------------------------------------------------------
   subarea   2 of  10          realization  343 of  450
--------------------------------------------------------------------
                  There is no SZ release
--------------------------------------------------------------------
   subarea   3 of  10          realization  343 of  450
--------------------------------------------------------------------
                  There is no SZ release
--------------------------------------------------------------------
   subarea   4 of  10          realization  343 of  450
--------------------------------------------------------------------
                  There is no SZ release
--------------------------------------------------------------------
   subarea   5 of  10          realization  343 of  450
--------------------------------------------------------------------
                  There is no SZ release
--------------------------------------------------------------------
   subarea   6 of  10          realization  343 of  450
--------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
!  Number of SeismicEvents = 0
!  Setting Seismic_flag=0 for Driftfail
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      574.9  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =     1443.2  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     30 at TPA time =   1415.4 yr
 *** failed WPs:  30   out of  343  ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
     ebsrel: running glass waste form
              Highest release rates from Sub Area 6
          Tc99    6.4001E+00 [Ci/yr/SA] at  1.524E+03 yr
          Ja241   3.3983E+00 [Ci/yr/SA] at  1.451E+03 yr
          Am241   1.6747E+00 [Ci/yr/SA] at  1.524E+03 yr
          Ni59    1.6206E+00 [Ci/yr/SA] at  1.524E+03 yr
          Ja243   1.0078E+00 [Ci/yr/SA] at  4.945E+03 yr
          Cs135   3.1658E-01 [Ci/yr/SA] at  1.524E+03 yr
exec: calling uzft
                Highest release rates from UZ
          Tc99    5.9557E+00 [Ci/yr/SA] at  1.601E+03 yr
          Ja241   5.8516E-01 [Ci/yr/SA] at  1.810E+03 yr
```

```
          Ja243   2.4675E-01 [Ci/yr/SA] at  4.945E+03 yr
          Cs135   1.0649E-01 [Ci/yr/SA] at  2.420E+03 yr
          Se79    3.5828E-02 [Ci/yr/SA] at  1.641E+03 yr
          Jc245   3.0954E-02 [Ci/yr/SA] at  1.682E+03 yr
exec: calling szft
              Highest release rates from SZ
          Tc99    3.6474E-01 [Ci/yr/SA] at  2.479E+03 yr
          Ja243   2.0445E-01 [Ci/yr/SA] at  6.560E+03 yr
          Ja241   4.8935E-02 [Ci/yr/SA] at  3.635E+03 yr
          Jc245   1.8583E-02 [Ci/yr/SA] at  3.549E+03 yr
          Jp239   1.2954E-02 [Ci/yr/SA] at  6.560E+03 yr
          Jc246   5.0461E-03 [Ci/yr/SA] at  3.549E+03 yr
----------------------------------------------------------------------
   subarea   7 of  10         realization  343 of  450
----------------------------------------------------------------------
                There is no SZ release
----------------------------------------------------------------------
   subarea   8 of  10         realization  343 of  450
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
!  Number of SeismicEvents = 0
!  Setting Seismic_flag=0 for Driftfail
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      423.5  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =     1740.1  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     81 at TPA time =   1723.3 yr
 *** failed WPs:  81   out of  931  ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
     ebsrel: running glass waste form
             Highest release rates from Sub Area 8
          Tc99    1.7553E+01 [Ci/yr/SA] at  1.810E+03 yr
          Ja241   9.5603E+00 [Ci/yr/SA] at  1.766E+03 yr
          Ni59    4.2797E+00 [Ci/yr/SA] at  1.810E+03 yr
          Am241   3.5463E+00 [Ci/yr/SA] at  1.810E+03 yr
          Ja243   3.1942E+00 [Ci/yr/SA] at  4.717E+03 yr
          Cs135   8.5441E-01 [Ci/yr/SA] at  1.810E+03 yr
exec: calling uzft
              Highest release rates from UZ
          Tc99    1.6831E+01 [Ci/yr/SA] at  1.810E+03 yr
          Ja241   2.0798E+00 [Ci/yr/SA] at  1.810E+03 yr
          Ni59    1.7755E+00 [Ci/yr/SA] at  2.420E+03 yr
          Cs135   8.0051E-01 [Ci/yr/SA] at  1.900E+03 yr
          Ja243   7.9779E-01 [Ci/yr/SA] at  4.717E+03 yr
          Se79    1.0589E-01 [Ci/yr/SA] at  1.854E+03 yr
exec: calling szft
              Highest release rates from SZ
          Tc99    1.1262E+00 [Ci/yr/SA] at  2.665E+03 yr
          Ja243   6.4420E-01 [Ci/yr/SA] at  6.113E+03 yr
          Ja241   2.0577E-01 [Ci/yr/SA] at  3.549E+03 yr
          Jc245   5.9237E-02 [Ci/yr/SA] at  3.466E+03 yr
```

Jp239   3.3365E-02 [Ci/yr/SA] at 6.113E+03 yr
Jc246   1.6245E-02 [Ci/yr/SA] at 3.466E+03 yr

---

subarea   9 of 10   realization 343 of 450

There is no SZ release

---

subarea 10 of 10   realization 343 of 450

There is no SZ release

---

exec: calling dcagw
Highest annual dose GW pathway
Am243   1.7048E+02 [mrem/yr] at 6.113E+03 yr
Am241   4.8341E+01 [mrem/yr] at 3.549E+03 yr
Cm245   1.5584E+01 [mrem/yr] at 3.466E+03 yr
Pu239   1.0486E+01 [mrem/yr] at 6.113E+03 yr
Cm246   4.1101E+00 [mrem/yr] at 3.466E+03 yr
Pu240   3.5894E+00 [mrem/yr] at 7.376E+03 yr
At end of TPI, annual dose GW pathway
Pu239   5.1974E+00 [mrem/yr]
Pu240   3.0855E+00 [mrem/yr]
Tc99   2.3719E-01 [mrem/yr]
I129   7.4767E-02 [mrem/yr]
Th230   2.0716E-02 [mrem/yr]
Se79   7.2515E-03 [mrem/yr]
sum 8.6265E+00 [mrem/yr]

****

FAULTING ON

---

subarea   1 of 10   realization 343 of 450

There is no SZ release

---

subarea   2 of 10   realization 343 of 450

---

exec: calling uzflow
exec: calling driftdriver
! Number of SeismicEvents = 0
! Setting Seismic_flag=0 for Driftfail
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
exec: time of drip shield mechanical failure =   529.7 yr
*** No Drip Shield Failure by General Corrosion ***
exec: calling nfenv
exec: calling ebsfail
ebsfail: No Corrosion Breach on WP Welded Areas
*** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
*** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from FAULTING   event =   13 at TPA time =   315.6 yr
*** failed WPs: 13   out of 1062 ***
exec: calling ebsrel
ebsrel: running spent fuel waste form
ebsrel: running glass waste form
Highest release rates from Sub Area 2

```
        Ja241   5.8897E+01 [Ci/yr/SA] at  1.854E+03 yr
        Ja243   7.9237E+00 [Ci/yr/SA] at  1.854E+03 yr
        Tc99    5.6030E+00 [Ci/yr/SA] at  1.854E+03 yr
        Ni59    1.3031E+00 [Ci/yr/SA] at  1.854E+03 yr
        Jp240   3.3461E-01 [Ci/yr/SA] at  4.607E+03 yr
        Jp239   3.0944E-01 [Ci/yr/SA] at  2.665E+03 yr
exec: calling uzft
             Highest release rates from UZ
        Ja241   5.8089E+01 [Ci/yr/SA] at  1.854E+03 yr
        Ja243   7.8150E+00 [Ci/yr/SA] at  1.854E+03 yr
        Tc99    5.5261E+00 [Ci/yr/SA] at  1.854E+03 yr
        Ni59    1.2853E+00 [Ci/yr/SA] at  1.854E+03 yr
        Jp240   3.3098E-01 [Ci/yr/SA] at  4.607E+03 yr
        Jp239   3.0564E-01 [Ci/yr/SA] at  2.665E+03 yr
exec: calling szft
             Highest release rates from SZ
        Ja243   1.7697E+00 [Ci/yr/SA] at  4.607E+03 yr
        Jp239   3.0448E-01 [Ci/yr/SA] at  4.830E+03 yr
        Jp240   2.4538E-01 [Ci/yr/SA] at  7.551E+03 yr
        Ja241   2.4310E-01 [Ci/yr/SA] at  4.607E+03 yr
        Tc99    1.1992E-01 [Ci/yr/SA] at  2.665E+03 yr
        Jc245   3.5008E-02 [Ci/yr/SA] at  4.607E+03 yr
--------------------------------------------------------------------
  subarea   3 of  10          realization  343 of  450
--------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
!  Number of SeismicEvents = 0
!  Setting Seismic_flag=0 for Driftfail
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
   exec: time of drip shield mechanical failure =      501.3  yr
   *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
   ebsfail: No Corrosion Breach on WP Welded Areas
   *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
   *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from FAULTING   event =     44 at TPA time =    315.6 yr
 *** failed WPs:  44   out of  2904  ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
    ebsrel: running glass waste form
          Highest release rates from Sub Area 3
        Ja241   1.2954E+02 [Ci/yr/SA] at  1.995E+03 yr
        Ja243   2.1592E+01 [Ci/yr/SA] at  1.995E+03 yr
        Tc99    1.8553E+01 [Ci/yr/SA] at  1.947E+03 yr
        Ni59    4.4106E+00 [Ci/yr/SA] at  1.947E+03 yr
        Am241   4.2936E+00 [Ci/yr/SA] at  1.947E+03 yr
        Cs135   9.6270E-01 [Ci/yr/SA] at  1.947E+03 yr
exec: calling uzft
             Highest release rates from UZ
        Ja241   1.2680E+02 [Ci/yr/SA] at  1.995E+03 yr
        Ja243   2.1136E+01 [Ci/yr/SA] at  1.995E+03 yr
        Tc99    1.8157E+01 [Ci/yr/SA] at  1.947E+03 yr
        Ni59    4.3164E+00 [Ci/yr/SA] at  1.947E+03 yr
        Am241   4.2019E+00 [Ci/yr/SA] at  1.947E+03 yr
        Cs135   9.4213E-01 [Ci/yr/SA] at  1.947E+03 yr
```

```
exec: calling szft
                Highest release rates from SZ
          Ja243   6.3994E+00 [Ci/yr/SA] at  4.499E+03 yr
          Ja241   1.0081E+00 [Ci/yr/SA] at  4.499E+03 yr
          Jp239   7.2522E-01 [Ci/yr/SA] at  4.607E+03 yr
          Jp240   5.6356E-01 [Ci/yr/SA] at  7.376E+03 yr
          Tc99    4.1866E-01 [Ci/yr/SA] at  2.729E+03 yr
          Jc245   1.2644E-01 [Ci/yr/SA] at  4.499E+03 yr
-----------------------------------------------------------------
   subarea   4 of  10         realization  343 of  450
-----------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
!  Number of SeismicEvents = 0
!  Setting Seismic_flag=0 for Driftfail
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      411.6  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Corrosion Breach on WP Welded Areas
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from FAULTING   event =     52 at TPA time =    315.6 yr
 *** failed WPs:  52   out of  1793  ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
     ebsrel: running glass waste form
             Highest release rates from Sub Area 4
          Ja241   1.5331E+02 [Ci/yr/SA] at  2.044E+03 yr
          Ja243   2.7377E+01 [Ci/yr/SA] at  2.044E+03 yr
          Tc99    2.1765E+01 [Ci/yr/SA] at  2.044E+03 yr
          Ni59    5.1160E+00 [Ci/yr/SA] at  2.044E+03 yr
          Cs135   1.1127E+00 [Ci/yr/SA] at  2.044E+03 yr
          Jp240   9.1777E-01 [Ci/yr/SA] at  4.607E+03 yr
exec: calling uzft
                Highest release rates from UZ
          Ja241   1.5023E+02 [Ci/yr/SA] at  2.044E+03 yr
          Ja243   2.6827E+01 [Ci/yr/SA] at  2.044E+03 yr
          Tc99    2.1328E+01 [Ci/yr/SA] at  2.044E+03 yr
          Ni59    5.0134E+00 [Ci/yr/SA] at  2.044E+03 yr
          Cs135   1.0904E+00 [Ci/yr/SA] at  2.044E+03 yr
          Jp240   9.0287E-01 [Ci/yr/SA] at  4.607E+03 yr
exec: calling szft
                Highest release rates from SZ
          Ja243   7.3449E+00 [Ci/yr/SA] at  4.499E+03 yr
          Ja241   1.1543E+00 [Ci/yr/SA] at  4.499E+03 yr
          Jp239   8.8288E-01 [Ci/yr/SA] at  4.717E+03 yr
          Jp240   6.8894E-01 [Ci/yr/SA] at  7.205E+03 yr
          Tc99    4.8788E-01 [Ci/yr/SA] at  2.796E+03 yr
          Jc245   1.4490E-01 [Ci/yr/SA] at  4.499E+03 yr
-----------------------------------------------------------------
   subarea   5 of  10         realization  343 of  450
-----------------------------------------------------------------
                  There is no SZ release
-----------------------------------------------------------------
   subarea   6 of  10         realization  343 of  450
```

```
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
