

# **Scientific Notebook**

## **TPA Validation Tests**

By

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## TPA 5.1 Module validation for SVTR

Account No:

Description: Validate the changes incorporated in the TPA 5.1 code for the module nfenv

### Objective:

To perform TPA validation as described in the document “ SOFTWARE VALIDATION PLAN FOR TOTAL SYSTEM PERFORMANCE ASSESSMENT”. The specific task described in the document that relates to the near field environment is provides below.

### Validation Task 5: Near Field Chemical and Temperature Conditions

Numerous changes have been implemented to *nfenv.f* and related input data and subroutines. These changes affect calculated drift-wall, drip-shield and waste-package temperatures, relative humidity, and the chemical environment.

**Scope:** *Review SCRs indicated in Table 6.1-1 and conduct additional testing as necessary to verify the following:*

- 1. When drift degradation occurs slowly, for reflux computations, the drift is considered open, and for faster rates of drift degradation, the drift is considered degraded. The appropriate dryout thickness data should be selected as a function of the specified drift degradation rate.*
- 2. 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.*
- 3. Temperature calculations appropriately account for and distinguish between time of ventilation and time of closure.*
- 4. Estimates of seepage versus time are consistent with reflux abstraction and the specified seepage onset temperature.*
- 5. Numerical resolution issues or time stepping algorithms that may affect sampled waste package, drip shield, or drift wall temperatures do not result in errors in temperature values used in calculations.*
- 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.*
- 7. Changes in pH, chloride and nitrate concentrations with time are correctly computed.*

*The validation team also may conduct any additional testing deemed appropriate to provide confidence that the near field environment functions are implemented as intended.*

Specific section of the Table 6.1.1 that relates to NFENV are provided below.

<b>Task</b>	<b>Functionality to be Tested</b>	<b>Relevant Software Change Reports</b>	<b>Validation Team</b>
P-5	<u>Near field chemical and temperature conditions: (nfenv.f)</u>	478, 480, 488, 520, 553, 555, 562, 589, 591, 604, 605, 622, 658	J. Myers K. Das M. Juckett R. Fedors *C. Manepally

Out of the seven validation test cases listed there, the first five concerns the near field thermal and hydrological aspects that will be covered in this document

### **Synopsis of the software change reports**

- (1) PA-SCR-478: Related to corrosion ; Not relevant
- (2) PA-SCR-480: Most relevant to NFENV. The diameter of leg-A (top) and leg-B (side) are calculated and incorporated for natural backfill. The thermal models are updated to account for it.
- (3) PA-SCR-488: Mostly related to other modules than NFENV. Related to NFENV is the change that is added to calculate relative humidity during the preclosure based on ground surface temperature rather than repository temperature
- (4) PA-SCR-520: The vapor pressure calculated in NFENV was providing erratic unphysical value. It was taken care by adding a smoothing function and fixing an upper bound of 374.3 deg C for relative humidity calculation
- (5) PA-SCR-533: Related to thermal diffusivity calculation in thermal mode-2. As it is not supported anymore it is not of interest.

- (6) PA-SCR-555: Mostly a cleanup activity with reflux-1 and 2 removed.
- (7) PA-SCR-562: Most of the changes relates to corrosion that are not relevant here. The only change of interest is the alteration of Thermal conductivity of the backfill material for model 1 and model 2. Model 2 considers convection directly instead of using an equivalent thermal conductivity. Earlier same thermal conductivity was being used for models 1 and 2 which was not correct. This change incorporates different conductivity values for backfill. Since model 2 is no more supported, this issue is also irrelevant.
- (8) PA-SCR-589: Most of the SCR is not related to nfenv. Only states that a new value of Thermal conductivity of YM rock was supplied which is of interest to NFENV
- (9) PA-SCR-591:Subareas had inconsistent temperature and the representative point for drift temperature was not located at the centroid. This was taken care by adding a script/code.
- (10) PA-SCR-604:Relates to the repository closure time. Added a passive ventilation period.
- (11) PA-SCR-605:Relates to updating drythick.dat file for degradaed and non-degraded drift case. Time of thermal pulse end period is also added there to compare it with the end time for thermal degradation.
- (12) PA-SCR-622: Cleanup of nfenv.f ; No technical issuse is addressed here.
- (13) PA-SCR-658: First part related to releaset.f and of no interest to the nfenv module. The second part tests that the seepage should be set to zero if the temperature at the drift wall or drip shield is more than the seepage threshold temperature

### **Software changes that are important**

PA-SCR-604:Relates to the repository closure time. Added a passive ventilation period

PA-SCR-605:Relates to updating drythick.dat file for degradaed and non-degraded drift case. Time of thermal pulse end period is also added there to compare it with the end time for thermal degradation

PA-SCR-658: First part related to releaset.f and of no interest to the nfenv module. The second part tests that the seepage should be set to zero if the temperature at the drift wall or drip shield is more than the seepage threshold temperature

PA-SCR-589: Most of the SCR is not related to nfenv. Only states that a new value of Thermal conductivity of YM rock was supplied which is of interest to NFENV

PA-SCR-520: The vapor pressure calculated in NFENV was providing erratic unphysical value. It was taken care by adding a smoothing function and fixing a upper bound of 374.3 deg C for relative humidity calculation

PA-SCR-488: Mostly related to other modules tha NFENV. Related to NFENV is the change that is added to calculate relative humidity during the preclosure based on ground surface temperature rather than repository temperature

PA-SCR-480: Most relevant to NFENV. The diameter of leg-A (top) and leg-B (side) are calculated and incorporated for natural backfill. The thermal models are updated to account for it.

## Tests that should be done

1. Suggested Test: *When drift degradation occurs slowly, for reflux computations, the drift is considered open, and for faster rates of drift degradation, the drift is considered degraded. The appropriate dryout thickness data should be selected as a function of the specified drift degradation rate*

Way to do it: Could not make much sense of the suggested task. I guess, it tells to check the proper drythick.dat for degraded and non-degraded scenario and see if the seepage rate is consistent with it.

2. Suggested Test: *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.*

Way to do it: Run it in small time window when degradation occurs (say from 0 years to 4 thousand years) and plot the temperatures vs rubble thickness for drip shield, waste package and drift wall; The time steps should be made small. BTW, drift wall temperature does not depend on drift degradation rate. These data should be available from thermal.dat or thermal.dbg as it is called now. This case can be run without drift degradation and compared with results with drift degradation

3. Suggested Test: *Temperature calculations appropriately account for and distinguish between time of ventilation and time of closure.*

Way to do it: Change TimeOfRepositoryClosure[yr] and TimeActiveVentilationEnds[yr] and run TPA for a small period of time (say for 0 to 1000 or even less years) and see how the temperature behaves for the waste package, drip shield and drift wall.

4. Suggested Test: *Estimates of seepage versus time are consistent with reflux abstraction and the specified seepage onset temperature.*

Way to do it: Change the distribution of Seepage threshold temperature and FlagSeepageThreshold and see the variation of qm3hit and qm3miss with time and check if they are consistent with the abstraction. Run it for the max, min and mean case to check it.

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

Way to do it: run it for different time steps (at least 5) and plot to see if they are consistent with each other or if any numerical error have affected the results

Date April 9 2007

## General change in the tpa.inp file

### Compliance period

1. It is kept at 10,000 years
2. The number of time steps is increased to 401
3. The ratio of first to, last time step is changed to 50.

```
**          ***>>> Simulation Times <<<***  
**  
constant  
DurationOfCompliancePeriod[yr]  
1.0e4  
constant  
MaximumTime[yr]  
1.0e4  
  
iconstant  
NumberOfTimeStepsInCompliancePeriod  
401  
**  
constant  
RatioOfLastToFirstTimeStepInCompliancePeriod  
50.0
```

### Output modes

- (1) Mode change to 2 to get user defined outputs
- (2) Selected the option so that nfenv.rlt and efenv.ech is created

```
**      ***>>> Output Print Options <<<***  
**  
iconstant  
OutputMode (0=None, 1=All, 2=UserDefined)  
2  
**  
iconstant  
UserDefinedLowerRealizationAppended  
1  
**  
iconstant  
UserDefinedUpperRealizationAppended  
1  
iconstant  
SelectAppendFiles  
2
```

In NFENV

(1) Set Flag to get the temperature.dbg flag

```
**  
**      ***>>> NFENV <<<***  
**  
  
iflag  
TabularTemperatureRHFlag (yes=1, no=0)  
1
```

## Test-2

*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*

Synopsis of the test: Three different test cases will be carried out to study the effect of accumulated rubble on temperature distribution of the waste package, drip shield and drift wall. The change in accumulated rubble height will be done by changing the balking factor.

Changes made in the tpa.inp file

General changes for all the cases

(1) Calculation confined only to subarea-1

```
iconstant
StartAtSubarea
1
**
** StopAtSubarea set to zero means include all subareas after StartAtSubarea
iconstant
StopAtSubarea
1
**
```

(2) Seismic scenario flag turned off to make a simpler calculation.

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

(3) Write all the results file to plot required data

Done for only realization1

Writes out all the data and echo files

```
**      ***>>>  Output Print Options  <<<***
**
iconstant
OutputMode(0=None,1=All,2=UserDefined)
1
**
iconstant
UserDefinedLowerRealizationAppended
1
**
iconstant
UserDefinedUpperRealizationAppended
1
**
** Select Append Files
** 0 = append all files
** 1 = uzflow.ech and uzflow.rlt only
** 2 = nfenv.ech and nfenv.rlt only
** 3 = ebsfail.ech and ebsfail.rlt only
** 4 = driftfail.ech, driftfail.rlt, mechfail.ech, and mechfail.rlt only'
** 5 = faulto.ech and faulto.rlt only
** 6 = volcano.ech and volcano.rlt only
** 7 = ebsrel.ech, ebsrel.rlt, ebsrel.cum only
```

```
** 8 = uzft.ech and uzft.rlt only
** 9 = szft.ech and szft.rlt only
** 10 = dcagw.ech and dcagw.rlt only
** 11 = ashplumo.ech and ashplumo.rlt only
** 12 = ashrmovo.ech and ashrmovo.rlt only
** 13 = dcags.ech and dcags.rlt only
** 14 = ashplume.cum only
** 15 = failt.cum only
** 16 = nefiiuz.cum and nefiisz.cum only
** 17 = releaset.cum only
** 18 = ggenii.cum only
** 19 = genv.cum only
** 20 = dcfgw.cum and dcfgs.cum only
** 21 = dsfail.ech and dsfail.rlt only
** 22 = files needed by the graphical post-processor
** rwr 2/26/07; SCR673; Reformat Input/Output/Intermediate Files
**      (add option to write all infilper.res time steps)
**      (instead of every 10th time step)
** 23 = infilper.cum only
**
iconstant
SelectAppendFiles
0
**
```

(4) Fraction allowed to degrade in chimney mode is set to 1.0 so that only chimney shaped material accumulation occurs

```
constant
FractionDriftDegradationOccursByChimney
1.0
```

(5) The TabulatTemperatrureRHFlag set to 1 so that thermal.dbg file is written out

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

Specific Changes in the input file

Bulking factor for subarea-1 is changed for rock type 1 and 2.

For rock type-1

```
**beta
constant
BulkingFactorRockTypeOneSubarea_1 []
1.15
```

\*\*1.0, 2.0, 23.1747, 92.6989  
\*\*

For rock type-2

\*\*beta  
constant  
BulkingFactorRockTypeTwoSubarea\_1 []  
1.15  
\*\*1.0, 2.0, 23.1747, 92.6989  
\*\*

Date April 11<sup>th</sup> 2007

## **Run-2**

*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.*

### **Task Objectives**

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

### **Scope of test-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 temperature and the drip shield temperatures will be compared for mode-1 and 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 (tempdw) 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).

### **Input files**

Use the mean value parameters for this run except for the bulking factors. See the input files in the accompanying CD.

### **Procedure**

#### (1) General changes in the input file

Obtained the tpa.inp file by converting the tpamean.out file from a general run of the TPA code in version tpa51betav.

```
(A) Set      StartAtSubarea=3
              StopAtSubarea=3
(B) Set      iflag
              SeismicDisruptiveScenarioFlag(yes=1,no=0)
              0
(C)Set       iflag
              VolcanismDisruptiveScenarioFlag(yes=1,no=0)
              0
(D) Set      iconstant
              StartAtRealization
              1
              **
              iconstant
              StopAtRealization
              1
```

#### (2) Test-case-2.1

```
(A) Set      **
              constant
              BulkingFactorRockTypeOneSubarea_3 []
              1.15
              **
(B) Set      **
              constant
              BulkingFactorRockTypeTwoSubarea_3 []
              1.15
              **
```

Note: In the tpa mean file, the beta distribution is replaced with a constant value distribution

which is used for the test.

(3) Test-case-2.2

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3 []  
                  1.20  
                  \*\*

(B) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeTwoSubarea\_3 []  
                  1.20  
                  \*\*

(2) Test-case-2.3

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3 []  
                  1.25  
                  \*\*

(B) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeTwoSubarea\_3 []  
                  1.25  
                  \*\*

\*\*\*\*\*Added on Date April 20<sup>th</sup> 2007

Some additional tests were performed for Thermal Mode=2 to analyze the sensitivity of the TPA code and its performance for two different models.