!  Number of SeismicEvents = 0
!  Setting Seismic_flag=0 for Driftfail
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      574.9  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: time of corrosion breach on welded areas =     1443.2  yr
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
    *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     30 at TPA time =   1415.4 yr
 *** failed WPs:  30   out of  343  ***
exec: calling ebsrel
     ebsrel: running spent fuel waste form
     ebsrel: running glass waste form
              Highest release rates from Sub Area 6
          Tc99    6.4001E+00 [Ci/yr/SA] at  1.524E+03 yr
          Ja241   3.3983E+00 [Ci/yr/SA] at  1.451E+03 yr
          Am241   1.6747E+00 [Ci/yr/SA] at  1.524E+03 yr
          Ni59    1.6206E+00 [Ci/yr/SA] at  1.524E+03 yr
          Ja243   1.0078E+00 [Ci/yr/SA] at  4.945E+03 yr
          Cs135   3.1658E-01 [Ci/yr/SA] at  1.524E+03 yr
exec: calling uzft
                Highest release rates from UZ
          Tc99    5.9557E+00 [Ci/yr/SA] at  1.601E+03 yr
          Ja241   5.8516E-01 [Ci/yr/SA] at  1.810E+03 yr
          Ja243   2.4675E-01 [Ci/yr/SA] at  4.945E+03 yr
          Cs135   1.0649E-01 [Ci/yr/SA] at  2.420E+03 yr
          Se79    3.5828E-02 [Ci/yr/SA] at  1.641E+03 yr
          Jc245   3.0954E-02 [Ci/yr/SA] at  1.682E+03 yr
exec: calling szft
                Highest release rates from SZ
          Tc99    3.6474E-01 [Ci/yr/SA] at  2.479E+03 yr
          Ja243   2.0445E-01 [Ci/yr/SA] at  6.560E+03 yr
          Ja241   4.8935E-02 [Ci/yr/SA] at  3.635E+03 yr
          Jc245   1.8583E-02 [Ci/yr/SA] at  3.549E+03 yr
          Jp239   1.2954E-02 [Ci/yr/SA] at  6.560E+03 yr
          Jc246   5.0461E-03 [Ci/yr/SA] at  3.549E+03 yr
----------------------------------------------------------------------
   subarea   7 of  10          realization  343 of  450
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
!  Number of SeismicEvents = 0
!  Setting Seismic_flag=0 for Driftfail
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
    exec: time of drip shield mechanical failure =      606.8  yr
    *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
    ebsfail: No Corrosion Breach on WP Welded Areas
    *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
```

```
   *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from FAULTING   event =     47 at TPA time =    315.6 yr
 *** failed WPs:  47   out of  696  ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
    ebsrel: running glass waste form
            Highest release rates from Sub Area 7
        Ja241   2.5334E+02 [Ci/yr/SA] at  1.766E+03 yr
        Ja243   2.9908E+01 [Ci/yr/SA] at  1.766E+03 yr
        Tc99    2.0476E+01 [Ci/yr/SA] at  1.766E+03 yr
        Ni59    4.8831E+00 [Ci/yr/SA] at  1.766E+03 yr
        Jp240   1.4234E+00 [Ci/yr/SA] at  4.607E+03 yr
        Jp239   1.2852E+00 [Ci/yr/SA] at  1.000E+04 yr
exec: calling uzft
              Highest release rates from UZ
        Ja241   3.1874E+01 [Ci/yr/SA] at  1.900E+03 yr
        Tc99    1.4877E+01 [Ci/yr/SA] at  1.854E+03 yr
        Ja243   4.6173E+00 [Ci/yr/SA] at  1.900E+03 yr
        Jp240   3.5088E-01 [Ci/yr/SA] at  4.717E+03 yr
        Jp239   3.1964E-01 [Ci/yr/SA] at  1.000E+04 yr
        Cs135   2.8023E-01 [Ci/yr/SA] at  2.363E+03 yr
exec: calling szft
              Highest release rates from SZ
        Ja243   2.0930E+00 [Ci/yr/SA] at  3.635E+03 yr
        Ja241   1.1759E+00 [Ci/yr/SA] at  3.549E+03 yr
        Tc99    6.5217E-01 [Ci/yr/SA] at  2.540E+03 yr
        Jp239   2.9754E-01 [Ci/yr/SA] at  1.000E+04 yr
        Jp240   2.9164E-01 [Ci/yr/SA] at  6.560E+03 yr
        Jc245   4.0913E-02 [Ci/yr/SA] at  3.635E+03 yr
----------------------------------------------------------------------
   subarea   8 of  10          realization  343 of  450
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
!  Number of SeismicEvents = 0
!  Setting Seismic_flag=0 for Driftfail
exec: calling nfenvFI
exec: calling dsfail
exec: calling mechdriver (drip shield)
   exec: time of drip shield mechanical failure =      423.5  yr
   *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
   ebsfail: time of corrosion breach on welded areas =     1740.1  yr
   *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
   *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     81 at TPA time =   1723.3 yr
 *** failed WPs:  81   out of  931  ***
exec: calling ebsrel
    ebsrel: running spent fuel waste form
    ebsrel: running glass waste form
            Highest release rates from Sub Area 8
        Tc99    1.7553E+01 [Ci/yr/SA] at  1.810E+03 yr
        Ja241   9.5603E+00 [Ci/yr/SA] at  1.766E+03 yr
        Ni59    4.2797E+00 [Ci/yr/SA] at  1.810E+03 yr
        Am241   3.5463E+00 [Ci/yr/SA] at  1.810E+03 yr
        Ja243   3.1942E+00 [Ci/yr/SA] at  4.717E+03 yr
        Cs135   8.5441E-01 [Ci/yr/SA] at  1.810E+03 yr
```

```
exec: calling uzft
          Highest release rates from UZ
      Tc99    1.6831E+01 [Ci/yr/SA] at  1.810E+03 yr
      Ja241   2.0798E+00 [Ci/yr/SA] at  1.810E+03 yr
      Ni59    1.7755E+00 [Ci/yr/SA] at  2.420E+03 yr
      Cs135   8.0051E-01 [Ci/yr/SA] at  1.900E+03 yr
      Ja243   7.9779E-01 [Ci/yr/SA] at  4.717E+03 yr
      Se79    1.0589E-01 [Ci/yr/SA] at  1.854E+03 yr
exec: calling szft
          Highest release rates from SZ
      Tc99    1.1262E+00 [Ci/yr/SA] at  2.665E+03 yr
      Ja243   6.4420E-01 [Ci/yr/SA] at  6.113E+03 yr
      Ja241   2.0577E-01 [Ci/yr/SA] at  3.549E+03 yr
      Jc245   5.9237E-02 [Ci/yr/SA] at  3.466E+03 yr
      Jp239   3.3365E-02 [Ci/yr/SA] at  6.113E+03 yr
      Jc246   1.6245E-02 [Ci/yr/SA] at  3.466E+03 yr
----------------------------------------------------------------------
  subarea   9 of  10         realization  343 of  450
----------------------------------------------------------------------
              There is no SZ release
----------------------------------------------------------------------
  subarea  10 of  10         realization  343 of  450
----------------------------------------------------------------------
              There is no SZ release
----------------------------------------------------------------------
exec: calling dcagw
          Highest annual dose GW pathway
      Am243   3.3000E+03 [mrem/yr]  at  4.499E+03 yr
      Pu239   5.0317E+02 [mrem/yr]  at  4.717E+03 yr
      Am241   4.7456E+02 [mrem/yr]  at  4.499E+03 yr
      Pu240   4.2184E+02 [mrem/yr]  at  7.376E+03 yr
      Cm245   6.2481E+01 [mrem/yr]  at  4.499E+03 yr
      Cm246   1.5361E+01 [mrem/yr]  at  4.499E+03 yr
     At end of TPI, annual dose GW pathway
      Pu239   4.5279E+02 [mrem/yr]
      Pu240   3.6418E+02 [mrem/yr]
      Th230   1.0670E+00 [mrem/yr]
      Tc99    6.4648E-01 [mrem/yr]
      I129    2.0680E-01 [mrem/yr]
      Se79    1.6758E-02 [mrem/yr]
        sum  8.1894E+02 [mrem/yr]
```

(Gives 4.4 rem/yr at 4,100 yr)

Notes: lhs.out files are the same; faulting fails about 150 WPs to give the 4.4 rem/yr dose (SA2 = 13; SA3 = 44; SA4 = 52; and SA7 = 52)

The SAV colloid retardation factor is 1.2 (~0.05 %-tile; mean value ~500; range 1 to ~5000) and sorption capacity is 0.0074 (~97th %-tile)

SA wet fraction is 0.67 and WPFLOWMULTFACTOR is 1.5; Affinity factors are 6.7 (Am), 8.2 (Cm) and 10.8 (Th)

Using mean value for SAV colloid retardation factor: PMD changed from 4,400 to 4.0 mrem/yr
Using mean value for sorption capacity: PMD changed from 4,400 rem/yr to 2,100 mrem/yr
Using mean values for both of the above: PMD changed from 4,400 rem/yr to 4.0 mrem/yr

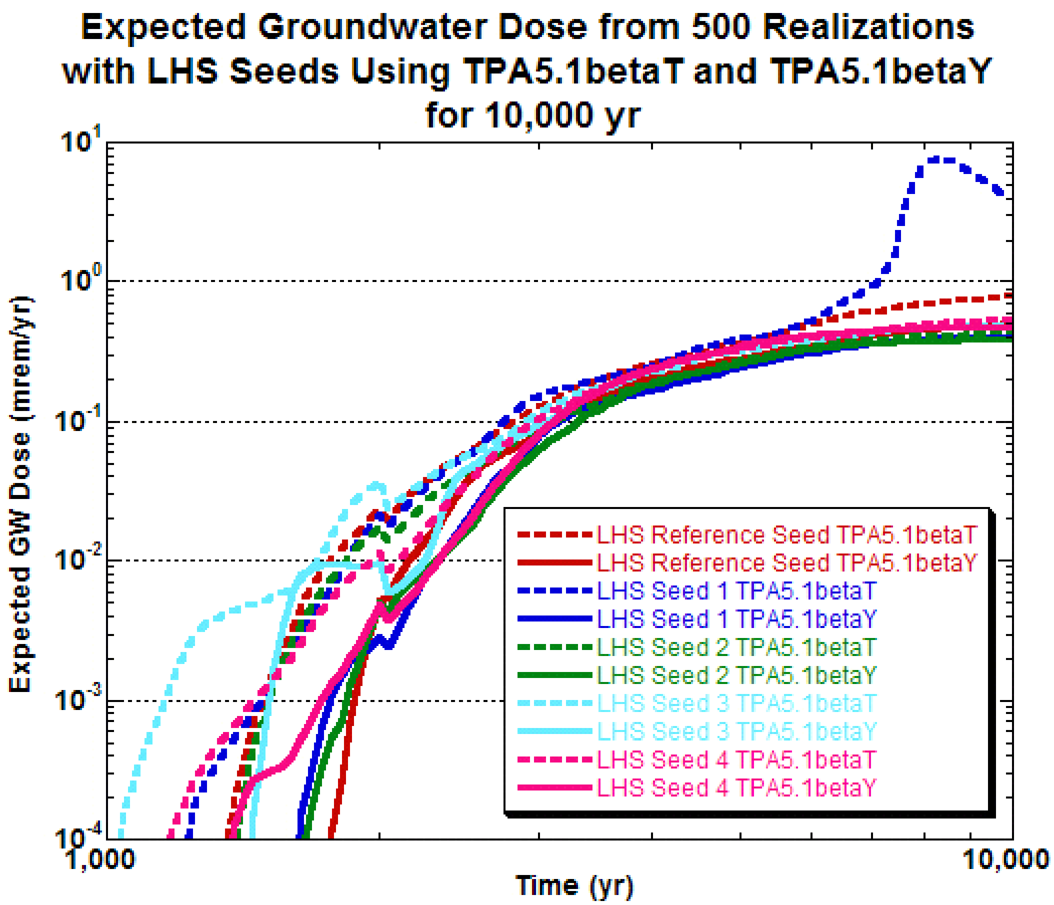
Running for 100,000 yr (instead of 10,000 yr) and using mean value for SAV colloid retardation factor: PMD was 40 mrem/yr and occurred at 100,000 yr

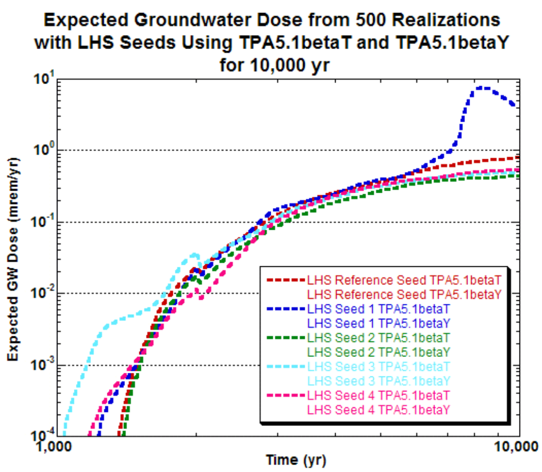
17. Differences Between Sampled Parameters in the *lhs.inp* Files for TPA51betaT and TPA51betaY.

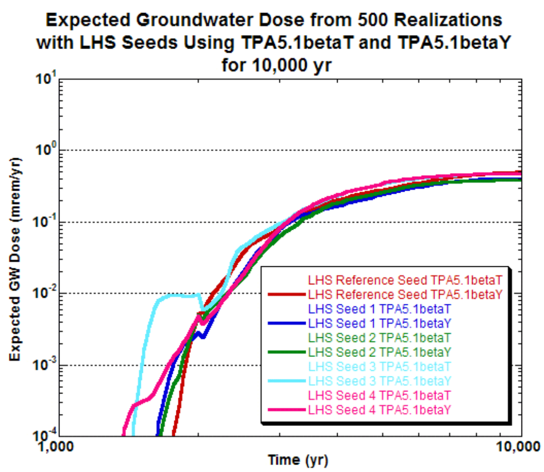
```
Comparing files lhs.inp and ..\LHS.INP
***** lhs.inp

LOGNORMAL   uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
   0.270000E+00    0.126000E+03
UNIFORM     uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum
***** ..\LHS.INP
LOGNORMAL   uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
   0.465000E+00    0.156000E+03
UNIFORM     uzflow_MeanAnnualPrecipitationMultiplierAtGlacialMaximum
*****

***** lhs.inp
LOGNORMAL   uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
   0.420000E+01    0.288000E+03
UNIFORM     BackfillParticleDiameter[m]
***** ..\LHS.INP
LOGNORMAL   uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
   0.357700E+01    0.285300E+03
UNIFORM     BackfillParticleDiameter[m]
*****

***** lhs.inp
BETA        BulkingFactorRockTypeOneSubarea_1[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_2[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_3[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_4[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_5[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_6[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_7[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_8[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_9[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_10[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_1[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_2[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_3[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_4[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_5[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_6[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_7[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
```

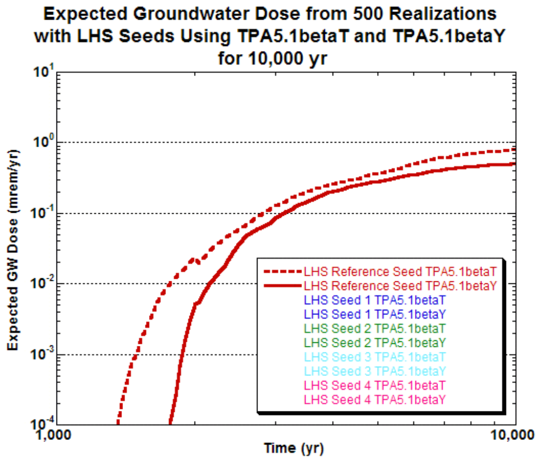
```
BETA        BulkingFactorRockTypeTwoSubarea_8[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_9[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_10[]
   0.100000E+01    0.200000E+01    0.231747E+02    0.926989E+02
LOGNORMAL   DegradationTimeRockTypeOneSubarea_1[yr]
***** ..\LHS.INP
BETA        BulkingFactorRockTypeOneSubarea_1[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_2[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_3[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_4[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_5[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_6[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_7[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_8[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_9[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeOneSubarea_10[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_1[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_2[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_3[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_4[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_5[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_6[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_7[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_8[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_9[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
BETA        BulkingFactorRockTypeTwoSubarea_10[]
   0.101000E+01    0.200000E+01    0.231747E+02    0.926989E+02
LOGNORMAL   DegradationTimeRockTypeOneSubarea_1[yr]
*****

***** lhs.inp
FINITEEXPONENTIAL TimeOfNextFaultingEventinRegionOfInterest[yr]
   0.100000E+03    0.100000E+05    0.200000E-04
UNIFORM     XLocationOfFaultingEventInRegionOfInterest[m]
***** ..\LHS.INP
FINITEEXPONENTIAL TimeOfNextFaultingEventinRegionOfInterest[yr]
   0.100000E+03    0.100000E+06    0.200000E-04
UNIFORM     XLocationOfFaultingEventInRegionOfInterest[m]
*****
```

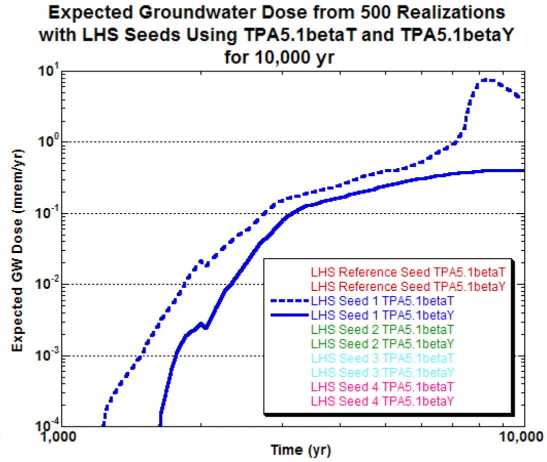
18. Plots of Expected Dose from 500 Realizations Using TPA51betaT and TPA51betaY and LHS Seeds for 10,000 yr.

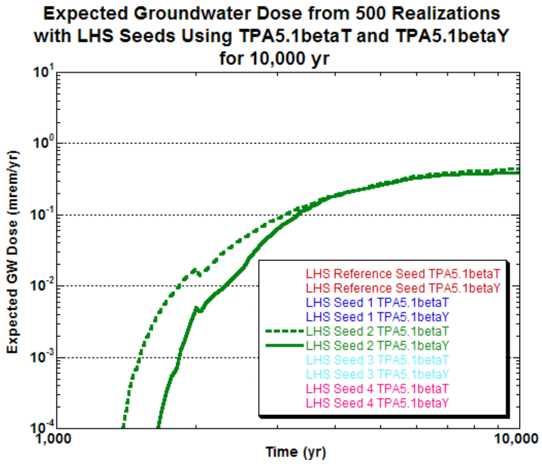


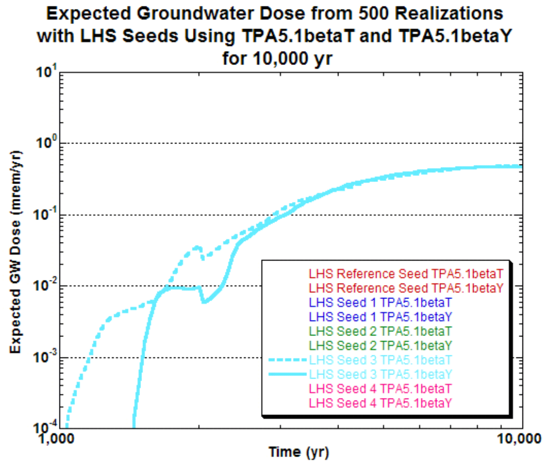


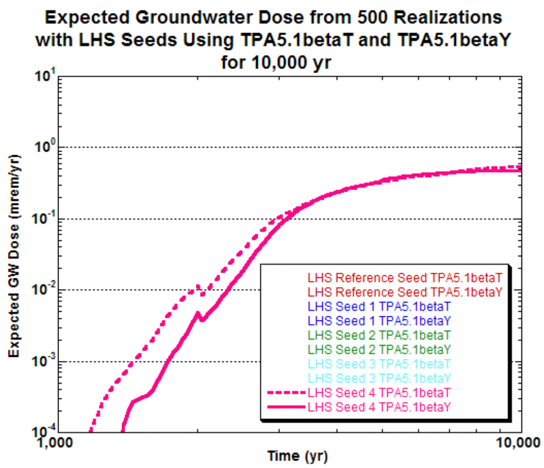



Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaT and TPA5.1betaY
for 10,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY

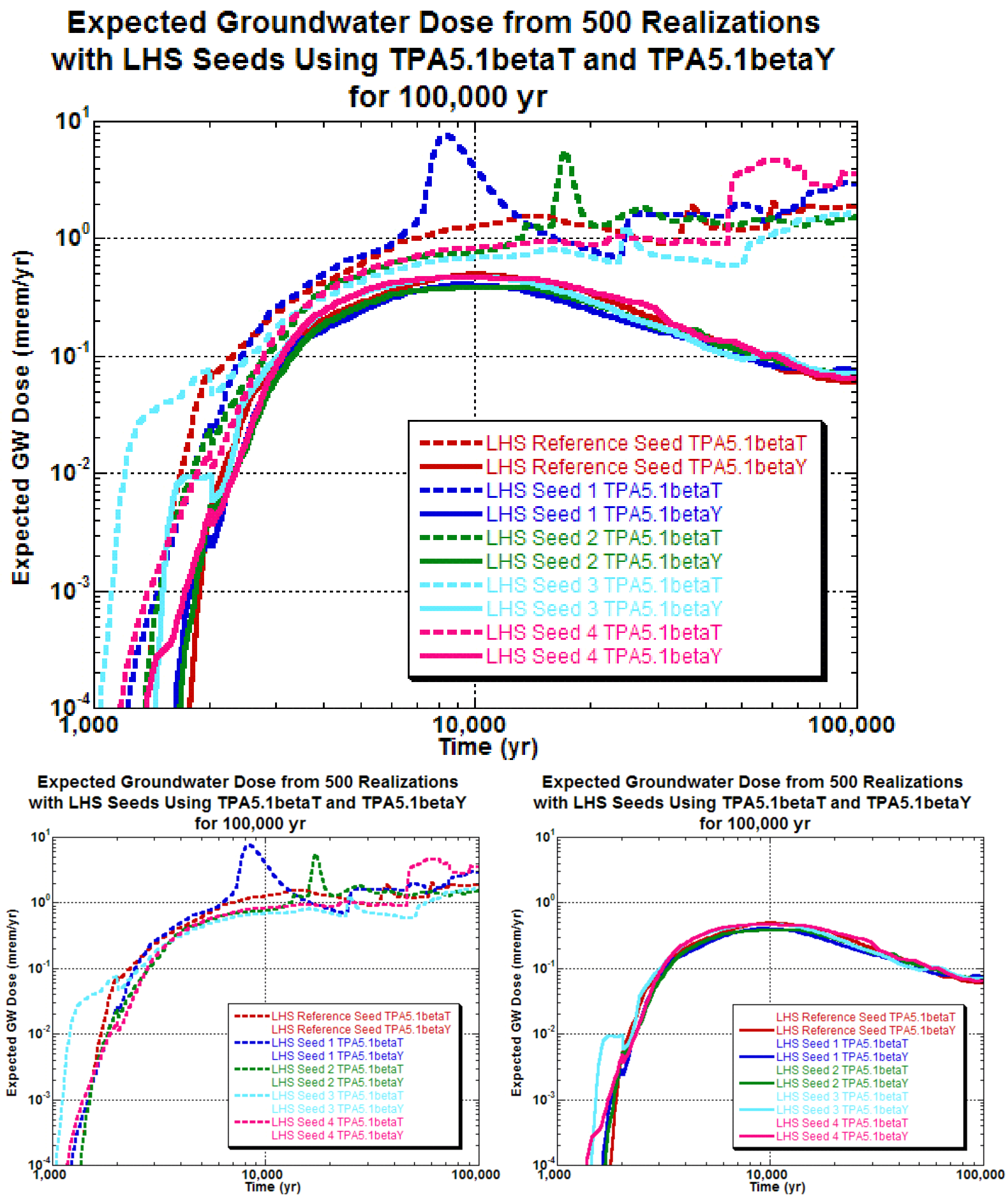

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaT and TPA5.1betaY
for 10,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY

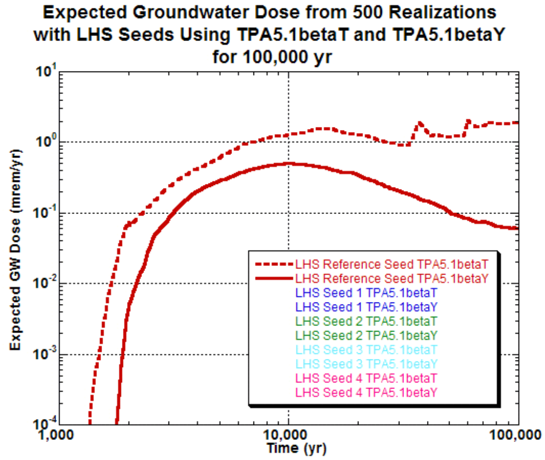

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaT and TPA5.1betaY
for 10,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY

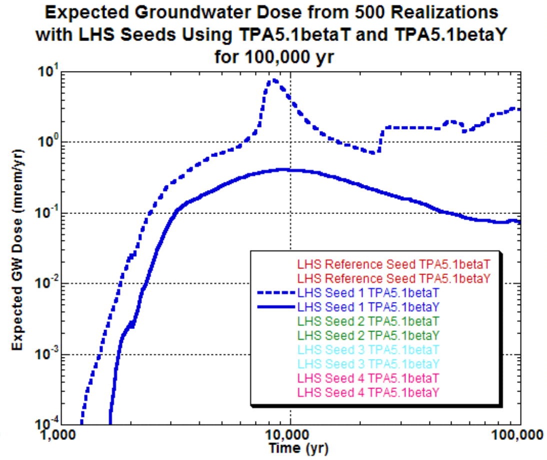

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaT and TPA5.1betaY
for 10,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY

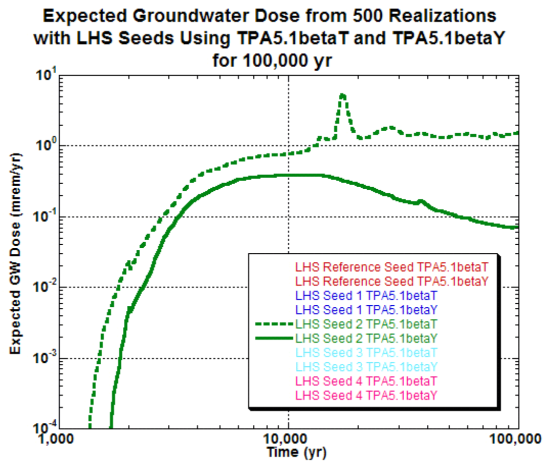

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaT and TPA5.1betaY
for 10,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY

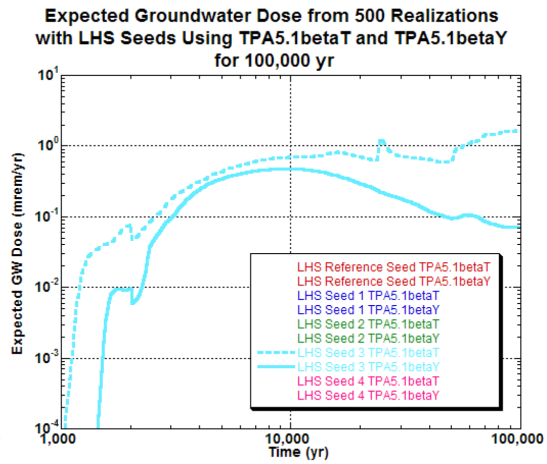
19. Plots of Expected Dose from 500 Realizations Using TPA51betaT and TPA51betaY and LHS Seeds for 100,000 yr.

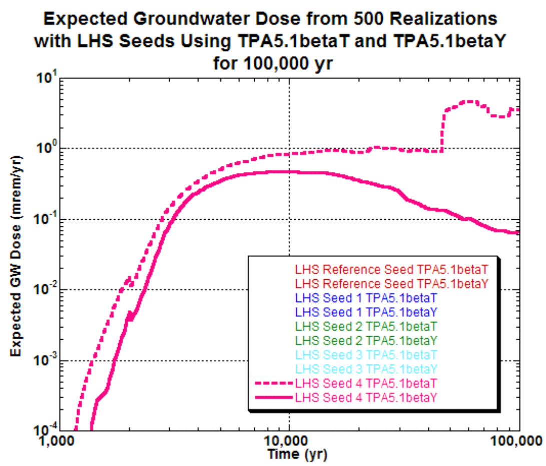



Expected Groundwater Dose from 500 Realizations with LHS Seeds Using TPA5.1betaT and TPA5.1betaY for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY


Expected Groundwater Dose from 500 Realizations with LHS Seeds Using TPA5.1betaT and TPA5.1betaY for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY


Expected Groundwater Dose from 500 Realizations with LHS Seeds Using TPA5.1betaT and TPA5.1betaY for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY


Expected Groundwater Dose from 500 Realizations with LHS Seeds Using TPA5.1betaT and TPA5.1betaY for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY


Expected Groundwater Dose from 500 Realizations with LHS Seeds Using TPA5.1betaT and TPA5.1betaY for 100,000 yr
Expected GW Dose (mrem/yr)
Time (yr)
LHS Reference Seed TPA5.1betaT
LHS Reference Seed TPA5.1betaY
LHS Seed 1 TPA5.1betaT
LHS Seed 1 TPA5.1betaY
LHS Seed 2 TPA5.1betaT
LHS Seed 2 TPA5.1betaY
LHS Seed 3 TPA5.1betaT
LHS Seed 3 TPA5.1betaY
LHS Seed 4 TPA5.1betaT
LHS Seed 4 TPA5.1betaY

20. Explanation for Differences in the GW, GS, and GWGS Expected Dose From TPA4.1 and TPA5.1betaT.

(all water contacts and enters the WP)
constant
Probability_WPWaterContact_GC-Flt-Ig
1.0
**
constant
Probability_WPWaterAllowance_GC-Flt-Ig
1.0

Number of WPs passed to EBSREL/RELEASET
(TPA51betaT: 10,000 yr and 401 realizations - basecase with volcanism flag on)

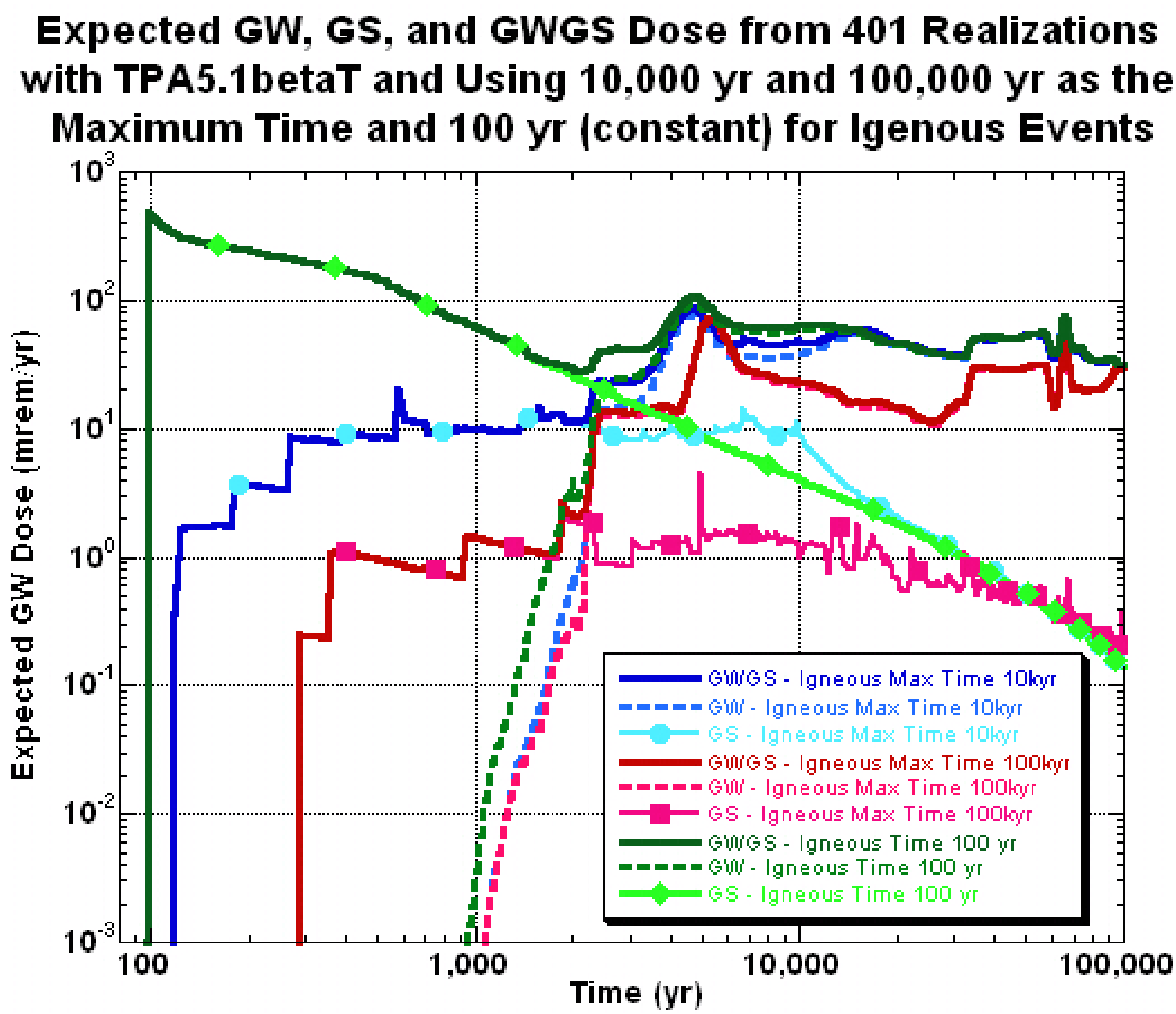
	#initial	#gencorr	#loccorr	#mechanical	#fault	#ign_act
Total WPs	252	0	41,069	19,034	0	1,544,887
Ave WPs/Real	0.6	0	102.4	47.5	0	3,852.6

Number of WPs passed to EBSREL/RELEASET
(TPA51betaT: 10,000 yr and 401 realizations - basecase NO volcanism)

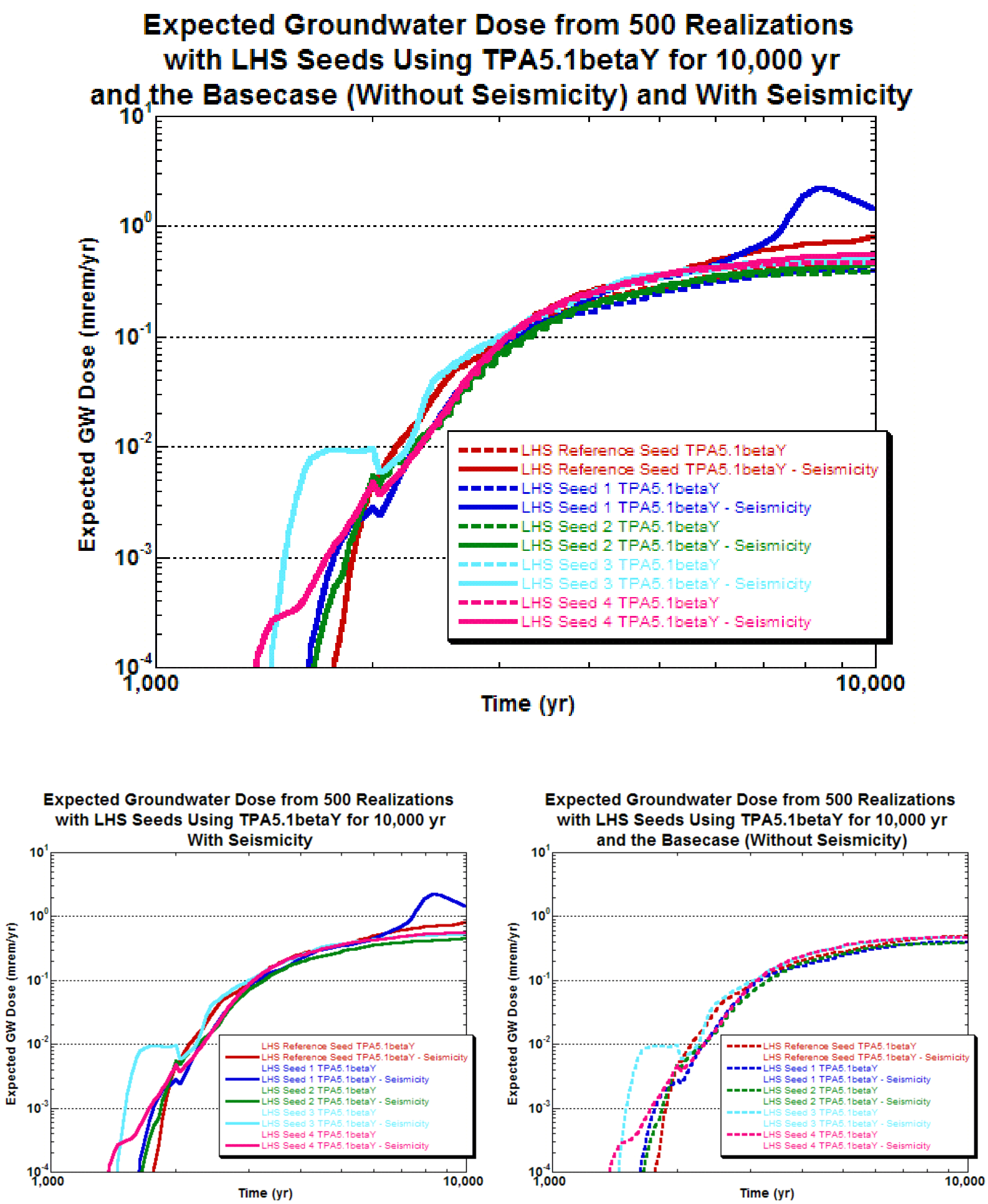
	#initial	#gencorr	#loccorr	#mechanical	#fault	#ign_act
Total WPs	252	0	59,419	20,456	0	0
Ave WPs/Real	0.6	0	148.2	51.0	0	0

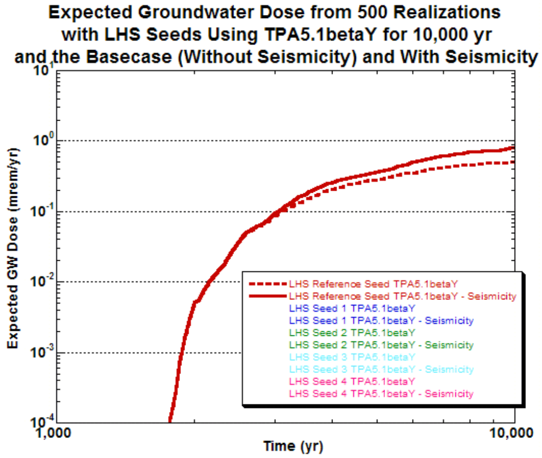
(Note: in the two runs above, the LHS parameters were the same; the only difference in the two runs was the volcanism flag was switched).