The tests are describe as follows

Test Case 2.4

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3 []  
                  1.15  
                  \*\*

(B) Set      \*\*  
              constant  
              BulkingFactorRockTypeTwoSubarea\_3 []  
              1.15  
              \*\*  
(C) Set      \*\*  
              iconstant  
              SelectThermalModel (1,2)  
              2

Test Case 2.5

(A) Set      \*\*  
              constant  
              BulkingFactorRockTypeOneSubarea\_3 []  
              1.20  
              \*\*  
(B) Set      \*\*  
              constant  
              BulkingFactorRockTypeTwoSubarea\_3 []  
              1.20  
              \*\*  
(C) Set      \*\*  
              iconstant  
              SelectThermalModel (1,2)  
              2

Test Case 2.6

(A) Set      \*\*  
              constant  
              BulkingFactorRockTypeOneSubarea\_3 []  
              1.25  
              \*\*  
(B) Set      \*\*  
              constant  
              BulkingFactorRockTypeTwoSubarea\_3 []  
              1.25  
              \*\*  
(C) Set      \*\*  
              iconstant  
              SelectThermalModel (1,2)  
              2

Date April 21<sup>st</sup> 2007

## **Run-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 its effect on the temperature profile. 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 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. 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.

### **Input files**

Use the mean value parameters for this run except for the bulking factors. See the input files in the accompanying CD.

## **Procedure**

### 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.

#### Test Case 3.1.1

Set  
constant  
TimeActiveVentilationEnds[yr]  
30.0

#### Test Case 3.1.2

Set  
constant  
TimeActiveVentilationEnds[yr]  
30.0

#### Test Case 3.1.3

Set  
constant  
TimeActiveVentilationEnds[yr]  
30.0

### 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.

#### Test Case 3.2.1

Set  
constant  
TimeOfRepositoryClosure[yr]  
60.0

#### Test Case 3.2.2

Set  
constant  
TimeOfRepositoryClosure[yr]  
100.0

#### Test Case 3.2.3

Set  
constant

TimeOfRepositoryClosure[yr]  
150.0

April 20th 2007

## **Run-5**

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

### **Objective**

Test 5 suggests to study the effect of integration parameters in temperature calculations. The Gauss Legendre integration is used to compute the drift wall temperature from the mountain scale heat transfer equation. The weighing factor of the integration will have some affect 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 *tpamean.inp* will be used. Cuurently a fixed value of Gauss-Legendre integration weighting factor of 20 is being used. The weighting factor for the Gauss-Legendre integration will be varied to three constants, 20; 50 and 100. Currently a value of 20 is being used for computational economy. This is the only parameter associated with numerics in the mountain scale model and will affect the integration. They seem to affect the drift wall temperature by creating oscillation and drop in temperature level by 20 deg centigrade immediately after the peak temperature.. The corresponding mean release and waste package temperature will be plotted to see if the results are sensitive to integration weighting factor.

### **Input files**

Use the mean value parameters for this run except for the bulking factors. See the input files in the accompanying CD.

## **Procedure**

The integration constants have been changed to four different values. The following parameters are set or changed in tpa.inp file.

Test Case 5.1

Set

```
iconstant  
NumberOfWeightsForGaussLegendreIntegration[]  
20
```

Test Case 5.2

Set

```
iconstant  
NumberOfWeightsForGaussLegendreIntegration[]  
50
```

Test Case 5.3

Set

```
iconstant  
NumberOfWeightsForGaussLegendreIntegration[]  
100
```

Test Case 5.4

Set

```
iconstant  
NumberOfWeightsForGaussLegendreIntegration[]  
200
```

Date April 27<sup>th</sup> 2007

## **Run-4**

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

### **Objective**

Test 4 suggests to study the sensitivity of seepage with the onset temperature. 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 deg C (194, 230 and 266 deg F) to study the sensitivity of the seepage rate with onset temperature. As constant values of the threshold temperatures will be used instead of sampling them, computing multiple realizations will not be necessary.

Results for these runs will be obtained from *nfenv.rlt* and *thermal.dbg*. The output variables, time, repository wall temperature (*temp<sub>rw</sub>*), drip shield temperatures (*temp<sub>dsA</sub>* and *temp<sub>dsB</sub>*) and the quantity of water hitting the waste package *qm<sub>3hit</sub>* will be used for analysis.

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 flanges of the drift 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 flange 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 flange diameters less than or equal to the original drift wall diameter and will be considered degraded otherwise. The rubble diameter in the flange, quantity of seepage, drip shield, and drift wall temperatures will be recorded in a file and the output will be used to study the drift degradation on seepage rate.

### **Input files**

Use the mean value parameters for this run except for the bulking factors. See the input files in the accompanying CD.

## **Procedure**

Two sets of tests have been performed for this analysis. In the first set of tests, the sensitivity of code to changes in seepage threshold temperature will be studied. The seepage threshold temperature will be changed to three constant values of 90, 110 and 130 deg C. For this set of run the input parameters are set so that there are no drift degradation. The purpose of this test is just to verify the effect of seepage threshold temperature on the onset of seepage process and whether the code handles it properly or not.

The second set of runs focuses on testing whether TPA compares the seepage threshold temperature with proper reference temperature. To test it, the TPA code will once run with slow degradation and once with fast degradation. To accomplish slow degradation, the degradation time for the rock will be set to a very high value and to accomplish fast degradation, it will be set to a low value. For both the cases, the seepage threshold temperature will be fixed at 130 deg C and the drift degradation scenario flag will be on. For the intact drift scenario, the seepage threshold temperature should be compared with the drift wall temperature whereas, for the degraded drift, it should be compared with the drip shield temperature.

### Cases 4.1

#### General setting for 4.1

```
iflag  
DriftDegradationScenarioFlag(yes=1,no=0)  
0
```

#### Test 4.1.1

Set

```
constant  
SeepageThresholdT[C]  
90.00000000000000
```

#### Test 4.1.2

Set

```
constant  
SeepageThresholdT[C]  
110.00000000000000
```

### Test 4.1.3

Set

constant  
SeepageThresholdT[C]  
130.00000000000000

### Cases 4.2

General setting for 4.2

constant  
SeepageThresholdT[C]  
110.00000000000000  
iflag  
DriftDegradationScenarioFlag(yes=1,no=0)  
1

### Test 4.2.1

Set

constant  
DegradationTimeRockTypeOneSubarea\_3[yr]  
10000000.00  
constant  
DegradationTimeRockTypeTwoSubarea\_3[yr]  
10000000.00

### Test 4.2.2

Set

constant  
DegradationTimeRockTypeOneSubarea\_3[yr]  
150.00  
constant  
DegradationTimeRockTypeTwoSubarea\_3[yr]  
150.00

Date 30<sup>th</sup> 2007

## **Run-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 dry out 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 proper dry out 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 (I) BF\_Out\_Dia entry in *thermal.dbg* and (ii) the value of the dryout thick. The *thermal.dbg* file is a standard output file. The dryout thickness will be obtained by modifying the *nfenv.f* file to output the dryout thickness for each time step.

We will also check for inconsistencies that occur because of the *dryout.dat* being derived from a base case degradation rate, and each realization of TPA sampling a degradation rate and time of completion. For this we can set different values for BulkingFactorRockTypeYYYYSubarea\_XX[] (where YYYY=One or Two; XX=1 to 10) and DegradationTimeRockTypeYYYYSubarea\_XX[yr] in DRIFTFAIL portion of *tpa.inp*.

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.

## **Input files**

Use the mean value parameters for this run except for the bulking factors. See the input files in the accompanying CD.

## **Procedure**

The following segment was added to the end of the subroutine thickness\_reader to get the interpolated thickness values out.

```
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  
  
close(idrycheck)
```

Three cases were studied to

Cases 1.1

TPA runs without any degradation and the thickness reader is supposed to read in data that is specified for use in an intact drift

```
set  
iflag  
SeismicDisruptiveScenarioFlag(yes=1,no=0)  
0
```

Cases 1.2

TPA runs with degradation and the time of degradation is before the end of thermal pulse. So,

the thickness reader is supposed to read in data that is specified for use in a degraded drift

```
set
  iflag
  SeismicDisruptiveScenarioFlag(yes=1,no=0)
  1

  constant
  DegradationTimeRockTypeOneSubarea_3[yr]
  200.000
  **

  constant
  DegradationTimeRockTypeTwoSubarea_3[yr]
  200.000
  **
```

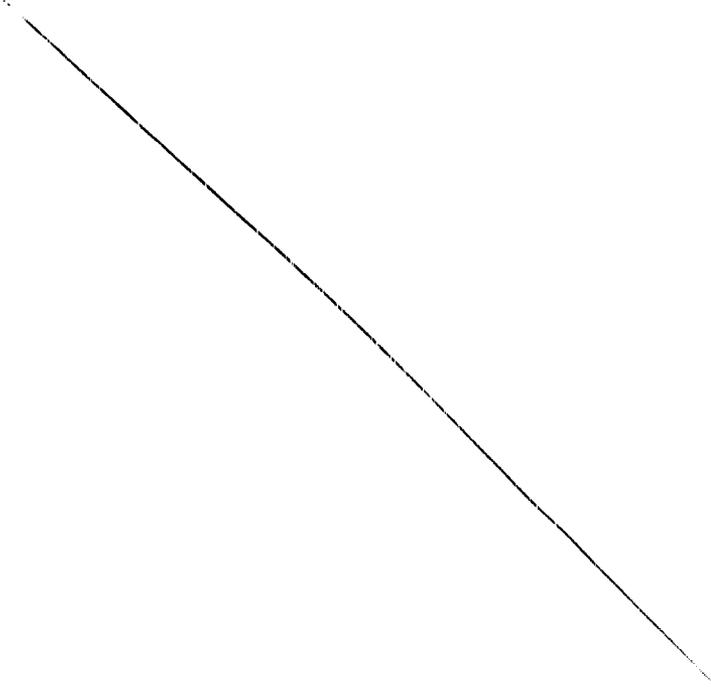
### Cases 1.3

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

```
set
  iflag
  SeismicDisruptiveScenarioFlag(yes=1,no=0)
  1

  constant
  DegradationTimeRockTypeOneSubarea_3[yr]
  1000000.000
  **

  constant
  DegradationTimeRockTypeTwoSubarea_3[yr]
  1000000.000
  **
```



KA

## Appendix-A

May 2<sup>nd</sup> 2007

### **TPA 5.1 Software Validation Task P-5 Test Results**

Following are test results for the validation test cases described in Attachment 1 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**

**Path for run directory:**

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

**Environment variable:**

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

**Special input files or modifications to input files required :** None

**Special diagnostic code modifications required :**

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 dry out thickness values that is being used in the computation in an output file. Note that the interpolated values of the dry out thickness are written out. This will provide a better understanding of what exact values of dry out zone thickness is 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.

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

```
set
  iflag
  SeismicDisruptiveScenarioFlag(yes=1,no=0)
  0
```

#### Case 1.2

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

```
set
  iflag
  SeismicDisruptiveScenarioFlag(yes=1,no=0)
  1

  constant
  DegradationTimeRockTypeOneSubarea_3[yr]
  200.000
  **

  constant
  DegradationTimeRockTypeTwoSubarea_3[yr]
  200.000
  **
```

#### 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

```
set
  iflag
  SeismicDisruptiveScenarioFlag(yes=1,no=0)
  1

  constant
  DegradationTimeRockTypeOneSubarea_3[yr]
  1000000.000
  **

  constant
  DegradationTimeRockTypeTwoSubarea_3[yr]
  1000000.000
  **
```

**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:**

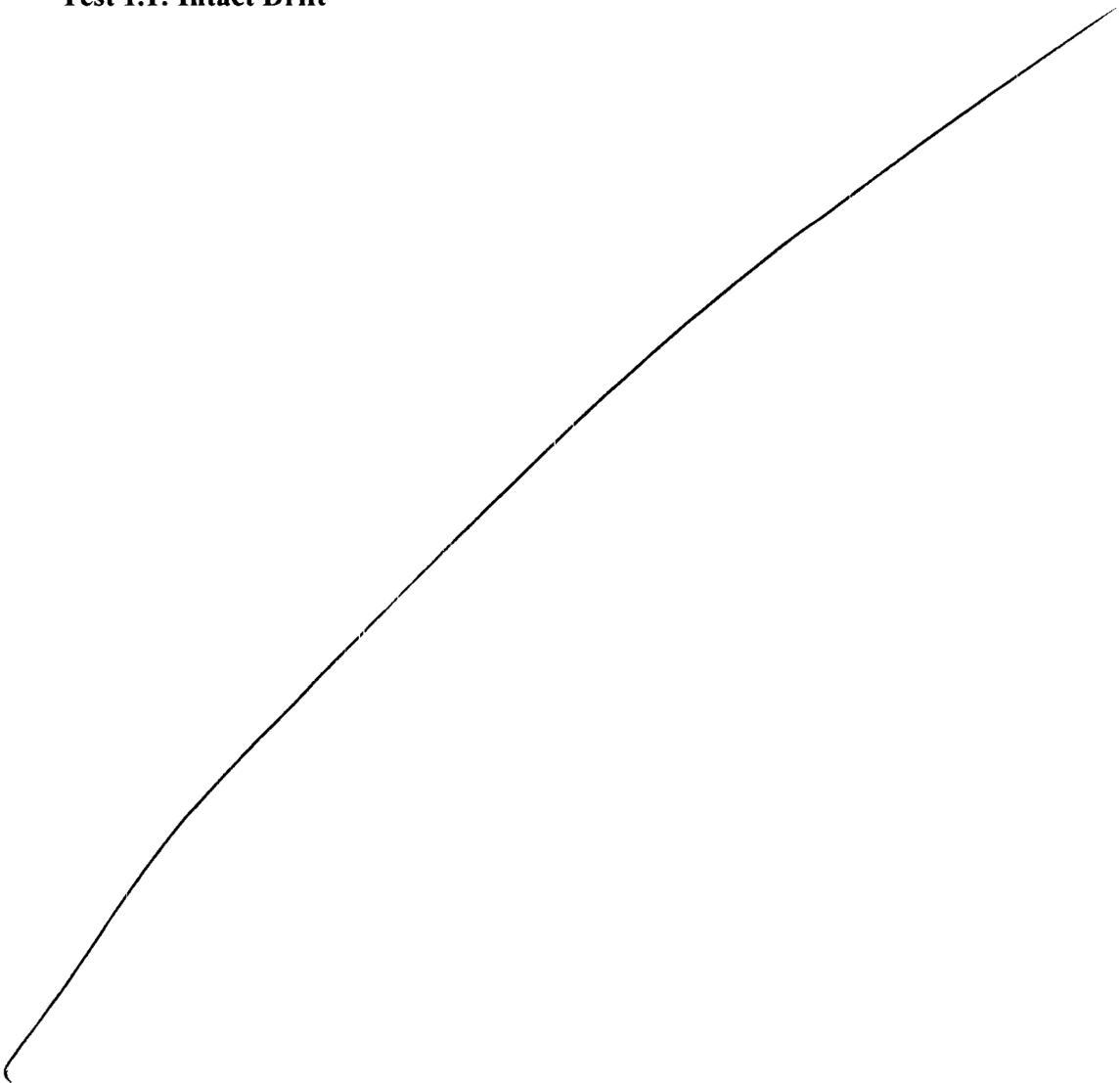
- 1) Execute the TPA code thrice, using the modified tpa.inp file and the new executable build with modified *nfenv.f*, and saving the results for examination.
- 2) Examine the dryout thickness values in the output files *drycheck.dat*. And *drythick.dat*