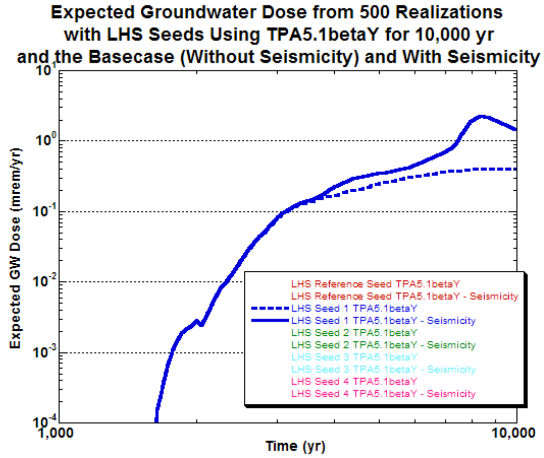
21. Plot of Expected Dose (GW, GS, and GWGS) From 401 Realizations Using TPA51betaT and Maximum Time for the Igneous Event of 10,000, and 100,000 yr and 100 yr (Constant).

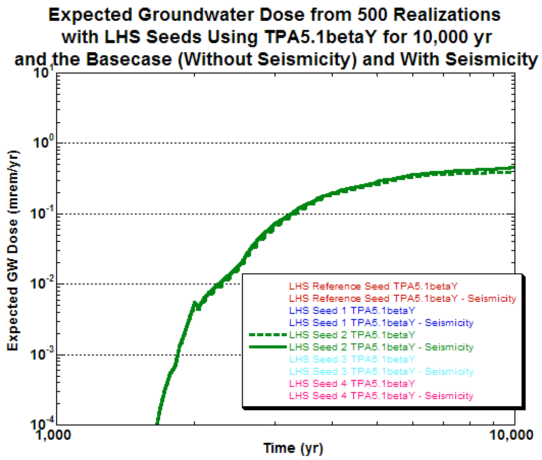


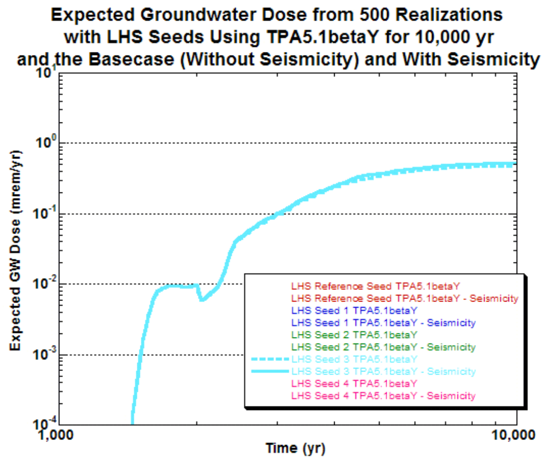
22. Plots of Expected Dose From 500 Realizations Using TPA51betaY and LHS Seeds With and Without Seismicity For 10,000 yr.

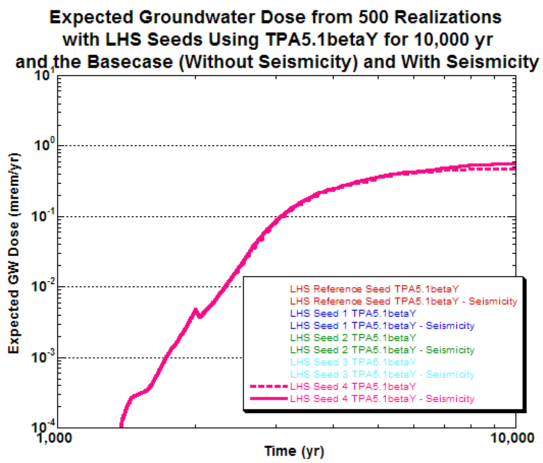



Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 10,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity

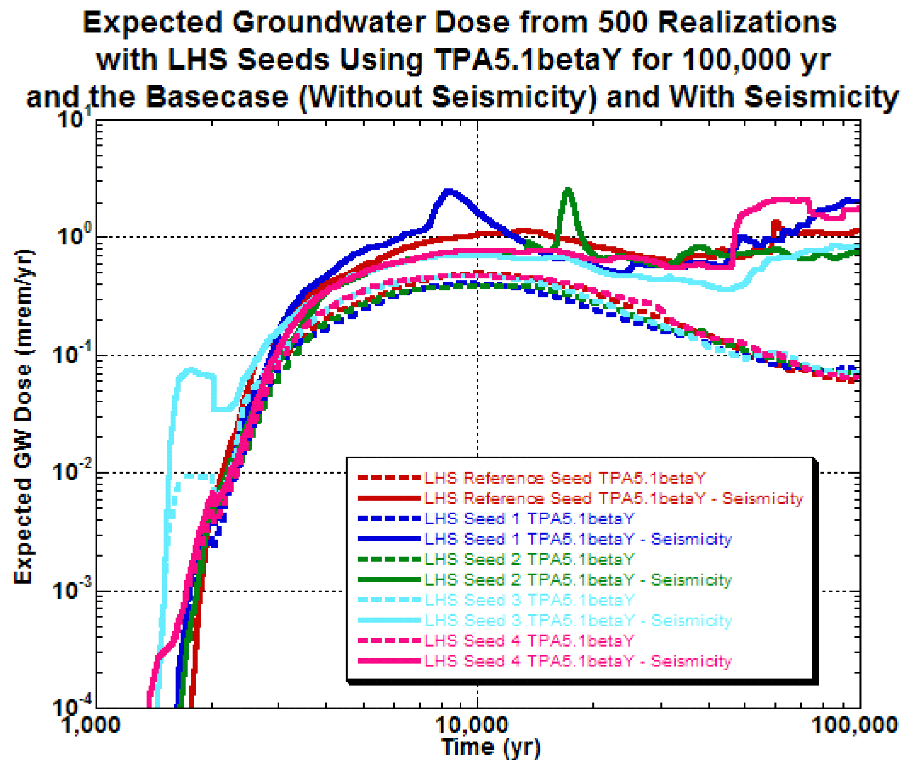

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 10,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity

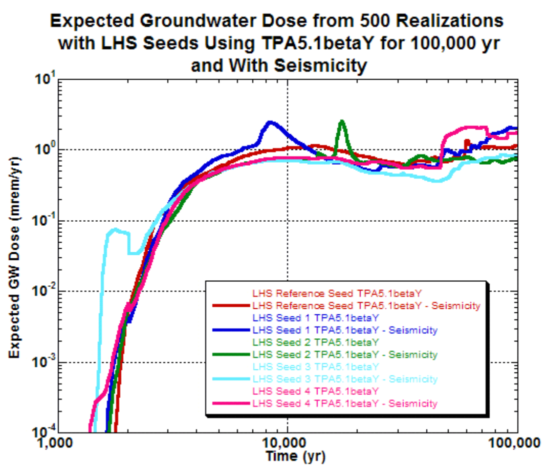

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 10,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity

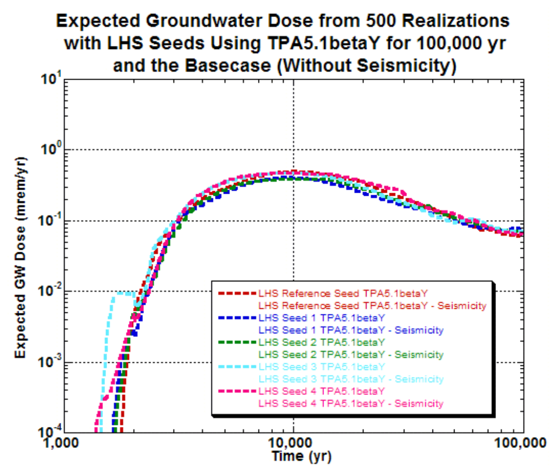

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 10,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity

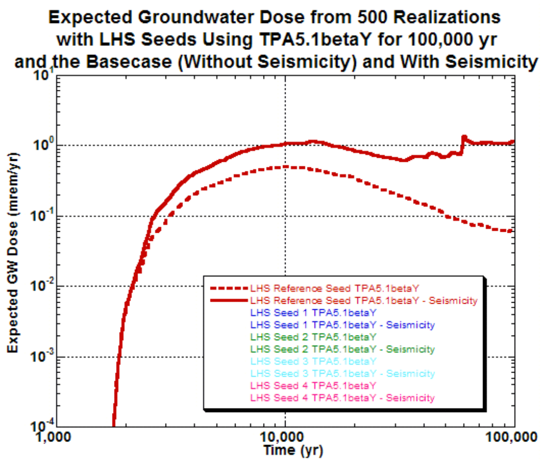

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 10,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity

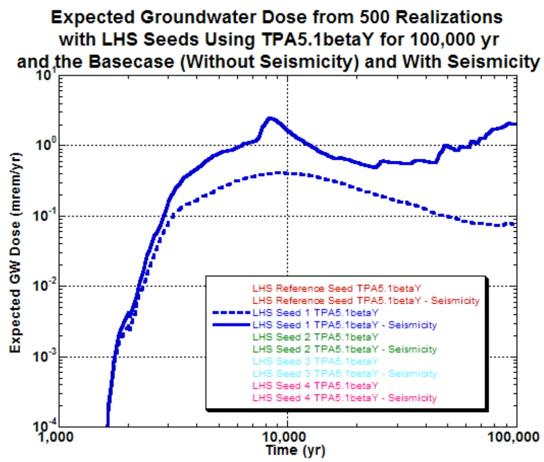
23. Plots of Expected Dose From 500 Realizations Using TPA51betaY and LHS Seeds With and Without Seismicity For 100,000 yr.

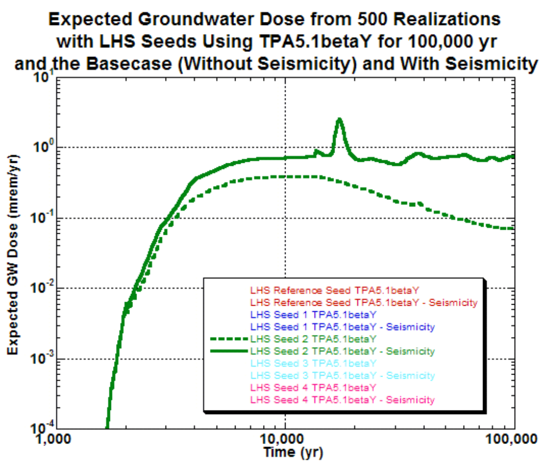


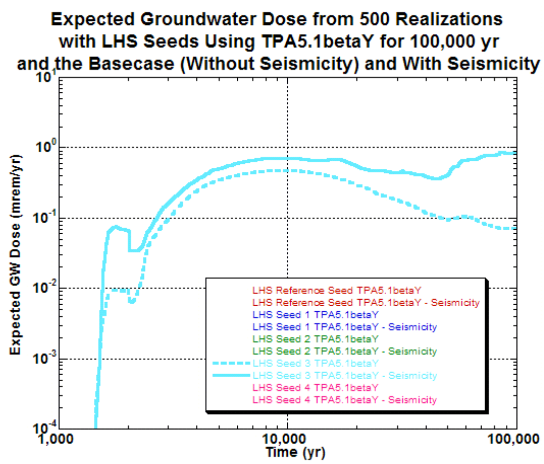


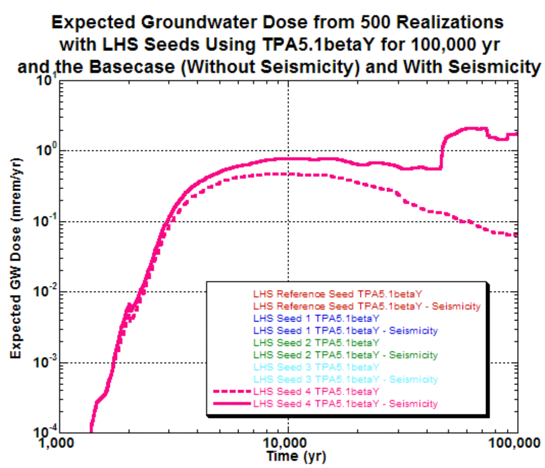



Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 100,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity

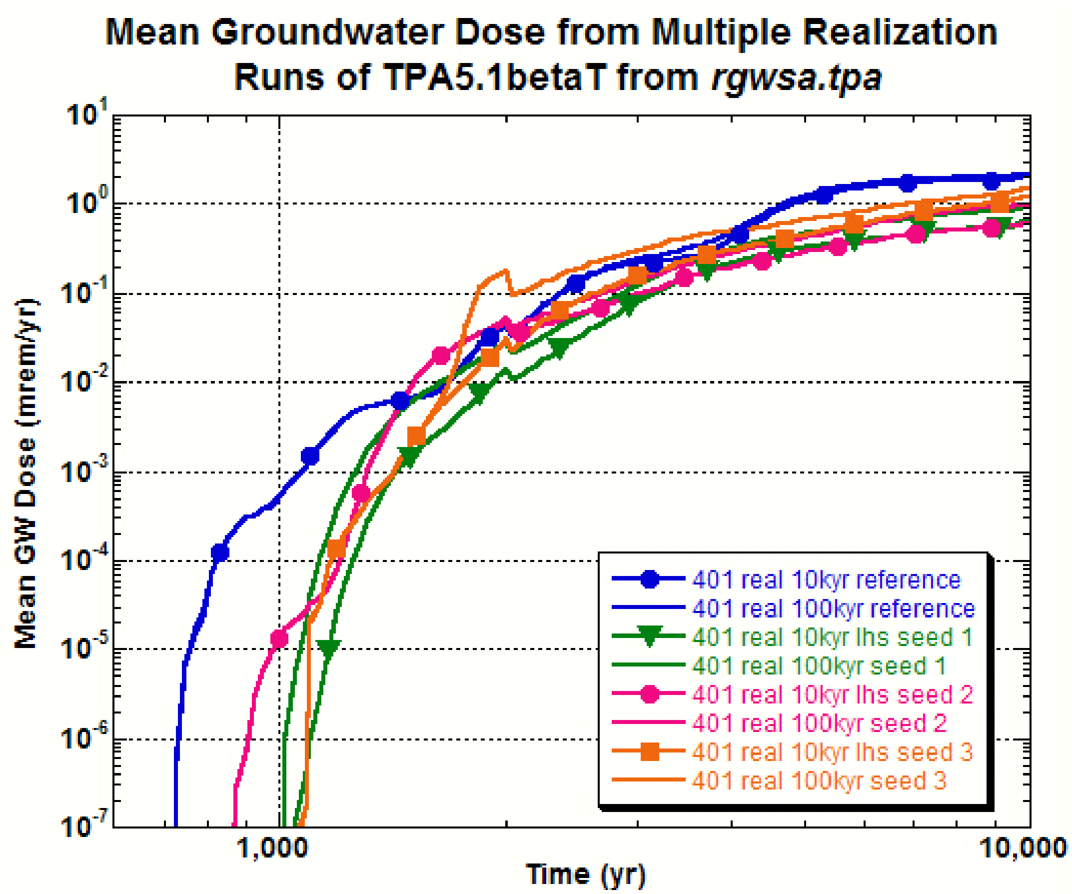

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 100,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity


Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 100,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity

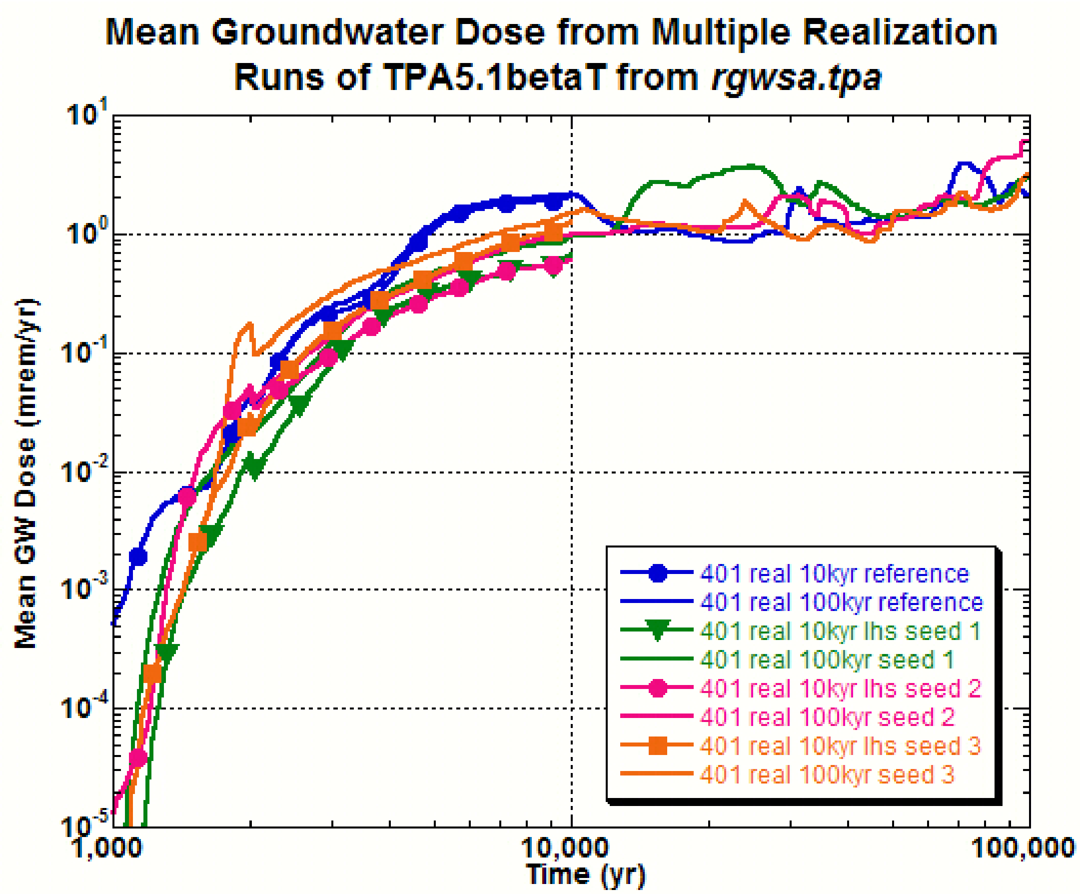

Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 100,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity


Expected Groundwater Dose from 500 Realizations
with LHS Seeds Using TPA5.1betaY for 100,000 yr
and the Basecase (Without Seismicity) and With Seismicity
Expected GW Dose (mrem/yr)
Time (yr)
1,000
10,000
100,000
LHS Reference Seed TPA5.1betaY
LHS Reference Seed TPA5.1betaY - Seismicity
LHS Seed 1 TPA5.1betaY
LHS Seed 1 TPA5.1betaY - Seismicity
LHS Seed 2 TPA5.1betaY
LHS Seed 2 TPA5.1betaY - Seismicity
LHS Seed 3 TPA5.1betaY
LHS Seed 3 TPA5.1betaY - Seismicity
LHS Seed 4 TPA5.1betaY
LHS Seed 4 TPA5.1betaY - Seismicity

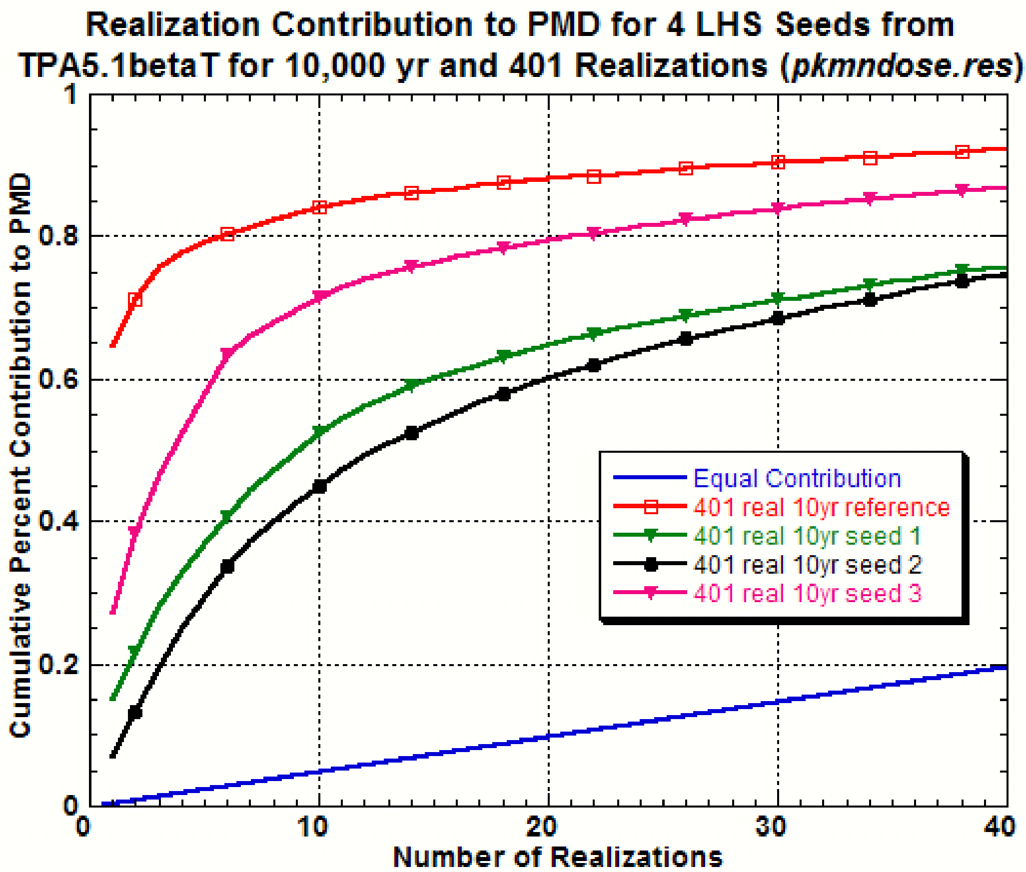
24. Plot of Mean Dose from 401 Realizations Using TPA51betaT and LHS Seeds for 10,000 yr.



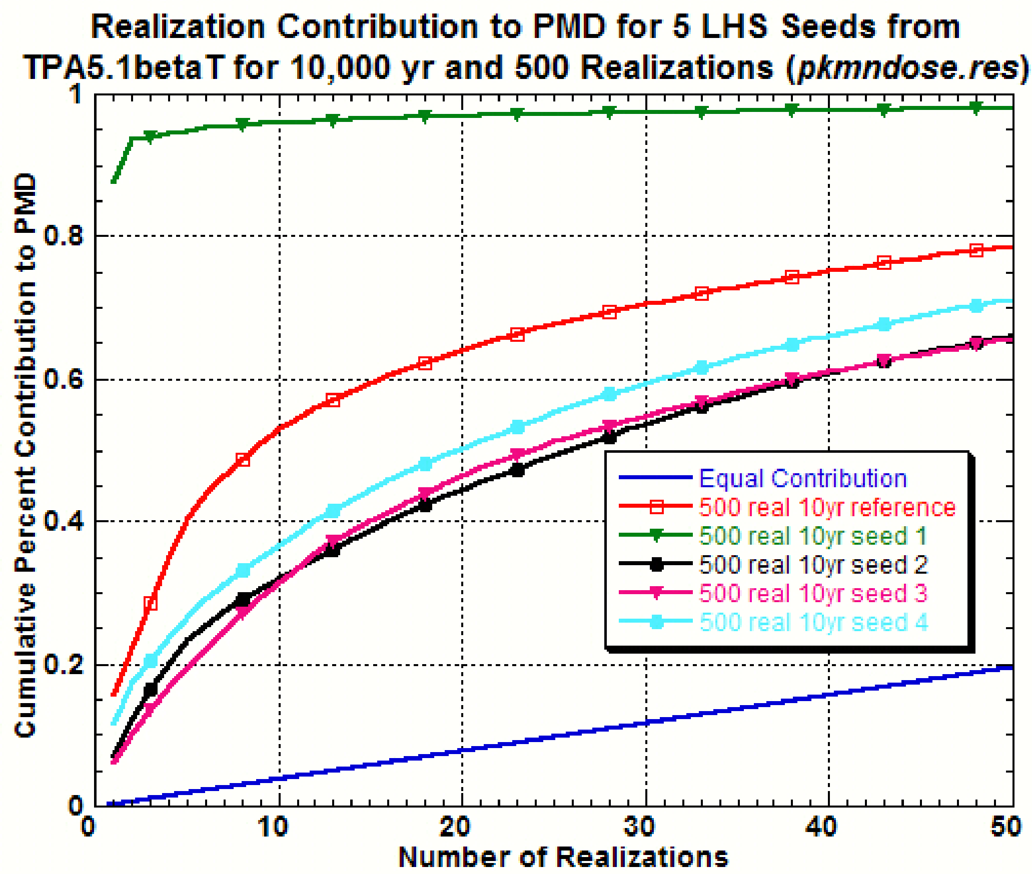
25. Plot of Mean Dose from 401 Realizations Using TPA51betaT and LHS Seeds for 100,000 yr.



26. Plot of Fraction Contribution to Peak Mean Dose by Realization from 401 Realizations Using TPA51betaT and LHS Seeds for 10,000 yr.



27. Plot of Fraction Contribution to Peak Mean Dose by Realization from 500 Realizations Using TPA51betaT and LHS Seeds for 10,000 yr



28. Understanding Results Using TPA5.1betaT from Realization 165 of 500 and LHS Seed1 for 10,000 yr.

Understanding Results - 10,000 yr / 500 realizations / Seed 1

PMD = 7.7 mrem/yr at 8,293 yr / 88% from Realization 165
(No releases in Subareas 1, 2, 6, and 9)

Dose
Highest annual dose GW pathway

Am243	2,856 mrem/yr	at 8,293 yr
Pu239	225 mrem/yr	at 8,490 yr
Cm245	96 mrem/yr	at 8,293 yr
Am241	94 mrem/yr	at 8,293 yr

Releases
Subarea 3 - Highest release rates from SZ
Ja243 10.6 Ci/yr/SA at 8,293 yr

WP failures
exec: failed WPs from MECHANICAL event = 1404 at TPA time = 5696.4 yr
*** failed WPs: 1404 out of 2904 *** (NOTE: Pallowance = 0.57)

Parameter Values
InitialSeepageReductionFractionByMechFailedWP
SFWettedFraction_MECH1 (These are correlated and equal to ~0.98)

29. More Understanding Results Using TPA5.1betaT from Realization 165 of 500 and LHS Seed1 for 10,000 yr.

Understanding Results

SA3 and Realization 165 of 500 with seed1 (PMD = 2,770 mrem/yr at 8293.3 yr)

There were no releases using sampled “mean values”. So used distributions for certain parameters and noted the following impacts on dose:

1. Force WP failures ContactAngleSubarea_3[degrees]
BulkingFactorRockTypeOneSubarea_3[]
(both were needed; resulted in ~1400 WP failures, instead of no WP failures)
PMD changed from 0.0 to 2.2 mrem/yr

2. SEISMIC Event hazardcurve modifications (this failed all WPs)

From reference:						To:					
1.0e-4	0.47	0.47	0.64	0.10	0.20	1.04e-4	2.44	4.75	0.53	0.30	0.60
1.0e-5	1.05	2.27	0.64	0.20	0.40	1.03e-4	2.44	4.75	0.53	0.30	0.60
1.0e-6	2.44	4.75	0.53	0.30	0.60	1.02e-4	2.44	4.75	0.53	0.30	0.60
1.0e-7	5.35	12.7	0.53	0.40	0.60	1.01e-4	2.44	4.75	0.53	0.30	0.60
1.0e-8	5.35	12.7	0.53	0.40	0.60	1.00e-4	2.44	4.75	0.53	0.30	0.60

PMD changed from 2.2 to 2.7 mrem/yr (because all WPs failed)

3. Flow uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr]
uzflow_HydraulicPropertyUncertaintyDeviation[N(0,1)]
uzflow_LongTermAverageFootprintAverageMAI[mm/yr]
SubAreaWetFraction
WastePackageFlowMultiplicationFactor
X0FmultCoefficient
PMD changed from 2.7 to 3.4 mrem/yr.

4. Colloid Retardation ColloidRetardationFactor_SAV_[]
ColloidRetardationFactor_STFF[]
PMD changed from 3.4 to 966 mrem/yr.

5. Water Contact SFWettedFraction_MECH1
InitialSeepageReductionFractionByMechFailedDS
InitialSeepageReductionFractionByMechFailedWP
PMD changed from 966 to 2,750 mrem/yr.

6. Colloid Sorption SorptionCapacity[moles/m3]
PMD changed from 2,750 to 1,960 mrem/yr.

7. SF Dissolution Preexponential_SFDissolutionModel2
PMD changed from 1,960 to 4,790 mrem/yr at 8896.6 yr.

DISCUSSION OF RESULTS

This section discusses information contained in Items 1 through 29, which are provided in the previous section. The items provide plots, tables, TPA input and output files, and analyses of results from the S-4 numerical stability validation tests and satisfies the testing objectives and requirements listed in the Software Validation Plan. That is, using the TPA5.1betaT code and consistent with the Test Procedure section, all test cases were completed and the analyses conducted, namely "…in *pkmndose.res*, analyses will be conducted to determine whether any single realization (or a few realizations) have a disproportionately high contribution to the peak mean dose; for these realizations, the TPA code outputs will be evaluated to determine the reasons for its disproportionately high contribution to the peak mean dose. For each type of test, the results will be plotted."

There are a number of plots which contain dose results for all realizations followed by corresponding dose results for one of the realizations. These plots are intended to show both the overall trend of dose results and also the dose results for one of the realizations.

Additionally, during S-4 validation testing activities, TPA code modifications were accomplished and the TPA code revised in releases TPA5.1betaU through TPA5.1betaY. Comparison S-4 testing was also conducted and plots generated to evaluate the effects of these modifications on TPA code results and numerical stability. These plots are also contained in this attachment.