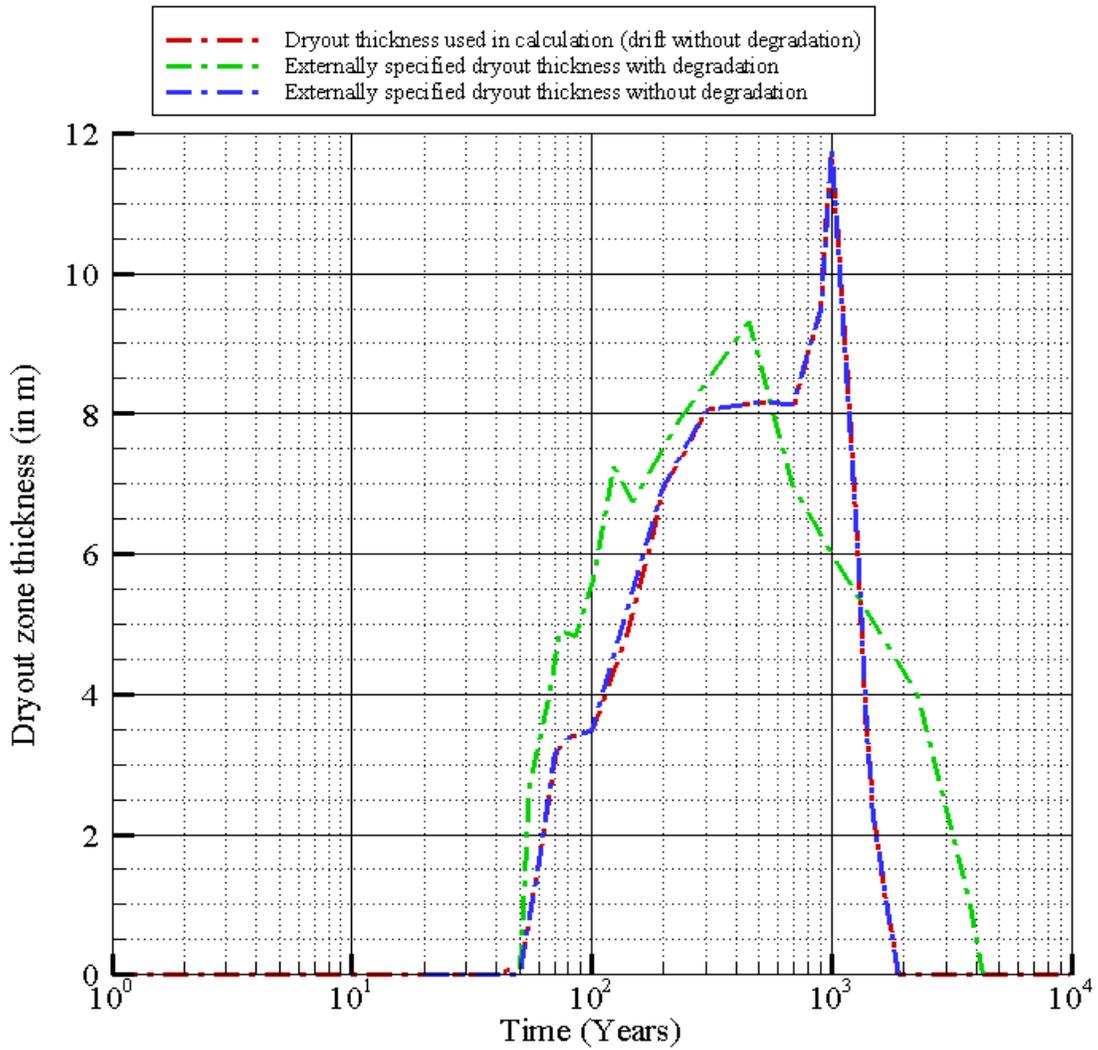
**Pass/Fail criteria:**

- 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 9degraded drift in *drythick.dat*
- 3) For test 1.1, the values recorded in *drycheck.dat* should match with data corresponding to intact drift in *drythick.dat*

**Test results:**

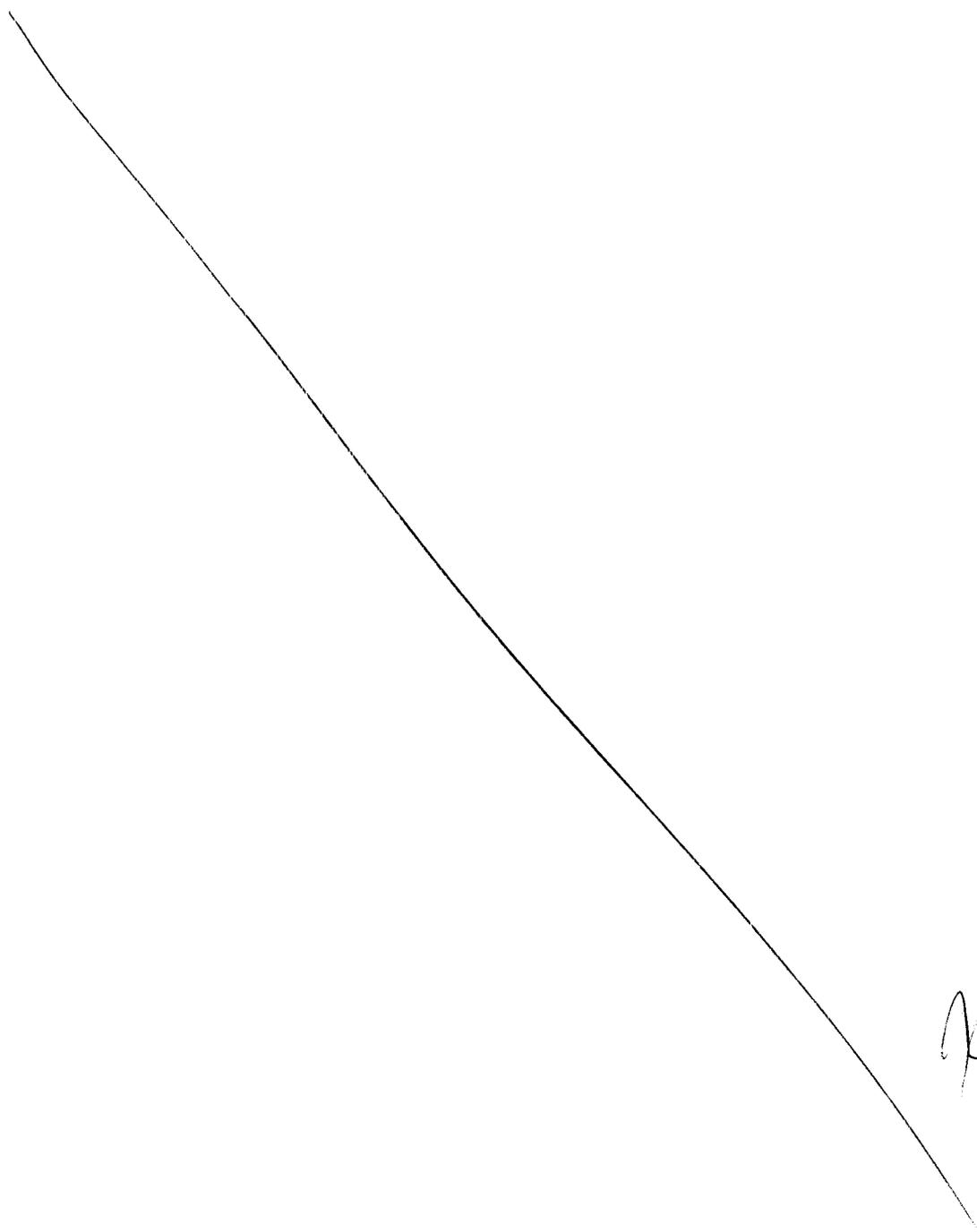
**Test 1.1: Intact Drift**

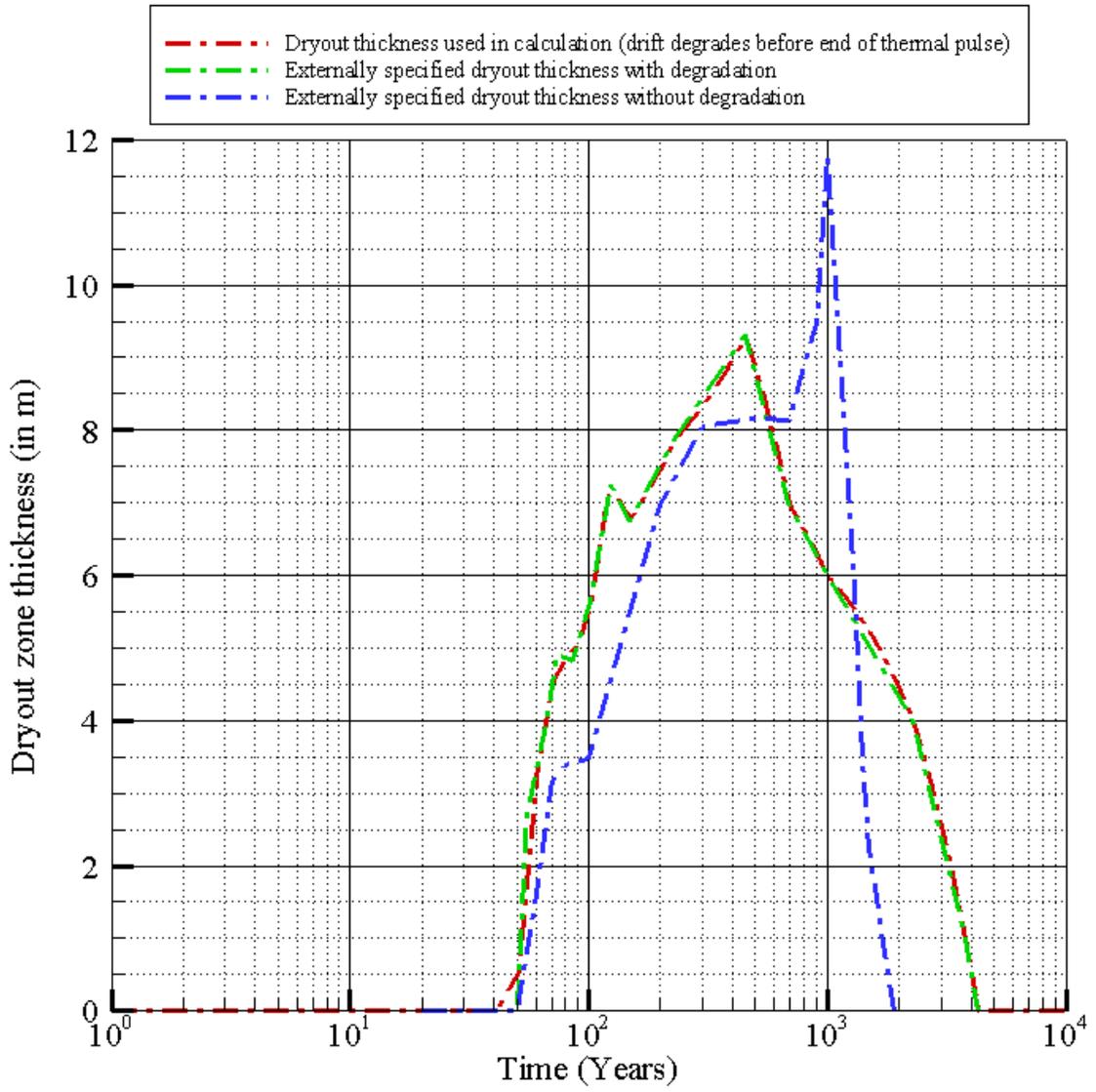




Observation: The dryout thickness values used in the computation matches exactly with the dryout values for the intact drift in *drythick.dat*

**Test 1.2: Total degradation before the end of thermal pulse**

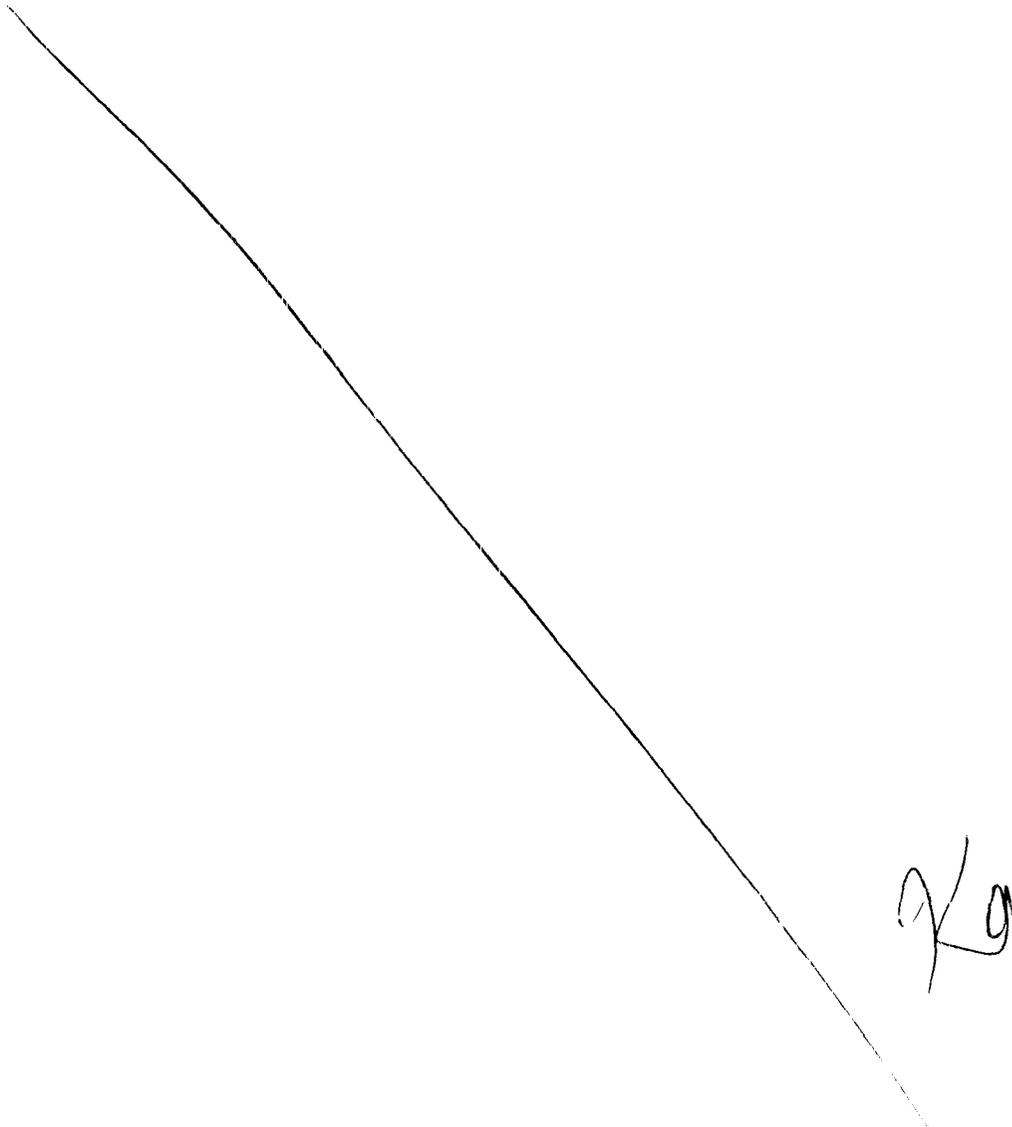


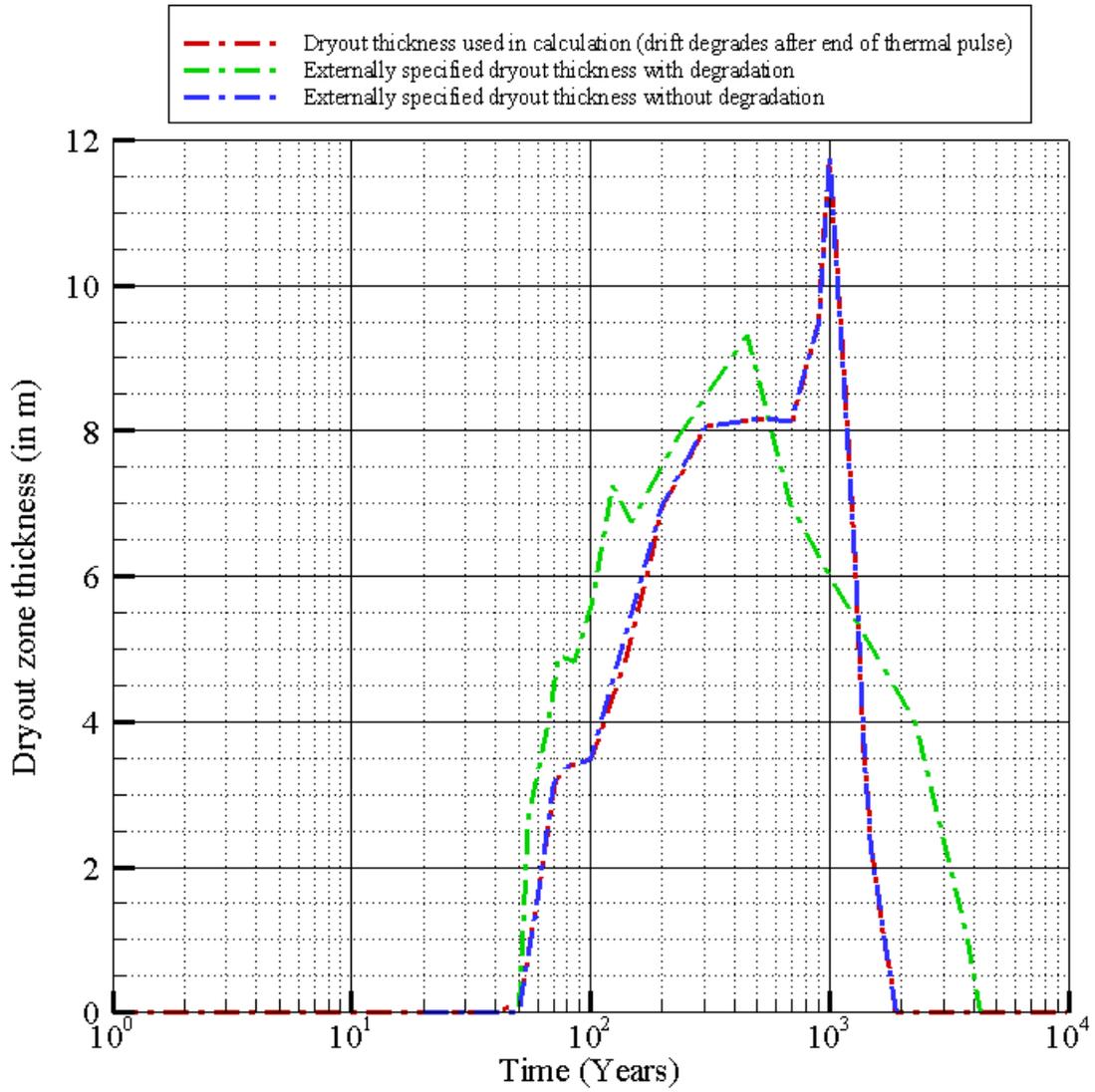


Observation: The dryout thickness values used in the computation matches exactly with the dryout values for the degraded drift in *drythick.dat*

May 4<sup>th</sup> 2007

**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*

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

May 8<sup>th</sup> 2007

**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 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.

(1) Test-case-2.1.1

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3[]  
                  1.15  
                  \*\*  
  
(B) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeTwoSubarea\_3[]  
                  1.15  
                  \*\*

(2) Test-case-2.1.2

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3[]  
                  1.20  
                  \*\*  
  
(B) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeTwoSubarea\_3[]  
                  1.20  
                  \*\*

(3) Test-case-2.1.3

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3[]  
                  1.25  
                  \*\*  
  
(B) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeTwoSubarea\_3[]  
                  1.25  
                  \*\*

(4) Test Case 2.2.1

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3[]  
                  1.15  
                  \*\*

(B) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeTwoSubarea\_3[]  
                  1.15  
                  \*\*

(C) Set       \*\*  
                  constant  
                  FractionAllowedToDegrade[]  
                  0.80  
                  \*\*

(5) Test Case 2.2.2

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3[]  
                  1.20  
                  \*\*

(B) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeTwoSubarea\_3[]  
                  1.20  
                  \*\*

(C) Set       \*\*  
                  constant  
                  FractionAllowedToDegrade[]  
                  0.80  
                  \*\*

(6) Test Case 2.2.3

(A) Set       \*\*  
                  constant  
                  BulkingFactorRockTypeOneSubarea\_3[]  
                  1.25

```
(B) Set      **
             **
             constant
             BulkingFactorRockTypeTwoSubarea_3[]
             1.25
             **
(©) Set      **
             **
             constant
             FractionAllowedToDegrade[]
             0.80
             **
```

**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 the sensitive to change 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*

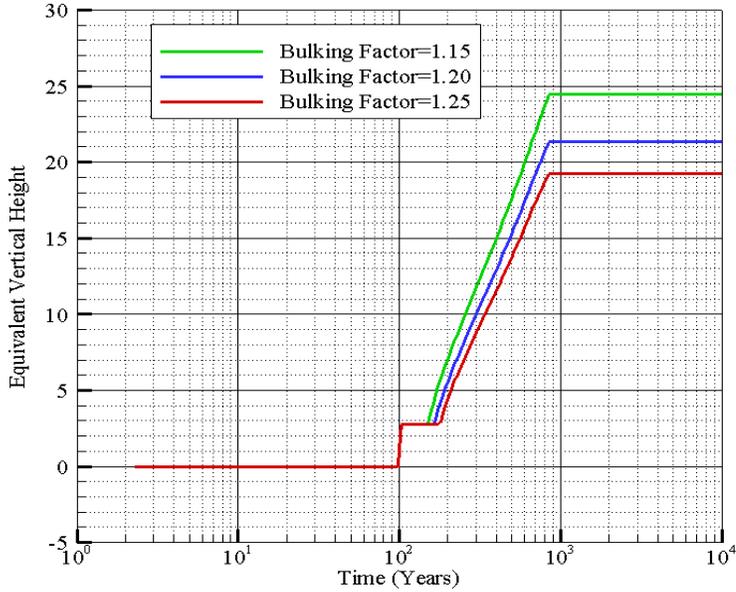
**Pass/Fail criteria:**

For all the cases, the temperature profile should show some sensitivity with change in rubble thickness or the bulking factor. It is expected that with lower values of thickness, the waste package temperature should be less and with a higher value of thickness, it should be more due to insulating effect of the rubble pile. 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 higher thickness of rubble on drip shield and should predict 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:**

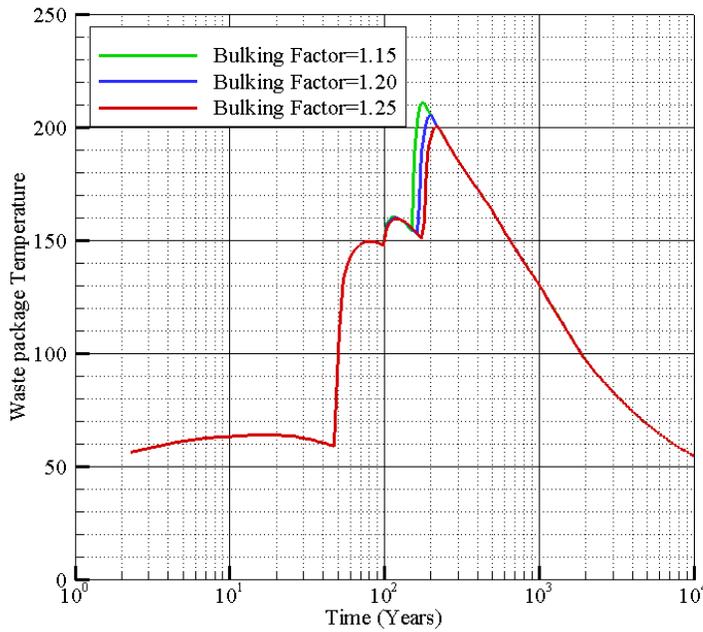
**Variation of drift height with bulking factor Thermal-Mode-1**