For every test related to the S-4 numerical stability task, all the input and output files, executables, source code, and data files are archived on DVDs for Task S-4. The top level of the subdirectory hierarchy structure on the DVDs is either number of realizations, scenario (faulting or igneous), time step, 1,000,000 yr (called NRC_1e6yr), or comparison runs. Subsequent levels consist of simulation time (only 10,000 and 100,000 yr) and LHS/SEISMIC seeds.

Item 1 of the Test Results section provides a matrix showing all of the tests identified in the S-4 Test Procedure. All of the 215 tests were completed and the results archived on DVDs. Each test utilized TPA5.1betaT with a *tpa.inp* file modified for either number of realizations, simulation period, values for LHS and SEISMIC seeds, number of time steps, and scenario evaluated (i.e., basecase, faulting, and igneous).

An indication of numerical stability in the peak mean dose is illustrated in Items 2 and 3 for the nominal scenario. For simulation times of 10,000 yr and 100,000 yr, Item 2 presents plots of peak mean dose and time of the peak mean dose with 401, 450, 500, 600, 700, 800, 900, and 1,000 realizations, five different LHS seeds (i.e., 1456789101.0, 1567894101.0, 1678945101.0, 1789456101.0, and 1894567101.0), and five different SEISMIC seeds (i.e., 1456789101.0, 1945678101.0, 1894567101.0, 1789456101.0, and 1678945101.0). The results from the 1,000,000 yr simulations in Item 2 are for 401, 600, and 1,000 realizations, four LHS seeds, and four SEISMIC seeds. Item 3 lists the values of the peak mean dose and time of the peak mean dose which are plotted in Item 2. Evaluation of these plots and tables suggests the peak mean dose is not entirely stable. For example, for 10,000 yr and 500 realizations, the five LHS seeds, named reference, seed 1, seed 2, seed 3, and seed 4, yield peak mean doses of 0.82, 7.66, 0.45, 0.50, and 0.54 mrem/yr, respectively. That is, the peak mean dose for seed 1 is approximately an order of magnitude greater than the peak mean dose from the other four seeds. The reason for this variability is attributable to a single realization and, later in this section, an analysis is presented to investigate this behavior. As will be seen, it is the result of relatively rare realizations that include a combination of early mechanical failures with sampled colloid transport parameters that result in rapid transport of colloid species. Based on this result, TPA Version 5.1BetaY included a change to remove seismic disruption from the nominal case so that it can be considered as a separate disruptive scenario using appropriate analytical techniques to estimate confidence in the mean dose estimates.

Similar to Items 2 and 3, the plots and tables in Items 4 and 5 provide an indication of numerical stability in the peak mean dose for the faulting and igneous disruptive scenario. For the igneous scenario, the ground surface, groundwater, and total (ground surface + groundwater) peak mean doses are presented in Items 4 and 5. For simulation times of 10,000 yr and 100,000 yr, Item 4 presents plots of peak mean dose and time of the peak mean dose with 401, 450, 500, 600, 700, 800, 900, and 1,000 realizations and the reference seed. The results from the 1,000,000 yr simulations in Item 4 include 401, 600, and 1,000 realizations and the reference seed. Item 5 lists the values of the peak mean dose and time of the peak mean dose which are plotted in Item 4. As with Items 2 and 3, an evaluation of the these plots and tables suggests the peak mean dose is not stable. For example, for 100,000 yr and 401, 450, 500, 600, 700, 800, 900, and 1,000 realizations with faulting, the peak mean doses are 3.99, 10.34, 2.12, 1.44, 3.94, 5.43, 4.87, and 4.99 mrem/yr, respectively. That is, the peak mean dose for 450 realizations is about 2–7 times greater than the peak mean doses from the other simulations. The reason for this variability is attributable to a single realization and, again, later in this section, an analysis is presented to identify reasons for this behavior.

The effects of time step size on the numerical stability of the mean groundwater dose are plotted in Item 6 for simulation times of 10,000, 100,000, and 1,000,000 yr, 401 realizations, the reference seed, and the TPA5.1betaT nominal case. Previous TPA code analyses typically used 201 time steps with an increasing time step size for simulation times of 10,000 yr. That is, the first time step was about 3 yrs and the time step size increased until the size of the last time step was about 300 yr. For simulation times of 100,000 yr, it was typical to use 401 time steps with the first 201 time steps set the same as for 10,000 yr, and then from 10,000 to 100,000 yr the remaining 200 time steps were uniform at 450 yr. The maximum number of time steps in the TPA code is 5001 and this test assesses numerical stability for that maximum number of time steps in 1,000,000 yr simulations. Note that for tests with simulation times greater than 10,000 yr and more than 201 time steps, the validation tests employed the same 201 time steps in the first 10,000 yr and the remaining time steps were used in 10,000 yr to the simulation end time. For purposes of this time step size test, the mean dose is considered to be numerically stable when visual examination of the plots in Item 6, for any particular simulation time, show the results for a given number of time steps are consistent with the results from the test having the largest number of time steps. Evaluation of the results in Item 6 suggests that numerical stability is achieved in 10,000 yr with at least 101 time steps, at least 401 time steps in 100,000 yr, and at least 1,001 time steps in 1,000,000 yr.

During validation activities, the TPA code was revised and versions TPA5.1betaU through TPA5.1betaY were released. To evaluate any impact of these modifications on the mean dose, especially in relation to the TPA5.1betaT code which was used for this validation testing, additional TPA code simulations were accomplished and the mean doses plotted. Items 7 and 8 display results from both TPA5.1betaT and TPA5.1betaW. In TPA5.1betaW, the mean doses in Item 7 and 8 exhibit delayed and decreased doses; although by the end of the 10,000 yr and 100,000 yr simulation times, the mean doses become more consistent. Item 8 also reveals the slight dependence of the results on simulation time. This dependence is expected and related to the differences between releases prior to 10,000 yr from waste packages failing after 10,000 yr during the 100,000 yr simulation. The differences between the mean dose from TPA5.1betaT and TPA5.1betaW are attributable to modifications related to the colloids source term and unsaturated zone filtering of colloids. Other changes were incorporated into the TPA code, but the changes were mainly related to reformatting and were not expected to affect the TPA code results.

Item 9 illustrates the relative magnitudes and timing of the ground surface and groundwater contributions to the total mean dose. Results are provided from 10,000, 100,000, and 1,000,000 yr using 401 realizations and the reference seeds. Furthermore, the simulations were conducted both with and without volcanism using TPA5.1betaT. The results show the mean dose is about 10 mrem/yr and is dominated by the ground surface contribution prior to 2,000 yr;

thereafter, the groundwater dose from intrusive volcanism dominates through 1,000,000 yr with a maximum of 50-100 mrem/yr. Note that, in these plots, the mean dose without volcanism (i.e., no extrusive and intrusive volcanism) is about 0.5 mrem/yr. These results highlight the large effect of both extrusive and intrusive waste package failures on mean dose.

Items 10 and 11 contain plots of the expected groundwater dose for 400, 450, 500, 600, 700, 800, 900, and 1,000 realizations in 10,000 and 100,000 yr using the reference seeds and the TPA5.1betaT code. These plots emphasize and further illustrate the conclusions from Items 2 and 3 regarding the lack of numerical stability in the dose and from Item 8 regarding the slight dependence of the dose on simulation time.

Items 12 and 13 contain plots of the expected groundwater dose, both with and without faulting, for 400, 450, 500, 600, 700, 800, 900, and 1,000 realizations in 10,000 and 100,000 yr using the reference seeds and the TPA5.1betaT code. Again, these plots emphasize and further illustrate the conclusions from Items 4 and 5 regarding the lack of numerical stability in the dose, most significantly in relation to dose results from the 450 realization simulation.

Items 14 and 15 contain plots of expected ground surface and groundwater dose, both with and without volcanism, for 400, 450, 500, 600, 700, 800, 900, and 1,000 realizations in 10,000 and 100,000 yr using the reference seeds and the TPA5.1betaT code. Once again, these plots emphasize and further illustrate the conclusions from Items 4, 5, and 9 regarding both the lack of numerical stability in the dose and the magnitudes and relative contributions of the ground surface and groundwater to the mean dose.

The information included in Item 16 is a detailed analysis of the faulting results presented in Items 4, 5, 12, and 13. This item examines Realization 343 out of 450, since this realization exhibits a disproportionately high contribution to the mean dose (over 90% of the peak mean dose). The screenprint is provided from the TPA5.1betaT basecase with and without faulting for 10,000 yr. The mean dose at 10,000 yr from this realization is 8.6 mrem/yr without faulting and 820 mrem/yr with faulting; whereas the peak mean dose is about 200 mrem/yr at about 6,000 yr without faulting and 4,400 mrem/yr at 4,100 yr with faulting. Following the screenprints in Item 15, Item 16 provides values for a number of *tpa.inp* file parameters and their associated quantiles, the number of waste packages failed by the faulting event, and the impacts on the peak mean dose of using mean values instead of the sampled values. The analysis identified the SAV (saturated zone alluvium) colloid retardation factor as the *tpa.inp* parameter with the greatest impact on peak mean dose. This parameter caused a more than three order of magnitude decrease in the peak mean dose when using the mean value (approximately 500) instead of the sampled value (1.2). These conditional results suggest stability of the mean could be improved by focusing future work on data or analyses to narrow the large range of uncertainty in the value of the colloid retardation factor. Because faulting is treated as a separate scenario class, these results are conditional and appropriate analytical techniques are required to understand the confidence bounds on the peak mean dose results and to express the results in terms of dose risk. Application of such techniques are beyond the scope of this validation exercise, which is aimed solely at understanding effects of faulting on stability of peak mean dose estimates.

The version of the TPA code released at the end of the testing was 5.1betaY. Items 17, 18, and 19 compare sampled parameters and results between TPA5.1betaT and TPA5.1betaY. Because of the potentially large numbers of mechanically-breached waste packages, it is significant, in terms of affecting the mean dose, to note that the flag for seismicity (a non-sampled parameter) was changed from “1 ” (ON) to “ 0” (OFF) in the TPA5.1betaY *tpa.inp* file. Attachment C of the S-4 validation task report provides additional discussion of the basis for turning off the seismic flag for the reference case. All of the changes in sampled parameter distributions are provided in Item 17. The minimum and maximum values of the UZFLOW parameters uzflow_FootprintAverageMeanAnnualInfiltrationAtStart[mm/yr] and uzflow_LongTermAverageFootprintAverageMAI[mm/yr] were modified; the minimum values for the MECHFAIL parameters BulkingFactorRockTypeOneSubarea_X, where X=1,10 (number of subareas), were modified; and the maximum value for the FAULTO parameter TimeOfNextFaultingEventinRegionOfInterest[yr] was increased. The number of sampled parameters was unchanged. These changes are expected to have only a small effect on the mean dose. Therefore, a meaningful comparison can be made between results from TPA5.1betaT and TPA5.1betaY, since the main differences between the TPA5.1betaT and TPA5.1betaY versions were turning the seismicity flag OFF and code modifications that were included in TPA5.1betaW (see the results in Items 7 and 8 for the effects of the TPA5.1betaW changes on mean dose). For Items 18 and 19, expected groundwater doses from the TPA5.1betaT and TPA5.1betaY codes are plotted for 500 realizations, the five LHS seeds, and 10,000 and 100,000 yr, respectively. The results, together with the results in Items 7 and 8 for TPA5.1betaW, indicate the mean dose is more stable in TPA5.1betaY and the increased stability is attributable to excluding the effects of seismicity.

Items 20 and 21 present information related to the ground surface and groundwater doses included in Items 4, 5, 9, 14, and 15. These results were generated using TPA5.1betaT for 401 realizations, the reference seed, with and without volcanism, and either 10,000 or 100,000 yr as the maximum time of the volcanic event. Item 20 shows there is an average of about 4,000 waste packages failed by intrusive volcanism. In separate calculations with the TPA4.1j code, there was an average of about 100 waste packages failed by intrusive volcanism. Additionally, all of the water that contacts waste package failed by intrusive volcanism enters the waste package (i.e., Pallowance = Pcontact = 1.0). It was verified that the simulations with and without volcanism used the same sampled parameter values. Item 21 shows the effects on the ground surface, groundwater, and total dose of increasing the maximum time of the volcanic events from 10,000 to 100,000 yr and also using 100 yr (constant) as the time of the volcanic event. As expected, by spreading the time of the igneous event out over 100,000 yr instead of 10,000 yr, the doses are also shifted out in time. Also, as expected, by setting the time of all volcanic events at 100 yr, the ground surface dose is shifted to an earlier time and the peak dose is greater. It is interesting is note that the groundwater dose is relatively insensitive to the time of the volcanic event. From discussions between NRC and Center staff, it was agreed that the maximum time of the volcanic events should be equal to the maximum simulation time.

Items 22 and 23 compare expected doses from the TPA5.1betaY code with and without seismicity. These items are a follow-up to the analyses in Items 17, 18, and 19. For this item, results are plotted using 500 realizations, five LHS seeds, with and without seismicity, and for 10,000 and 100,000 yr, respectively. The plots are consistent with the previous discussion for Items 17, 18, and 19 and verify that the effects of turning seismicity OFF in the TPA5.1betaY code are that the dose is more stable and the increased stability is attributable to the effects of seismicity.

Items 24 and 25 contain plots of the mean dose from TPA5.1betaT for 401 realizations, four LHS seeds, and 10,000 and 100,000 yr, respectively. As with a number of items discussed previously, the results plotted in Items 24 and 25, especially for 100,000 yr, exhibit instability in the behavior of the mean dose.

Items 26 through 29 are useful in identifying whether a few realizations dominate the mean dose, and once identified, in analyzing those dominate realizations to determine the reasons for the high-dose behavior. The fraction each realization contributes to the peak mean dose is plotted in Item 26 for 401 realizations and Item 27 for 500 realizations using TPA5.1betaT, 10,00 yr, and LHS seeds. From these plots, the realization with the highest contribution to the peak mean dose is about 10-30% of the peak mean dose, except for two cases in which the contributions are about 65% (401 realizations with the reference seed) and 90% (500 realizations and LHS seed 1). The latter is analyzed in detail in Items 28 and 29 to identify the reasons for the high dose in this one realization. Realization 165 out of 500 showed a peak dose of about 2,800 mrem/yr occurring at 8,300 yr. The initial analysis is provided in Item 28, while the follow-up analyses is included in Item 29. Both of these items discuss the reasons contributing to the high dose. Waste package failure is certainly needed and there are a large number of mechanically failed waste package in this realization. However, other conditions are needed to transport the radionuclides from the EBS to the receptor location. The *tpa.inp* file parameters which were identified as having an influence on the high dose are listed in Item 29. Just as with the discussion in Item 16, the *tpa.inp* parameter with the largest effect on the peak dose was the SAV colloid retardation factor. This parameter had an almost three orders of magnitude effect on the peak dose when the sampled value for the parameter was used instead of the mean value. That is, the peak dose was 996 mrem/yr (sampled value) compared to 3.4 mrem/yr (mean value).

CONCLUSIONS

The conclusions from the S-4 validation testing are summarized below. The information provided throughout this attachment forms the bases for the following conclusions.

1. Using the TPA5.1betaT code and different LHS and SEISMIC seeds, the mean dose results for the nominal scenario are not numerically stable for the time periods and number of realizations assessed in the testing (i.e., 10,000, 100,000, and 1,000,000 yr and 401, 450, 500, 600, 700, 800, 900, and 1,000 realizations). It was not possible to establish a reasonable range of numerical stability and convergence based on these tests.

2. Using the TPA5.1betaT code and the reference seeds, the mean dose results for the igneous and faulting cases of the disruptive scenario are not numerically stable for the time periods and number of realizations assessed in the testing (i.e., 10,000, 100,000, and 1,000,000 yr and 401, 450, 500, 600, 700, 800, 900, and 1,000 realizations). It was not possible to establish a reasonable range of numerical stability and convergence based on these tests.

3. For time step size, results indicate numerical stability of the mean dose is achieved in 10,000 yr with at least 101 time steps, in 100,000 yr with at least 401 time steps, and in 1,000,000 yr with at least 1,001 time steps. The criterion for numerical stability, for a given number of time steps and simulation time, is consistency with the results for the maximum number of time steps evaluated in the test.

4. In detailed analyses intended to identify *tpa.inp* file parameters with large impacts on the peak mean dose for specific realizations, the SAV colloid retardation factor was a highly influential parameter. In two separate analyses, the SAV colloid retardation factor resulted in about three orders of magnitude decrease in dose when using the mean value compared to the sampled value.