**Observation**

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

**Variatio  
tempera  
factor**

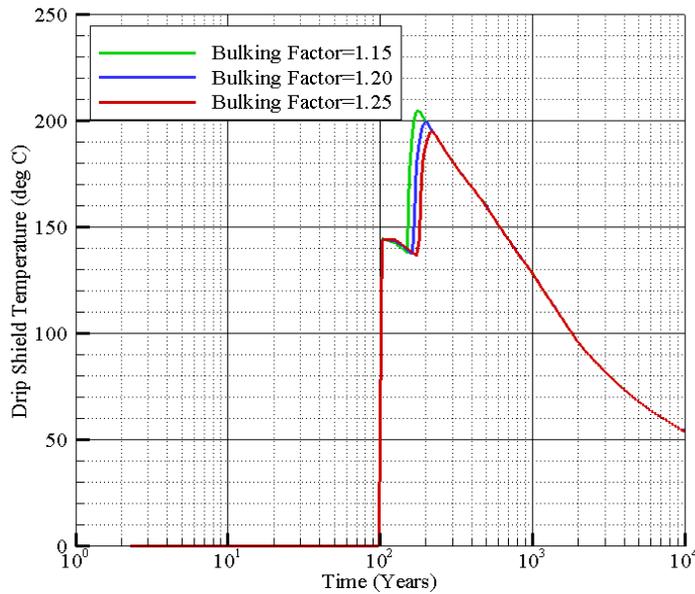


**n of waste package  
ture with bulking  
in Thermal-Mode-1**

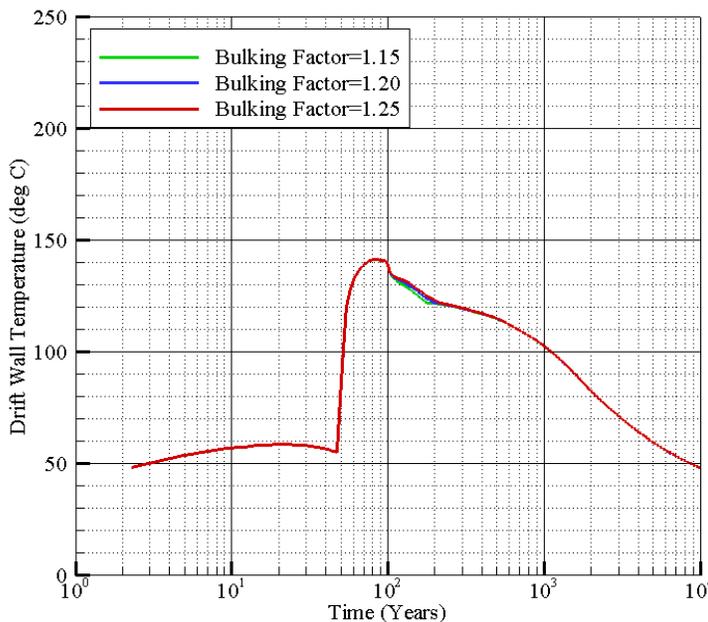
### Observation

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

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



O  
C  
aff  
di  
sh  
fa  
te  
  
V  
te  
fa



### Observation

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

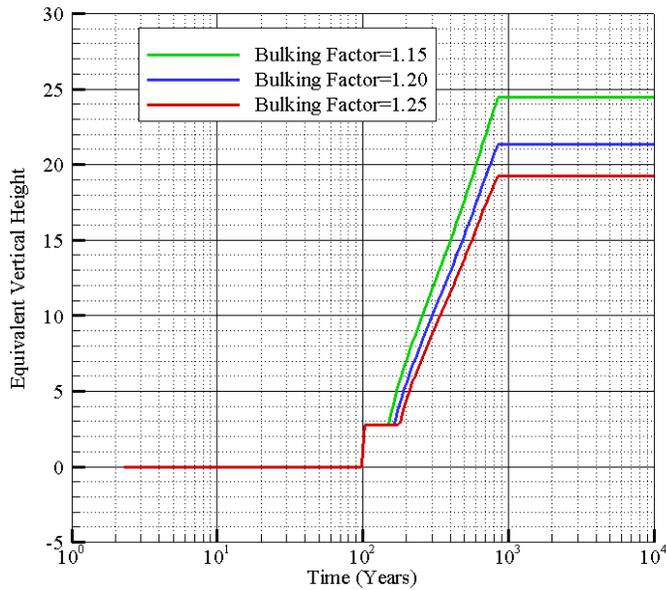
### Variation of drift wall temperature with bulking factor in Thermal-Mode-1

May 9<sup>th</sup> 2007

**Observation**

Change in bulking Factor does not change the drift wall temperature

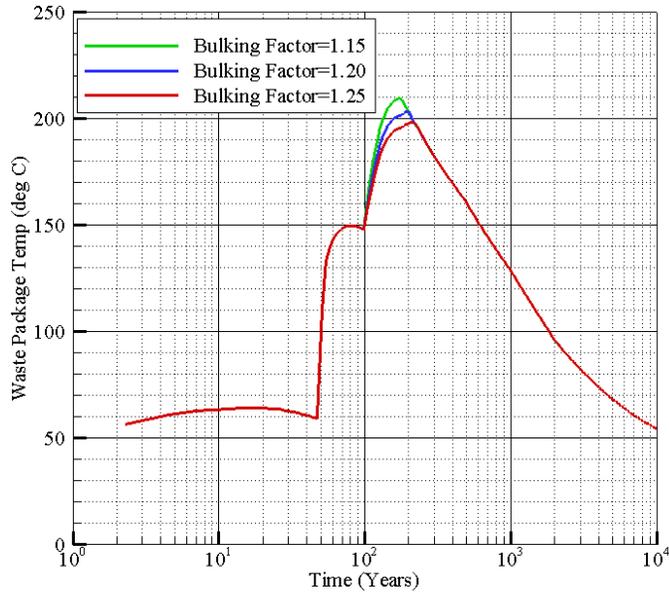
**Variation of drift height with bulking factor Thermal-Mode-2**



**Observation**

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

**Variation  
temperat  
factor in**

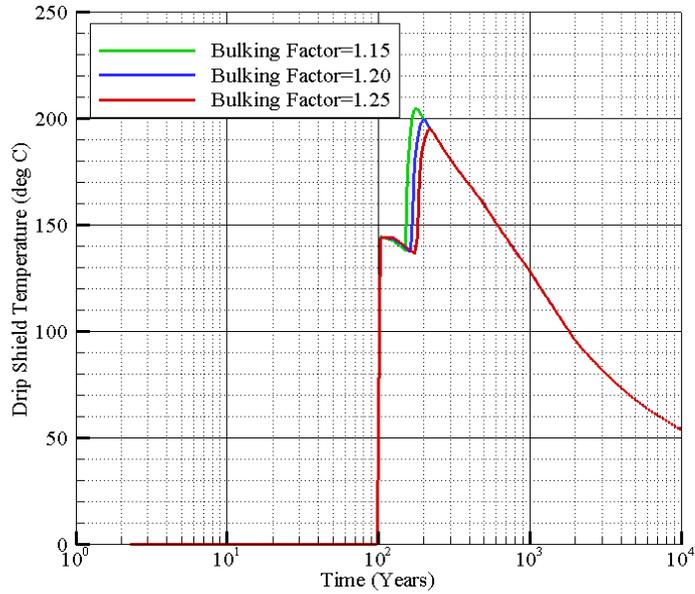


**of waste package  
ure with bulking  
Thermal-Mode-2**

**Observation**

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

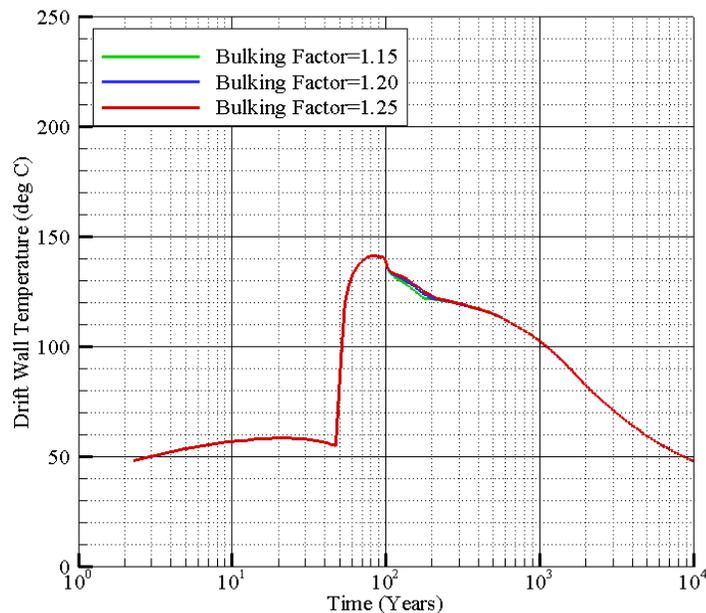
**Variation of drip shield temperature with bulking factor in Thermal-Mode-2**



### Observation

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

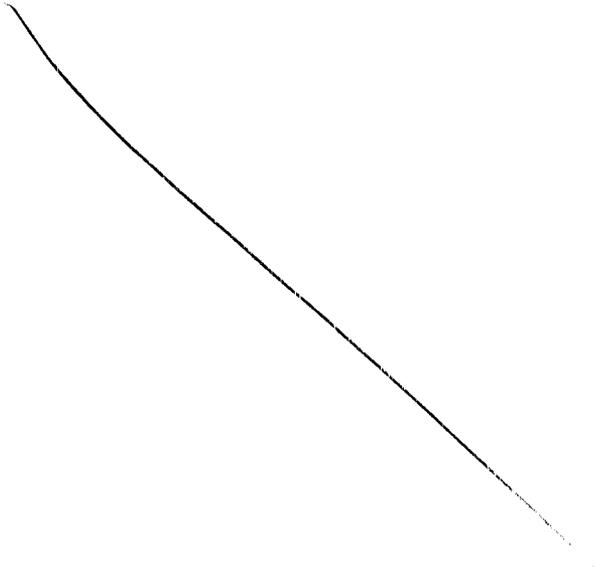
### Variation of drift wall temperature with bulking factor in Thermal-Mode-2



**Observation**

Change in bulking Factor does not change the drift wall temperature

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



A handwritten signature in black ink, consisting of several loops and a vertical line at the end, likely representing the initials 'KA'.

May 10<sup>th</sup> 2007

### 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 are generally used for the calculations. Specific input changes made for each specific case is described below;

### 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.

#### Test Case 3.1.1

Set  
constant  
TimeActiveVentilationEnds[yr]  
30.0

#### Test Case 3.1.2

Set  
constant  
TimeActiveVentilationEnds[yr]  
30.0

#### Test Case 3.1.3

Set  
constant  
TimeActiveVentilationEnds[yr]  
30.0

### 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.

#### Test Case 3.2.1

Set  
constant  
TimeOfRepositoryClosure[yr]  
60.0

#### Test Case 3.2.2

Set  
constant  
TimeOfRepositoryClosure[yr]  
100.0

#### Test Case 3.2.3

Set  
constant  
TimeOfRepositoryClosure[yr]  
150.0

**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. Lowering this period will result in less heat removal and higher temperature. Similarly, a longer period of active ventilation means higher heat removal rate and lower temperature at the 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 a jump in higher waste package temperature immediately after closure. 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.

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

**Constraints:** None

**Output files to compare or examine:** *thermal.dbg*

**Test Procedure:**

- 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*

**Pass/Fail criteria:**

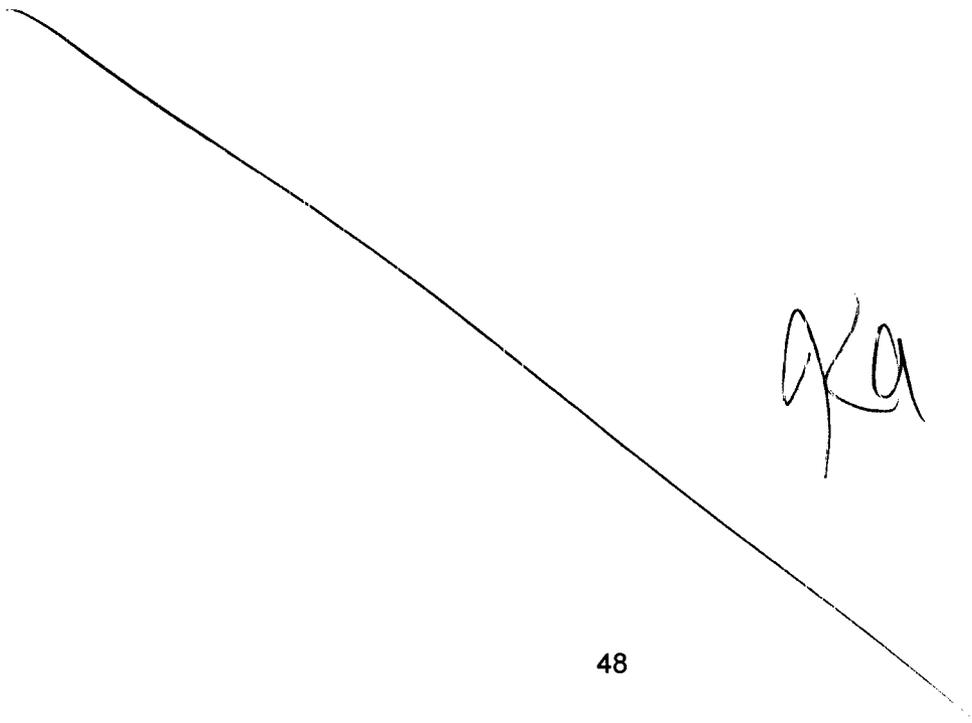
- (1) Lower value of active ventilation must result in subsequent higher temperature in drift components and drift wall as less heat is being removed by forced convection.
- (2) Repository closure results in a jump in waste package temperature immediately after the closure. Early closure will cause this spike to happen early and a late closure will have this spike late.

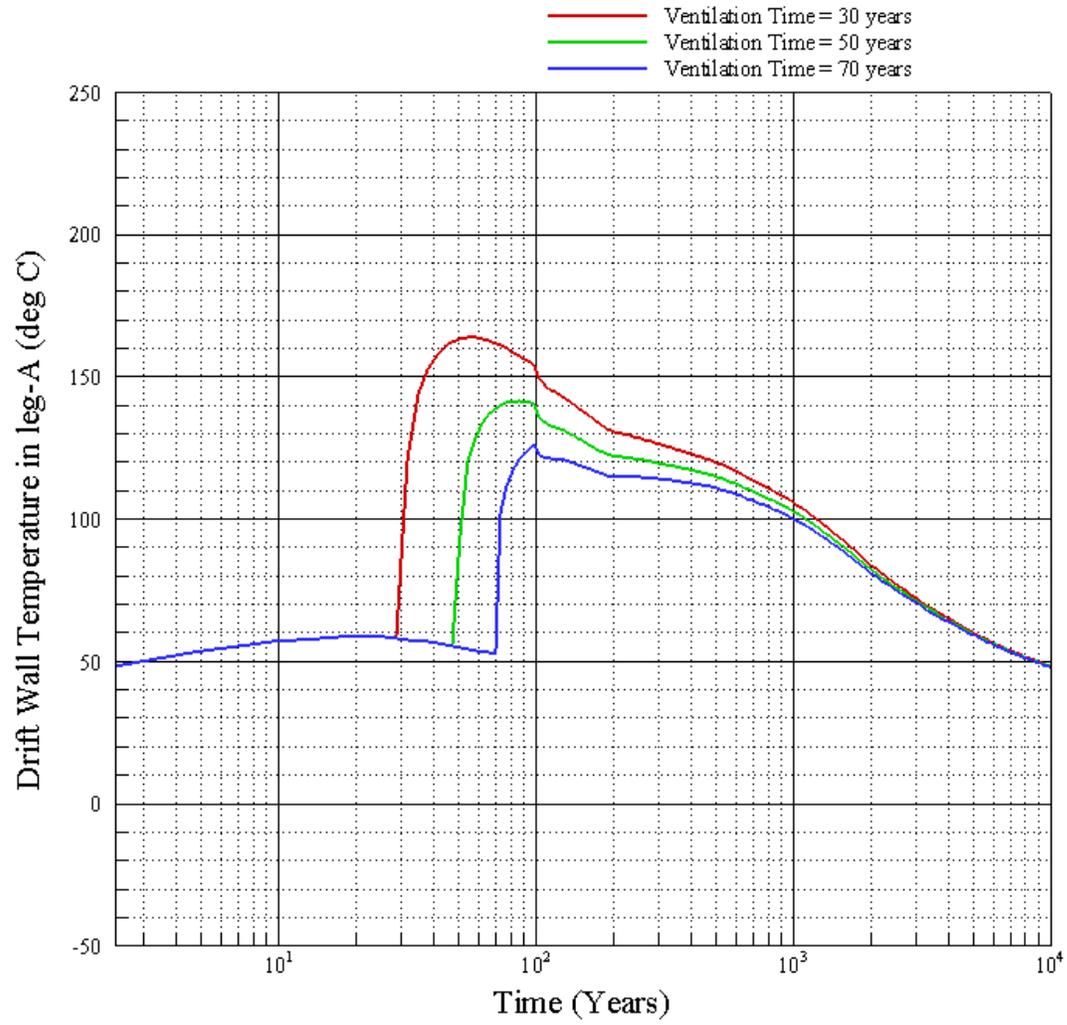
(3) Change in closure time should not affect the wall temperature distribution.

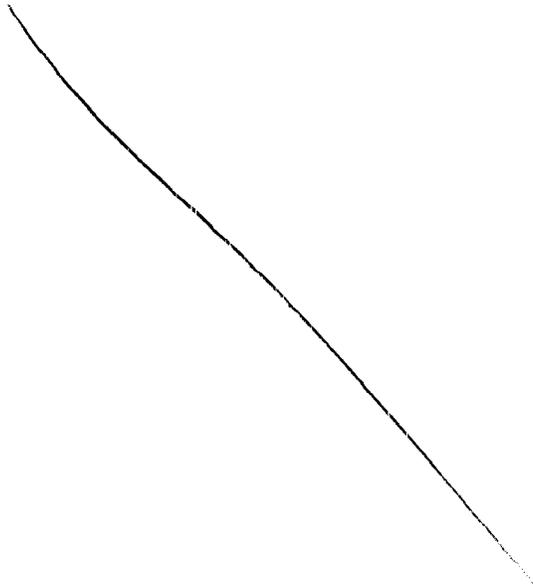


**Test results:**

**Effect of active ventilation time on drift wall temperature**



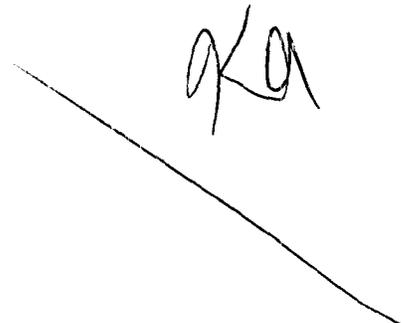




AKa

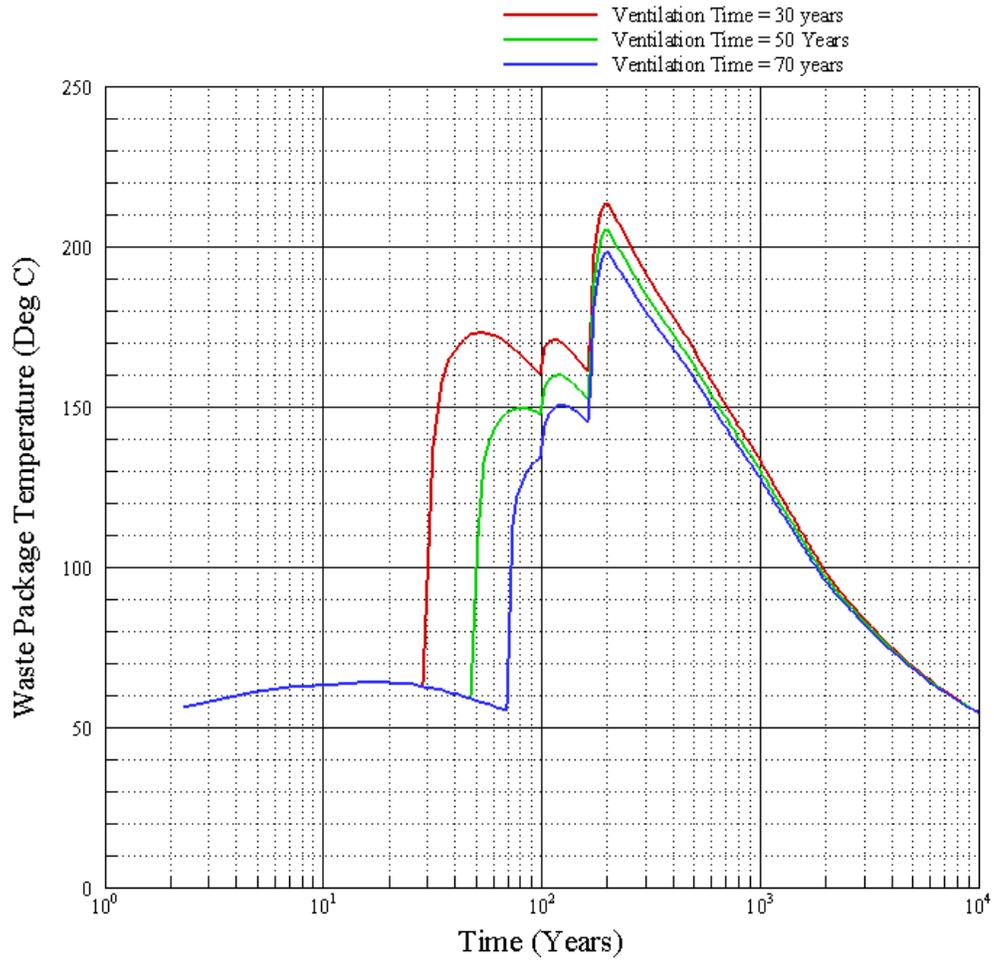
**Observation**

The drift wall temperature shows a jump immediately after the active ventilation period. Lower active ventilation time results in higher drift wall temperature.



AKa

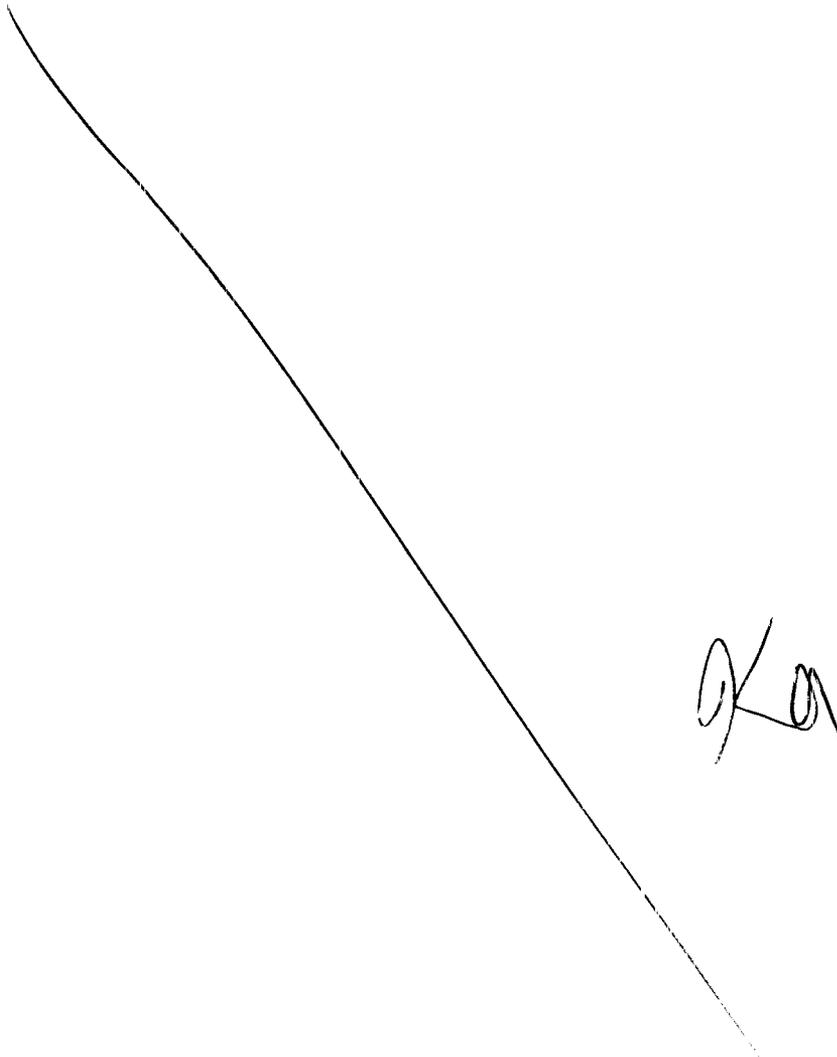
### Effect of active ventilation time on waste package temperature