5. Based on results from TPA5.1betaT in items 1 and 2 above, it was deemed necessary to consider seismic disruption as a separate scenario class, which is reflected in TPA5.1betaY code, which does not include seismic disruption in the nominal case. Comparison of TPA5.1betaT and TPA5.1betaY results show that the mean dose is stable when seismicity is not active.

6. Analyses of realizations with doses that dominant the mean dose, combined with the stable results from TPA5.1betaY, indicate stability of the mean dose is most affected by *tpa.inp* file input parameters (e.g., SAV colloid retardation factor) and seismicity (i.e., mechanically breached waste packages). Thus, the numerical stability of the mean dose is explainable based on the input parameters and model.

Following the change to remove seismic disruption from the nominal case in TPA5.1betaY code, the mean dose results exhibit reasonable statistical stability for a variety of simulation time periods of interest. Therefore, the stated criterion of Task S-4 is met. Attachments B and C follow, which contain supplemental analyses to further probe numerical stability convergence of the Igneous Extrusive Model scenario (Attachment B) and to evaluate the potential effects on convergence from seismic induced waste package mechanical failures (Attachment C).

The input files and results of these tests are archived on four DVDs labeled “TPA Version 5.1 Task S-4, Attachment A.”

TEST EVALUATION (PASS/FAIL): **PASS**

Attachment B
TPA Version 5.1 Validation Task S-4
Convergence of Igneous Extrusive Models

TEST PROCEDURES

1. Execute TPA5.1 version BetaU for the two extrusive igneous models ASHPLUME/ASHREMOVO/DCAGS and TEPHRA/ASHREMOB.

2. Compare convergence of the mean doses produced by the TEPHRA/ASHREMOB model for 200, 500, 1000 and 1700 realizations.

3. Compare convergence of the ASHPLUME/ASHREMOVO/DCAGS model for 1000 realizations and two different random seeds.

4. Compare raw sampling results for the mean dose from ASHPLUME/ASHREMOVO/DCAGS to the mean produced by the "convolution" approach. Use either 100 or 200 realizations per event time.

All TPA runs were limited to 10,000 years because the peak mean doses are likely to occur in this range.

TEST CRITERIA

Results of these tests should show how well-converged the mean dose is for the stated number of realizations in the tests. Differences between the two models should be explained. Results from raw sampling of the ASHPLUME/ASHREMOVO/DCAGS model should also be compared to the convolution approach and differences between the two results explained.

SOFTWARE USED IN EXERCISES

A set of short FORTRAN codes and DOS batch files was developed to facilitate the use of the convolution approach, and for demonstrating the differences between the two models for fixed event times. Program CHANGEAGE.for was used to alter the tpa.inp file by changing the year of burial (AverageCalendarYearAssumedForEmplacement[A.D.]) with the event time held constant at 100 years. The calender date of waste burial was changed for each of the 20 runs, with either 100 or 200 realizations per run. In addition, there was a program to convolute the output files for the 20 event times (program CVOLC4.exe), and a DOS batch file to execute the programs (RUNVOLC.bat) for the 20 runs.

DESCRIPTION OF TEST RESULTS

There are two alternative models for extrusive volcanism in TPA 5.1:

- The original methodology, ASHPLUME/ASHREMOVO/DCAGS, henceforth referred to as ASHPLUME, which is based on a volcanic plume that is always directed toward the RMEI, and

- The TEPHRA/ASHREMOB methodology, henceforth referred to as "TEPHRA", which accounts for a distribution of wind directions, and for remobilization of deposited ash by fluvial and aeolian processes.

There are several sets of runs compared:

- Runs for the TEPHRA model, used to calculate the mean dose average over all realizations for 200, 500 and 1000 realizations. Note that the calculated dose for this case used the random sampling ("raw" sampling) of the event time (TimeOfNextVolcanicEventinRegionOfInterest[yr]), and produced a non-smooth output for the mean dose from the output file *rgssa.tpa* produced from the TPA code. The peak-of-the-mean dose was therefore estimated visually from the output curve. Furthermore, the dose calculated was conditional, assuming that the event happened exactly once per 10,000-year computational interval, and had to be multiplied by 0.001 to correct it to a recurrence frequency of 10^{-7} per year.

- 1000-vector "raw" sampling of the ASHPLUME model was used to calculate the mean dose averaged over all realizations. As in the case described above, the TPA code used the random sampling of event time, which produced an even-more irregular curve, so the peak-of-the-mean dose was estimated visually. This figure was plotted from the *rgssa.tpa* file, also correcting for the recurrence frequency by multiplying dose by 0.001.

- A mean dose curve for the ASHPLUME model was generated by the convolution method; i.e., generate mean dose curves with a fixed event time but different burial ages, then convolute the curves into a mean dose curve representing a random event time. This required the generation of 20 mean dose curves, each with 100 realizations.

- The same convolution method as above, but using 200 realizations rather than 100 realizations.

CONVERGENCE OF THE TEPHRA MODEL RESULTS

Figure 1 shows the convergence of the mean dose for the default TEPHRA model using 200, 500, 1000 and 1700 realizations. The 1700-realization results were synthesized by concatenating the 200, 500 and 1000-realization results, assuming that the runs are approximately statistically independent. Figure 1 illustrates that the mean has reached a nearly stable state by 1700 realizations for the TEPHRA model. This will be shown not to be the case for the ASHPLUME model, but the differences can be explained adequately. However, see the discussion on the advisability of using equally spaced time intervals for these calculations.

CONVERGENCE OF THE ASHPLUME MODEL RESULTS

Mean dose curves are shown in Figure 2 for the ASHPLUME model using 1000 vectors and two random seeds. These results are also compared to the TEPHRA results for 1000 realizations as a reference and to the convolution results for the ASHPLUME model. The following observations can be drawn from these calculations:

- The peak-of-the-mean dose from the TEPHRA methodology is about 0.01 millirem (1E-5 rem), whereas the peak-of-the-mean dose from the ASHPLUME methodology is higher [e.g., approaching 0.03 millirem (3E-5 rem) with the convolution approach in Figure 2.

- The peak for the TEPHRA model occurs later than the peak for ASHPLUME. This is to be expected because the time constant for remobilization is much longer than the ash deposition and removal processes in the ASHPLUME methodology.

- Using "raw" sampling of event time for the ASHPLUME methodology gives irregular, but still useful results if at least 1000 realizations are used. Figure 3 shows the ASHPLUME results with two different random seeds.

- Convolution results are also shown in Figure 3 for 20 unequally spaced event times and 100 realizations. Results using 200 realizations produced nearly identical results, indicating that 100 realizations is adequate for this calculation.

- In Figure 3, the mean dose curve derived with the convolution approach appears to fall off more quickly with time than the raw sampling approach. However, this appears to be a computational artifact of the raw sampling with variable time steps. Since the time steps increase with time, the relatively high but short-lived peaks produced by the ASHPLUME model cannot be resolved adequately at the high end of the time scale. This leads to an artificial lengthening of the tails of the dose curves for later event times, which has the effect of increasing the apparent mean dose. Figure 4 shows the calculation of the mean dose from raw sampling with the default variable time steps (201 steps) and an alternative run for the same case, but using 1000 equally spaced time steps, which more accurately capture the shape of the dose results for later events. The latter case agrees more closely with the convolution approach with regard to the fall-off of mean dose with time.

- Figure 5 shows the mean doses averaged over 100 realizations for both the ASHPLUME and TEPHRA models at several fixed event times. Although the ASHPLUME results show a much higher peak than the TEPHRA results for the same event times, the doses decay much faster. The longer time constant exhibited by the TEPHRA model lead to a smoother output than the ASHPLUME case for the total mean dose curve.

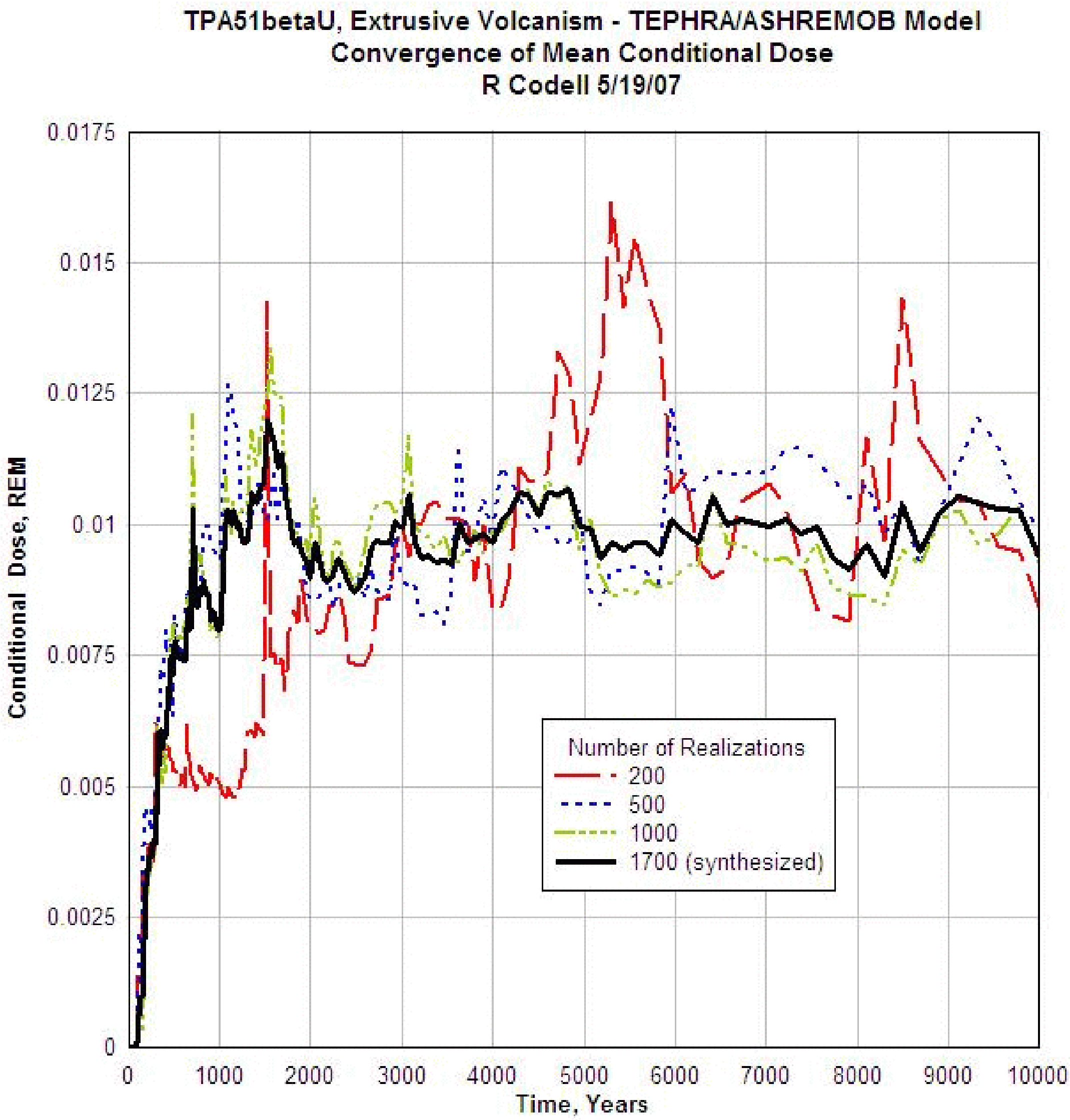


Figure 1. Convergence of the mean dose for the TEPHRA model, using 200, 500, 1000, and 1700 realizations, and unequal time steps (1700 realizations concatenated from other results; see text).

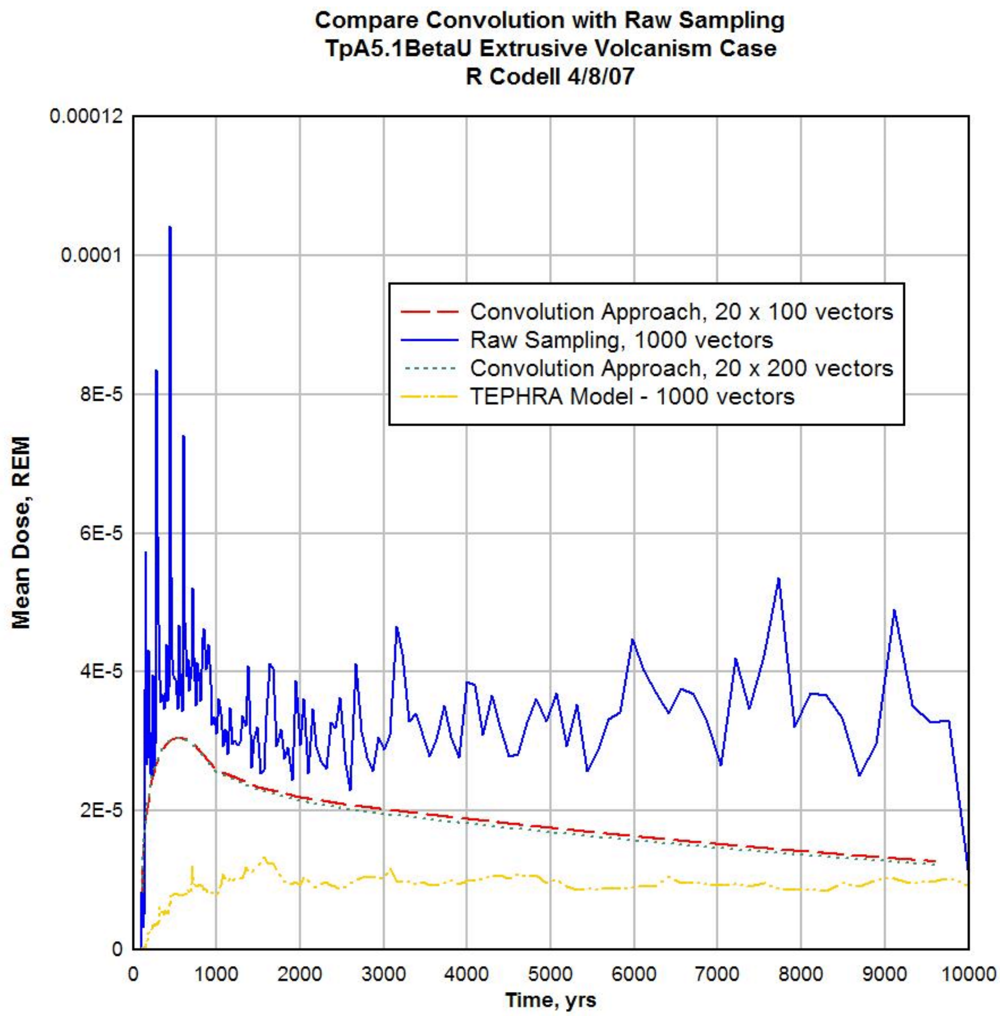


Figure 2. Comparison of ASHPLUME and TEPHRA models for extrusive volcanism using uneven time steps, and convolution results (20 event times, 100 realizations).

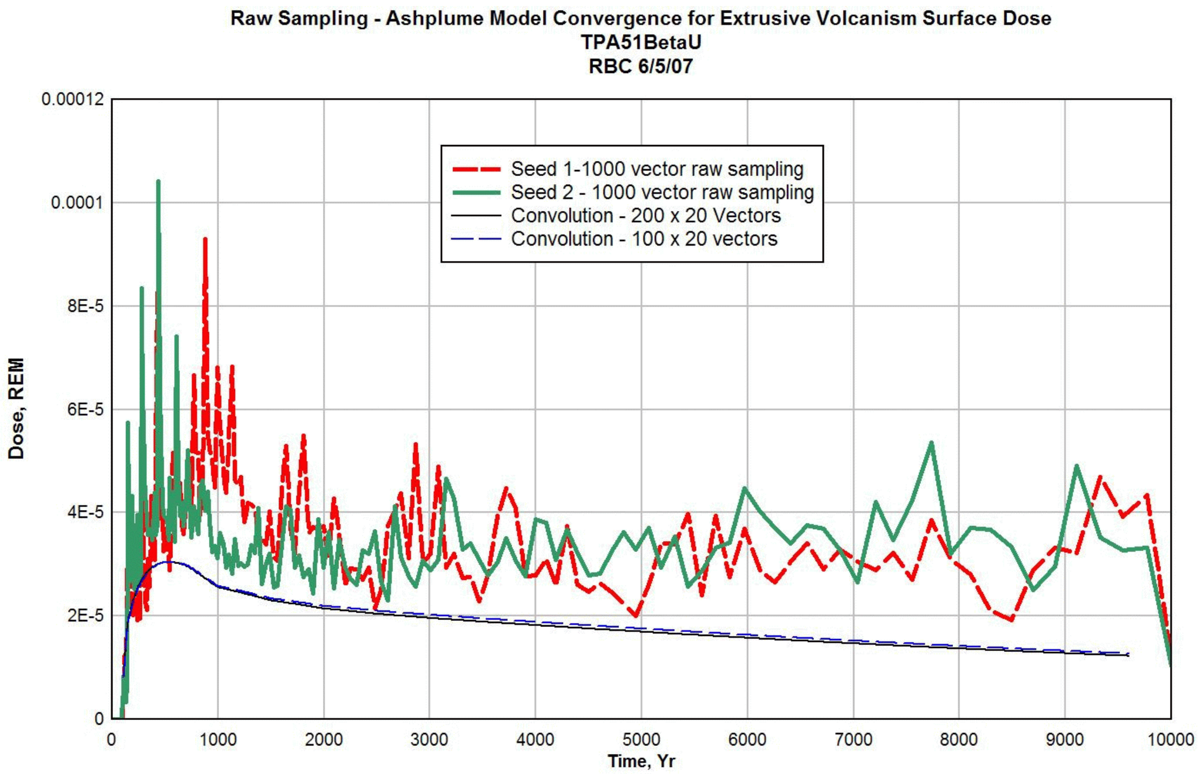


Figure 3. ASHPLUME for 1,000 realizations and two random seeds compared to convolution results.