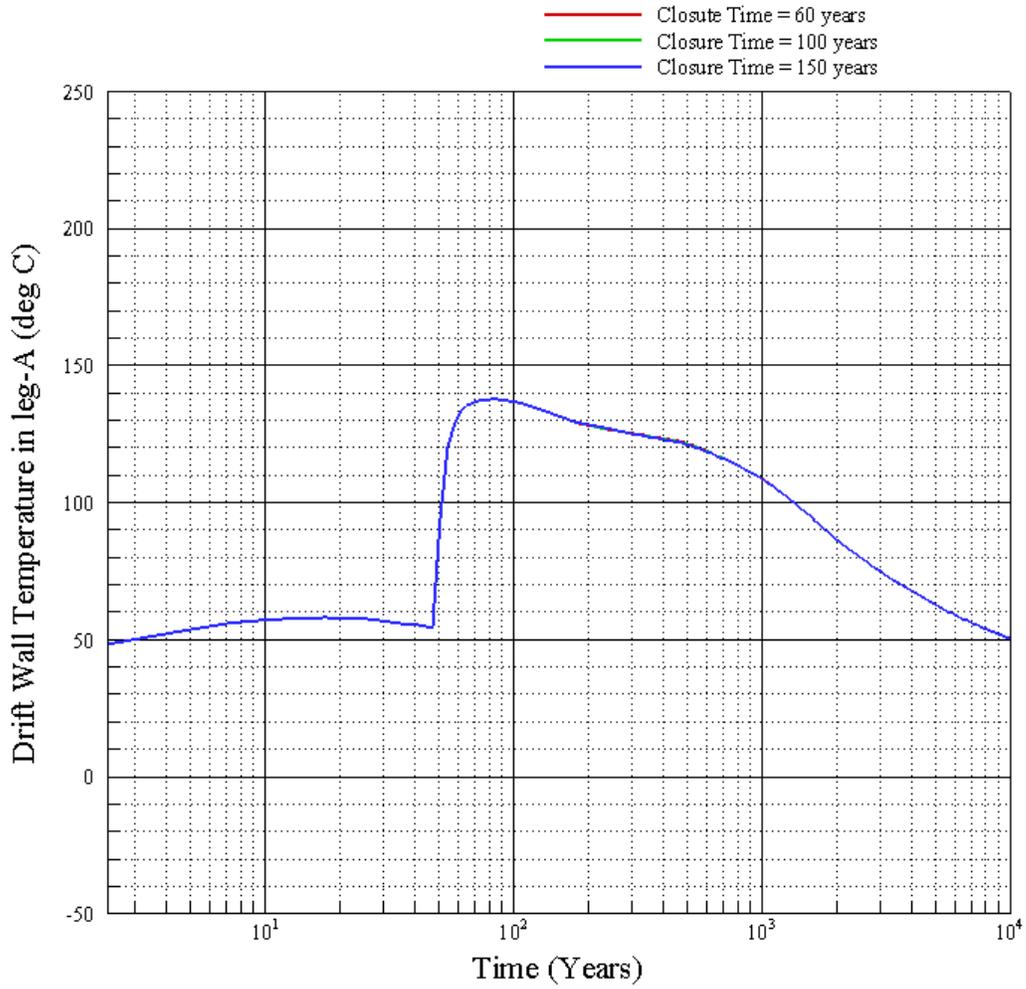


#### Observation

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

### Effect of repository closure time on drift wall temperature



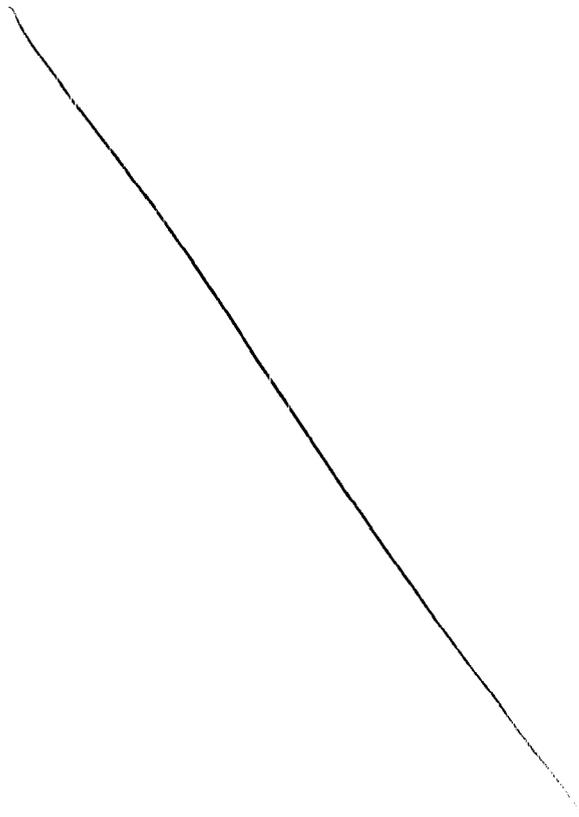


**Observation**

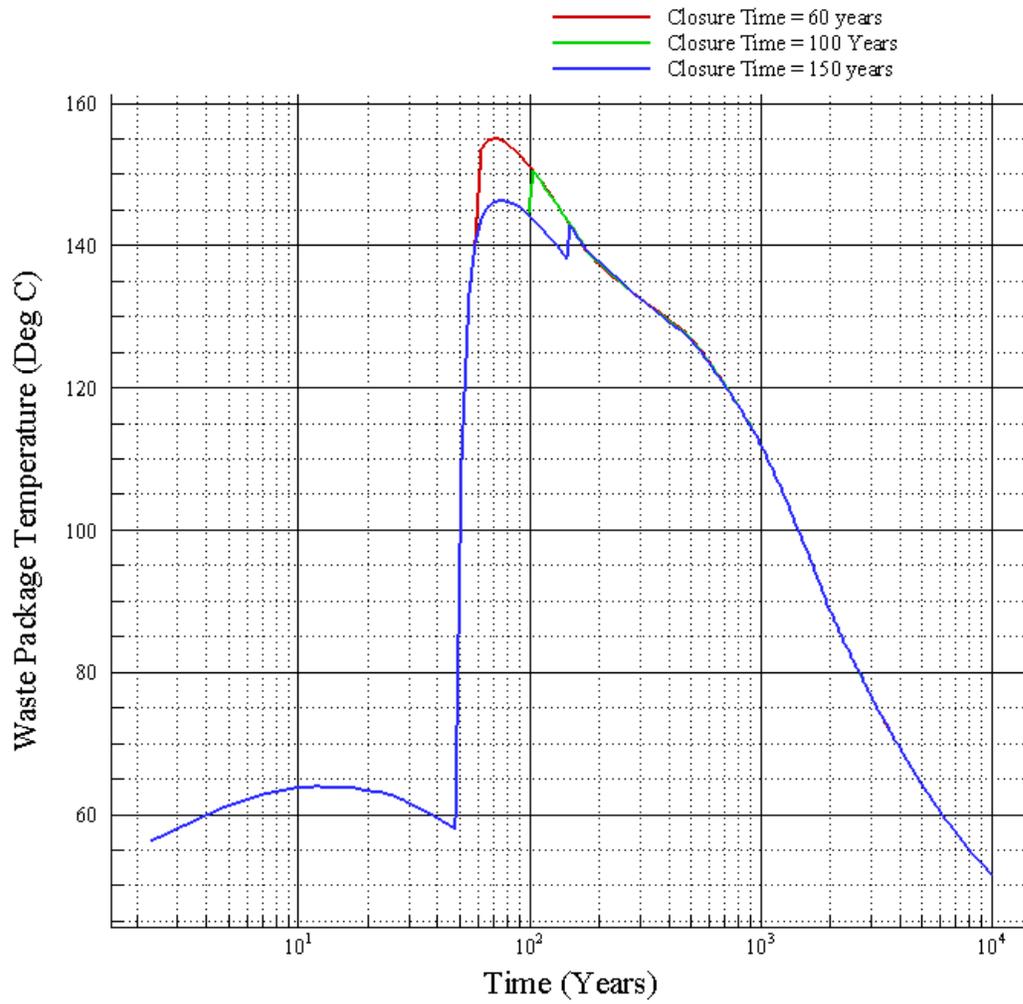
Change in closure time should not affect the wall temperature distribution. All the lines are coincident.

May 14th 2007

**Effect of repository closure time on waste package temperature**



KA



### 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=90  
Test case 4.2 :        Cuda: D\TPA\TEST-4\SeepThT=110  
Test case 4.3 :        Cuda: D\TPA\TEST-4\SeepThT=130  
Test case 4.4 :        Cuda: D\TPA\TEST-4\Intact  
Test case 4.5 :        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

**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 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
enddo
close(iseepcheck)
endif
```

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

**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 “seepcheck.dat” that is created with the code above is also written out.

Tests 4.1, 4.2 and 4.3 studies the effect of change in seepage threshold temperature on the quantity of water contacting the waste package . For these tests, the drift degradation switch is turned off, i.e. no drift degradation takes place. Tests 4.4 and 4.5 explores the use of seepage threshold temperature in the code with and without drift degradation. Test 4.4 simulates a drift without degradation and 4.5 simulates it with degradation.

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

Test 4.1