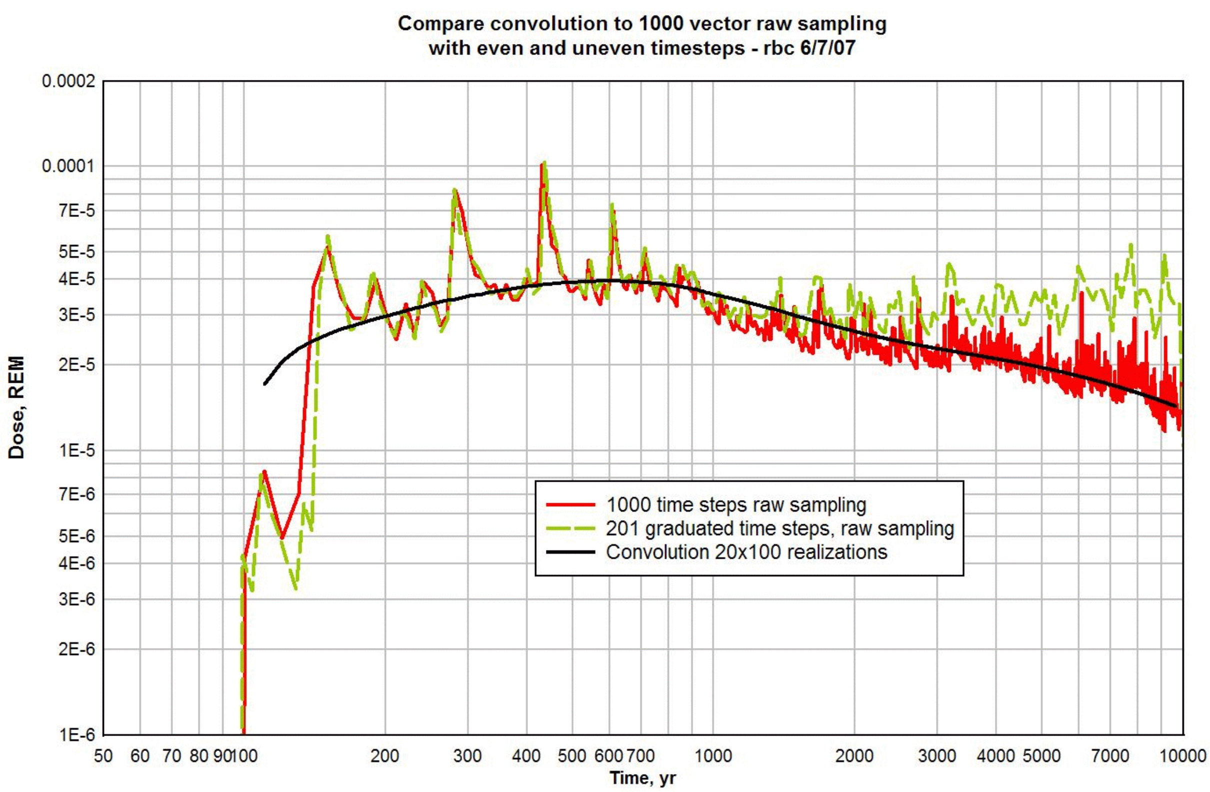


Figure 4. Comparison of convolution results with 1,000 vectors using even and uneven time steps.

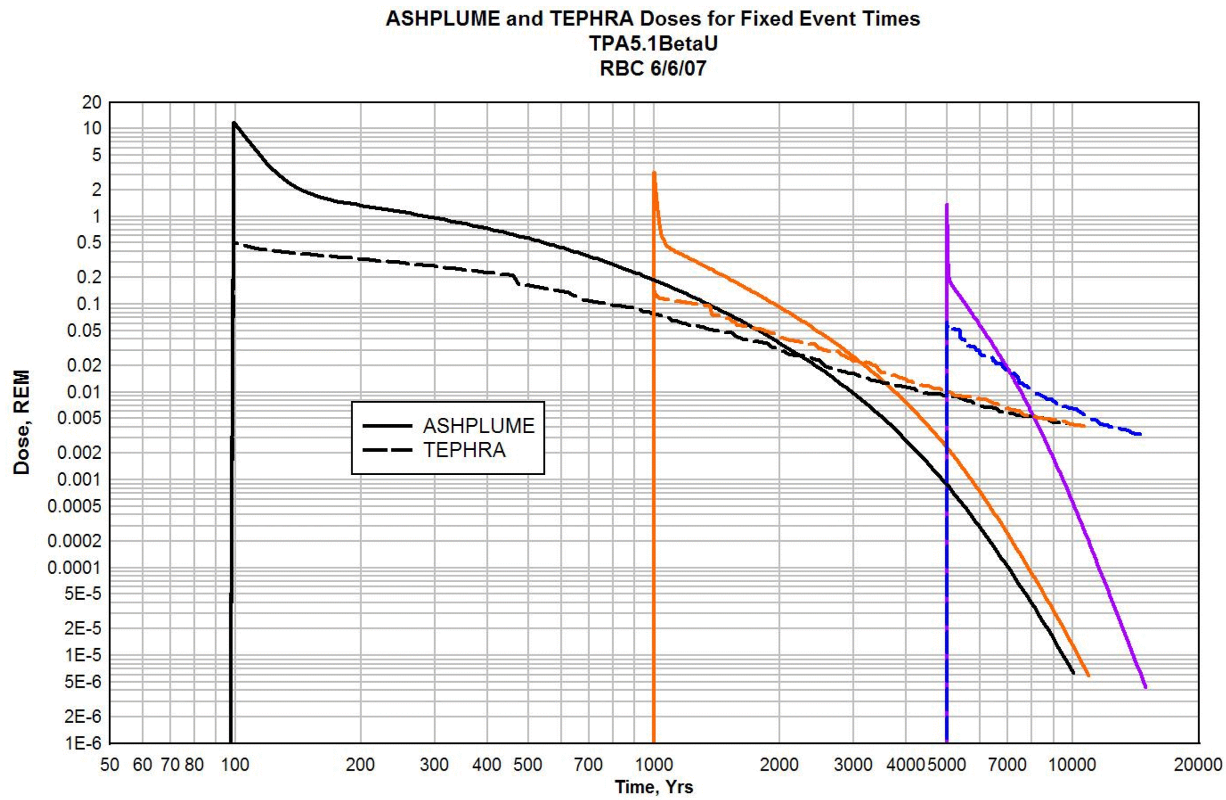


Figure 5. Mean conditional surface doses for fixed event times comparing ASHPLUME to TEPHRA

CONCLUSIONS

These results demonstrate that the TEPHRA/ASHREMOB model converges faster than the ASHPLUME/ASHREMOVO/DCAGS model, but that the disparity between the two convergence results can be well explained by the differences in the time constants for the two models. This part of the test criteria is therefore PASSED.

When calculating the mean dose curve for extrusive volcanism over the entire time period using raw sampling, it is important to use a large number (1000) of regularly spaced time steps, especially for the ASHPLUME model, which has sharper and shorter-lived peaks. The default, variable time stepping (201 steps) appears to be adequate for calculating the peak-of-the-mean for the ASHPLUME model when the peak occurs in the first 100 years, but overestimated dose for times later than 100 years. For the TEPHRA model, in which the peak occurs later than the ASHPLUME result, peak of the mean may be overestimated. Therefore, it is recommended to use at least 1000 regularly spaced time steps for all igneous extrusive simulations if raw sampling is to be employed.

Inspection of results from these analyses of the convergence of the ASHPLUME model appear to be consistent and explainable. Therefore, this part of the test criteria is considered to be PASSED.

The input files and results of these tests are archived on DVDs for TPA Version 5.1 Validation Task S-4, Attachment B.

TEST EVALUATION (PASS/FAIL): **PASS**

Attachment C

TPA Version 5.1 Validation Task S-4

Additional Testing to evaluate the convergence of results from seismic-induced waste package mechanical failures.

TEST PROCEDURE

Execute several sets of 500 realization reference case runs for 10^4 yr. Then examine the dose consequences of the realization runs for outlier results which can be attributed to seismic events. If an outlier occurs, investigate the cause of the outlier and its implication to the stability of the mean dose consequence.

TEST CRITERION

The degree of variability in simulation peak mean dose results cause by seismic activity should be explainable. If special analytical methods are required to evaluate the mean when seismic disruption of waste packages is considered, then it may be necessary to treat seismic activity as a separate scenario class from the nominal case.

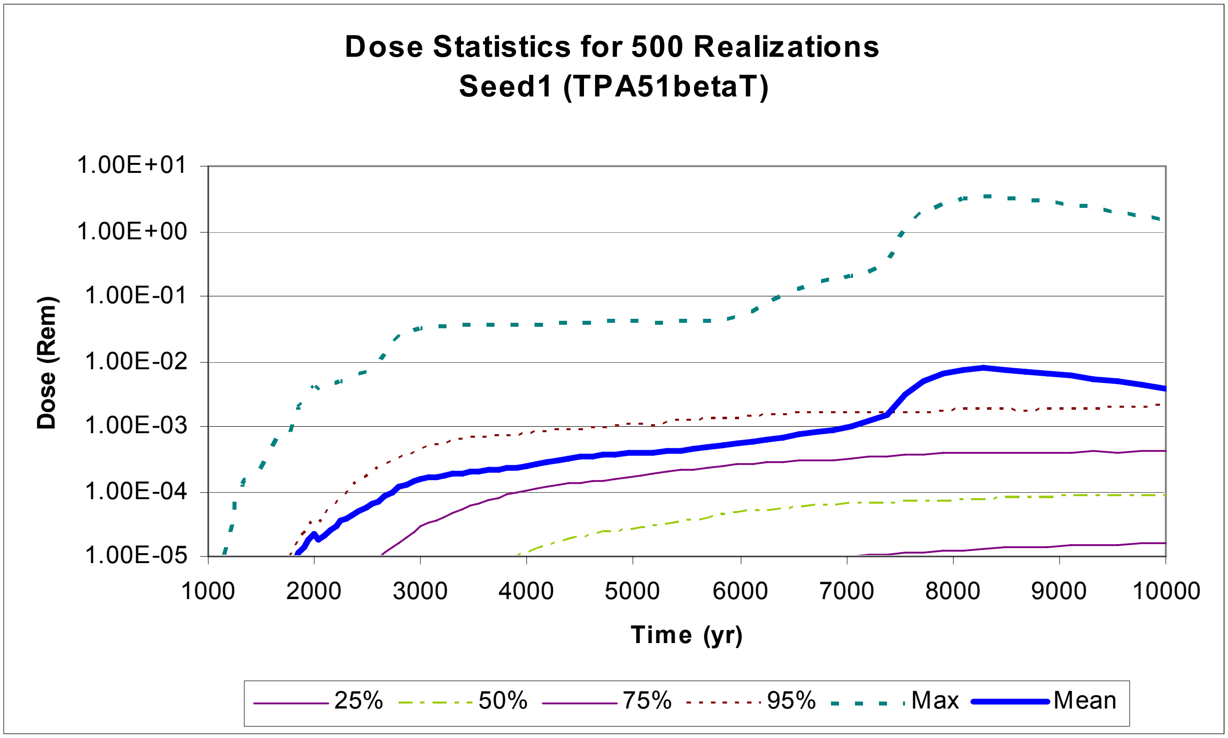
TEST RESULTS

The TPA version 5.1betaT code was executed for five sets of 500 realizations, where the seed for the LHS was changed to different values for each of the sets, and where each set was run with and without seismicity. The sets were labeled: reference, seed1, seed2, seed3 and seed4. The mean dose for these realizations are listed in the table below.

Peak Mean Dose for TPA51betaT

Case	Peak Mean Dose with Seismicity (mrem)	Peak Mean Dose without Seismicity (mrem)	Time of Peak Mean Dose with Seismicity (yr)	Time of Peak Mean Dose without Seismicity (yr)
Reference	0.817 mrem	0.493 mrem	10,000 yr	10,000 yr
Seed1	7.66 mrem	0.416 mrem	8,290 yr	10,000 yr
Seed2	0.451 mrem	0.375 mrem	10,000 yr	10,000 yr
Seed3	0.499 mrem	0.427 mrem	10,000 yr	10,000 yr
Seed4	0.544 mrem	0.435 mrem	9,540 yr	9540 yr

The peak mean dose for all five sets of realizations that do not include seismicity all appear to be well converged. However, when the seismicity is included in the evaluation of dose consequences, seed1 stands out as an obvious outlier. Seed1 has a peak mean dose which is an order of magnitude greater than any of the other results. A close examination of the results of seed 1 (with seismicity), shows that a single realization, 165 of 500, has a peak dose of 3.3555 rem (at 8290 yr). This single realization contributes 6.711 mrem to the peak mean dose; thus approximately 90% of the peak mean dose can be attributed to a single realization. The following plot shows the dose consequence of seed1.



An examination of the remaining four sets of realizations shows that the contribution from seismicity ranges from 0.1 to 0.3 mrem. This disparity in seismic dose consequences, 6.7 mrem vs. 0.3 mrem is striking and indicative of poor convergence for seismic consequences.

It is observed that under these sampling conditions, when seismicity was evaluated, the occurrence of seismic events (both the timing and magnitudes of the events) were the same for all five sets of TPA runs (the seismic sampling routine is controlled by a separate random number seed). Thus the lack of dose convergence is not the result of seismic event sampling, which may in its own right contribute to poor dose convergence.

This lack of convergence can be attributed to a relative under sampling of LHS-controlled parameters during seismic events. This under sampling can be illustrated as follows: Because seismic events occur with low frequency (1 in 10,000 yr) and the probability that the event will result in mechanical breaching of waste packages is low, about 2 or 3 % of realizations (in 10,000 yrs) will experience some degree of WP failures. Thus, the LHS sampled parameters represented during seismic induced WP failure will be a small subset of the total LHS sampling. Thus for a 500 realization set, only about 15 realizations will have seismic consequences. And because each of these 15 realizations may have significant WP failure, the sub sampling of the LHS parameters may result in obviously poor convergence of the mean dose.

This result depicts the difficulty of a direct evaluation of the mean consequence for seismicity. Because of this difficulty, seismic events have been removed from the nominal scenario reference case and will be treated as a disruptive scenario class using appropriate analytical methods to bound the confidence in the peak mean dose estimate. A method that may be useful in this regard has been developed to evaluate system performance using a disaggregated approach, in which the impact of seismicity is evaluated separately from other failure scenarios. Documentation of this approach for estimating the mean consequences for seismic and other disruptive events this approach can be found in the following reference.

Pensado, O. and Mancillas, J. “Estimates of Mean Consequences and Confidence Bounds on the Mean Associated With Low-Probability Seismic Events in Total System Performance Assessments.” CNWRA Intermediate Milestone 06002.01.352.705. Paper prepared for submission to Proceedings of the 11th International Conference on Environmental Remediation and Radioactive Waste Management (ICEM2007). September 2-6, 2007; Bruges, Belgium. 2007.

The input files and results of these tests are archived on DVDs for TPA Version 5.1 Validation Task S-4, Attachment C.

TEST EVALUATION (PASS/FAIL): PASS