```
Set    DriftDegradationScenarioFlag(yes=1,no=0)
      0
      constant
```

SeepageThresholdT[C]  
90.00000000000000

Test 4.2

Set DriftDegradationScenarioFlag(yes=1,no=0)  
0  
constant  
SeepageThresholdT[C]  
110.00000000000000

Test 4.3

Set DriftDegradationScenarioFlag(yes=1,no=0)  
0  
constant  
SeepageThresholdT[C]  
130.00000000000000

Test 4.4

Set constant  
SeepageThresholdT[C]  
110.00000000000000  
iflag  
DriftDegradationScenarioFlag(yes=1,no=0)  
1  
constant  
DegradationTimeRockTypeOneSubarea\_3[yr]  
10000000.00  
constant  
DegradationTimeRockTypeTwoSubarea\_3[yr]  
10000000.00

Test 4.5

Set constant  
SeepageThresholdT[C]  
110.00000000000000  
iflag

DriftDegradationScenarioFlag(yes=1,no=0)  
1  
constant  
DegradationTimeRockTypeOneSubarea\_3[yr]  
150.00  
constant  
DegradationTimeRockTypeTwoSubarea\_3[yr]  
150.00

**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:**

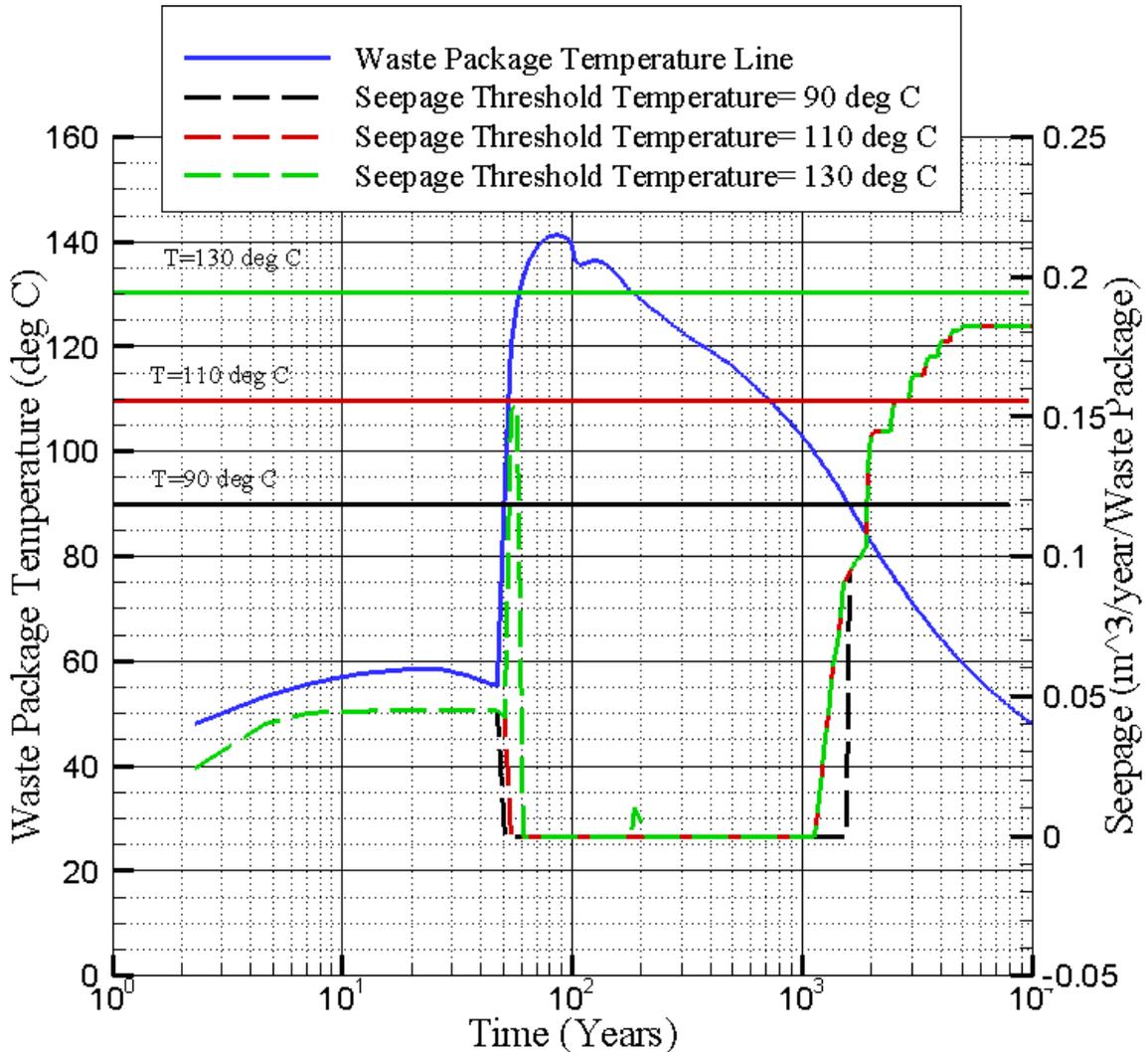
- 1) Execute the TPA code six times, using the modified tpa.inp file and the new executable build with modified *nfenv.f*, and saving the results for examination.
- 2) Examine the drift wall temperature and qm3hit from the *nfenv.rlt* file and observe the temperature at which seepage starts.
- 3) Examine 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 only contact the waste package when the drift wall temperature is at or below the seepage threshold temperature.
- 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:**

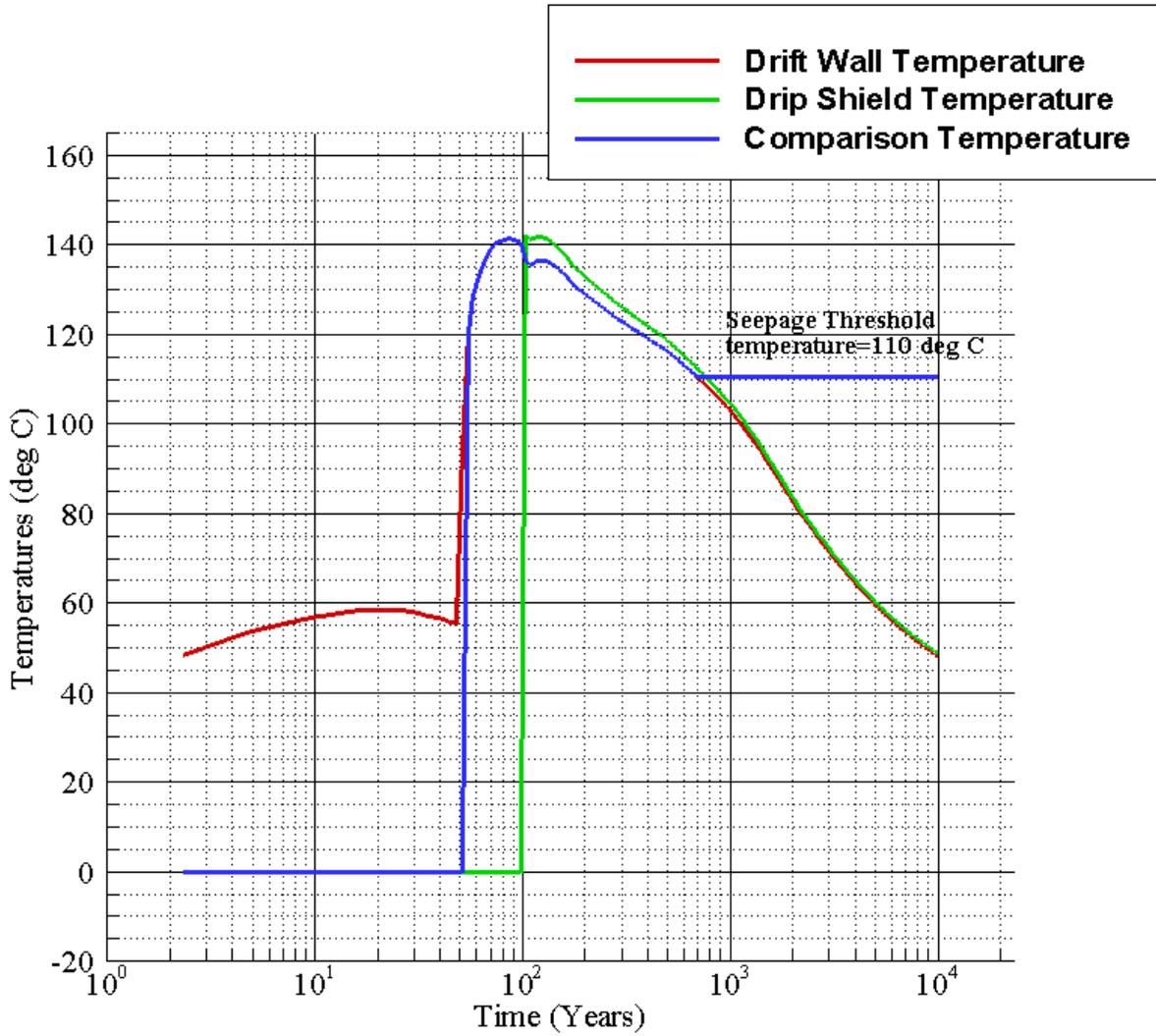
**Effect of Seepage Threshold Temperature on the quantity of water contacting the waste package.**



**Observation**

The dotted lines show the seepage that contacts the waste package. The solid lines show different temperatures. The dotted green line shows the seepage with seepage threshold temperature=130 deg C. The seepage starts when the drift wall temperature reaches 130 deg C. (At the intersection of the horizontal continuous green line indicating the constant T=130 deg 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.

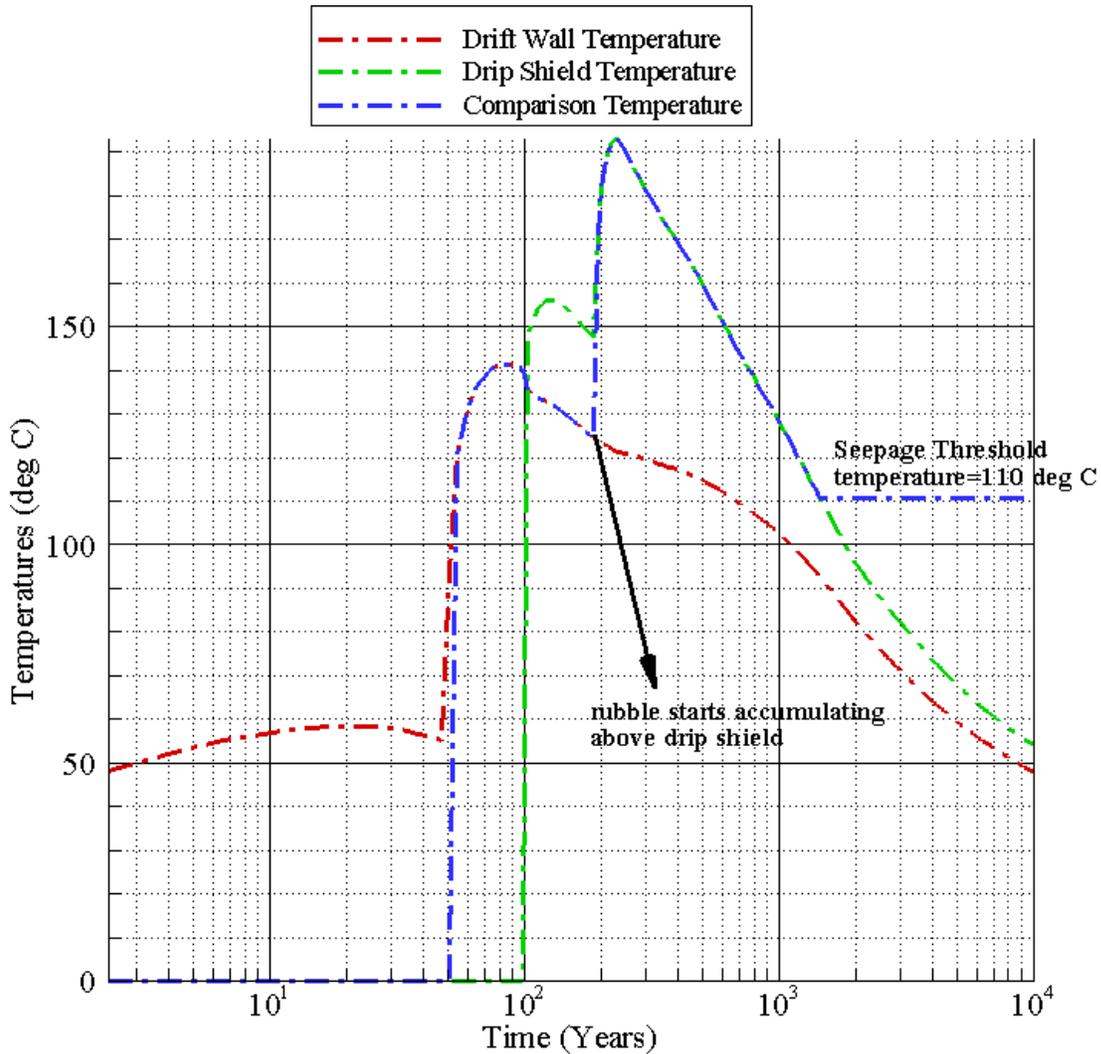
### The comparison temperature for an intact drift



### 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 an intact drift.

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

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**Test 4. 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-Legendre integration is varied between 10 and 200. Specific input changes made for each specific case is described below;

Case 5.1

\*\*

iconstant

NumberOfWeightsForGaussLegendreIntegration[]

10

\*\*

Case 5.2

\*\*

iconstant

NumberOfWeightsForGaussLegendreIntegration[]

20

\*\*

Case 5.3

\*\*

iconstant

NumberOfWeightsForGaussLegendreIntegration[]

30

\*\*

Case 5.4

\*\*

iconstant

NumberOfWeightsForGaussLegendreIntegration[]

40

\*\*

Case 5.5

\*\*

iconstant

NumberOfWeightsForGaussLegendreIntegration[]

50

\*\*

Case 5.6

\*\*

iconstant  
NumberOfWeightsForGaussLegendreIntegration[]  
60  
\*\*

Case 5.7  
\*\*

iconstant  
NumberOfWeightsForGaussLegendreIntegration[]  
100  
\*\*

Case 5.8  
\*\*

iconstant  
NumberOfWeightsForGaussLegendreIntegration[]  
200  
\*\*

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

**Constraints:** None

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

**Test Procedure:**

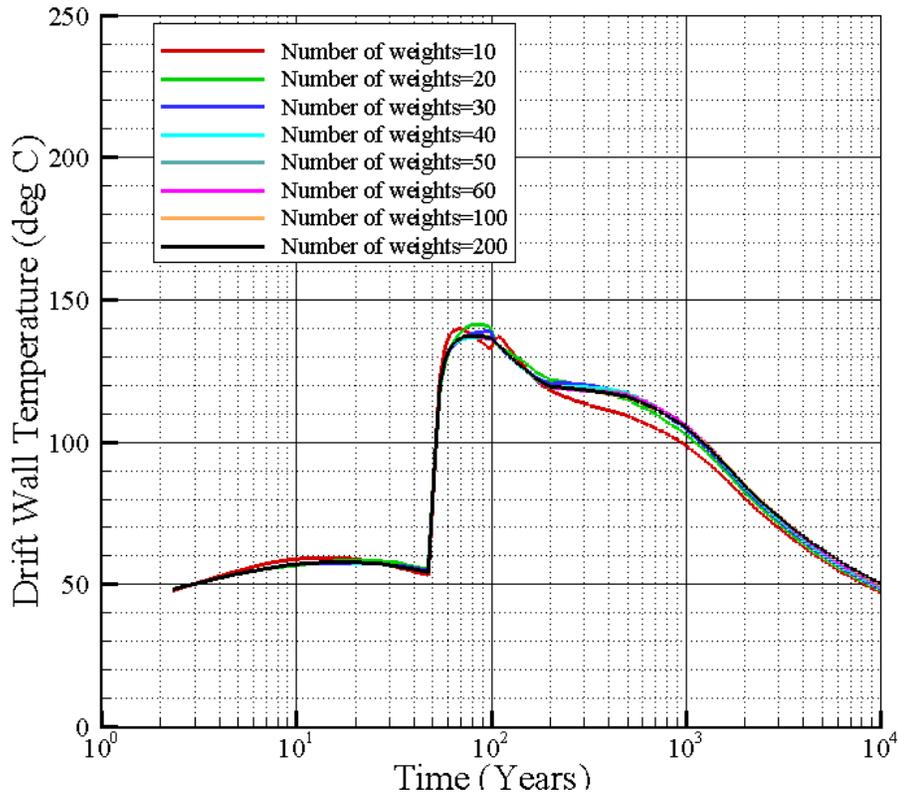
- 1) Execute the TPA code eight times, using the modified tpa.inp file and the standard tpa executable .
- 2) Plot the drift wall, waste package and drip shield temperature to see what effect the number of weighting factors for integration has

**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**

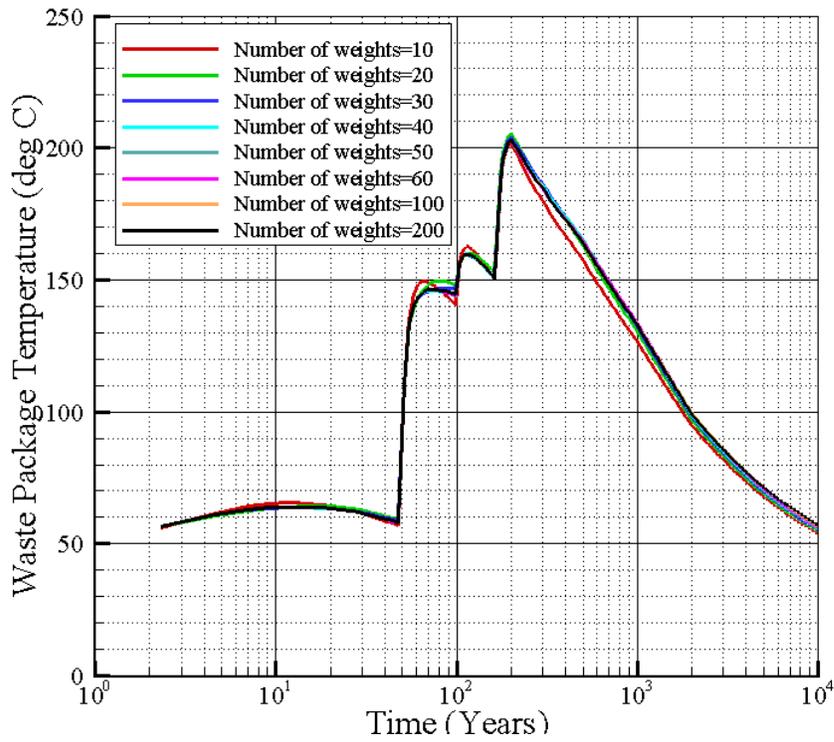


**Observation**

The temperature calculations are affected when the number of weights is 10. At higher number of weights, the calculations do not change

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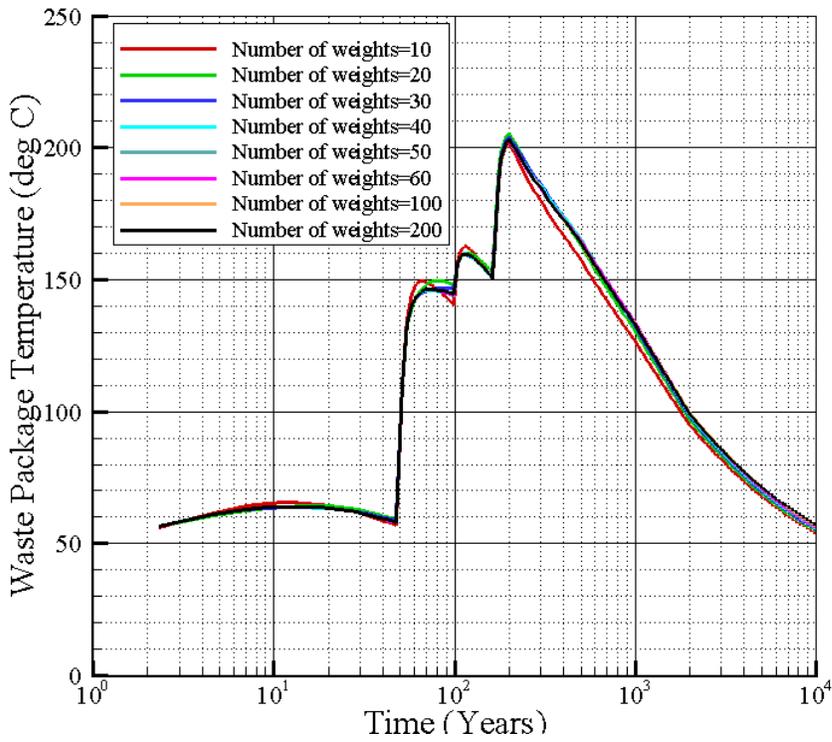
**Effect of the number of weighting factors on waste package temperature**



**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**



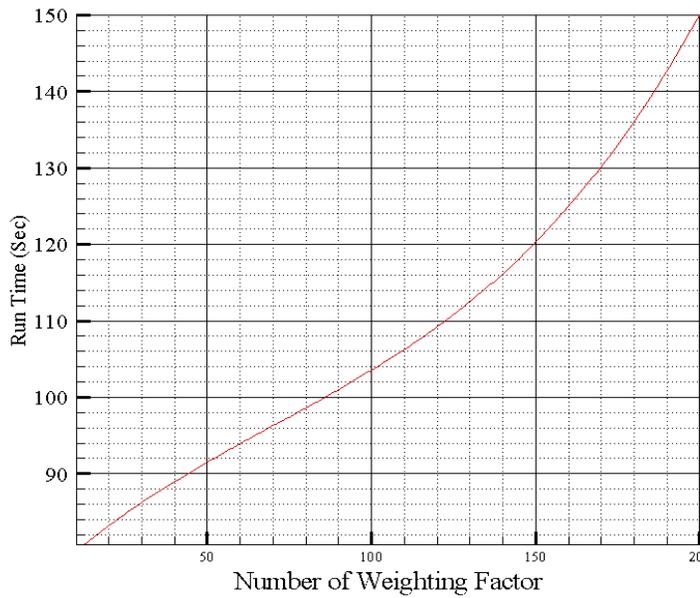
**Observation**

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

***Test 4 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.

## ADDITIONAL INFORMATION FOR SCIENTIFIC NOTEBOOK NO. 862E

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