SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 610	2. Software Title and Version: TPA 5.1	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *exec.f, driftfail.f, driftdriver.f tpa.inp*

The new MECHFAIL module requires the vertical pressure of rock rubble as a function of time as well as the vertical pressure of the rock rubble during seismic events. This information is not available in the current drift degradation subroutine called **eqvdia()**. A new routine is required to replace subroutine **eqvdia()** that will calculate drift heights, equivalent diameters for the radial geometry, and vertical pressures. Two drift failure mechanisms are specified: Chimney and Trapezoidal. Refer to Ibarra, L., et. al., "Drip Shield - Waste Package Mechanical Interaction (Staff Working Draft)," January 2006.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
L. Ibarra Date: 2-22-06	R. Janetzke Date:2-22-06

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*): A standalone module called *driftfail.f* has been incorperated into the TPA code. This module calculates vertical pressures from accumulated rubble that results from the degradation of the emplacement drift. The degraded drift can take one of two shapes: a simple chimney shape or a trapezoidal shape. This module calculates vertical pressures at TPA time intervals and during seismic events. In addition this module calculates drift equivalent diameters and drift heights.

The standalone is called by the subroutine driftdrive in the executive module. The subroutine driftdrive prepares the driftfail.inp file and executes the standalone code. The standalone then performs its calculations and returns that data in the file *driftfail.dat*. After the calculations are completed the subroutine driftdrive returns the data contained in driftfail.dat to the executive module.

8. Implemented by:	Date:
J. Mancillas	4-6-06

9. Description of Acceptance Tests:

Tested a modified version of tpa5.0.2q on Windows machine, "tpa," and UNIX machine, "spock." Version 5.0.2q was used with updated driftfail.f and driftdrive.f files. Discussion of test results included in Attachment 1.

All process level and system level tests successfully PASSED.

10. Tested by:	Date:
G. Adams	4-7-06

UPDATE REQUIREMENTS for TPA.INP

SCR 610

Status ***(ADD, DELETE, MODIFY TO, MODIFY FROM)***	**Module**	**Parameter Name**	**Description** ***(Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.)***	**Distribution**	**Range**	**Justification** ***1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.***	**Source**
Modify From	tpa.inp	DripShieldHeight[m]		Constant	2.51		
Modify To	tpa.inp	DripShieldEqvHeight[m]	Equivalent height of the drip shield	Constant	2.508		
Modify From	tpa.inp	DripShieldWidth[m]		Constant	2.505		
Modify To	tpa.inp	DripShieldEqvWidth[m]	Equivalent width of the drip shield	Constant	2.082		

ADD	tpa.inp	TrapezoidBaseAngle	angle used to calculate the width of the chimney during trapezoidal degradation	Constant	50.7	Angle chosen to give a chimney width of approximately 10 m	
ADD	tpa.inp	FractionDriftDegradationOccursByChimney	Fraction of drift degradations which occur by the chimney mechanism	Constant	0.75		
ADD	tpa.inp	SeismicMinimumBulkingFactor	Lowest value a bulking factor can be seismicly reduced to.	Constant	1.15		
ADD	tpa.inp	DriftDegradationGeometrySelectionValue	Randomly selected value used to determine which drift degradation method is selected	Uniform	0.0,1.0		

Attachment 1

Description of Acceptance Tests

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

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

For the process level tests, the "drift height above the invert" percentage errors between the tpa generated results and the spreadsheet calculations were consistently greater than the percentage errors between other spreadsheet and tpa generated values. There was a difference in the technique for averaging and calculating the resulting drift heights between the code and the spreadsheets. This larger percentage error occurs during the early period of drift degradation. Even with this larger percentage error, the results were within the test criteria of 1% error and therefore the tests passed.

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

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

The test plan and test results are included in document, "Test Plan and Test Results for TPA SCR #610." Supporting files are included on a CD labeled, "Test Plan and Test Results for TPA SCR #610."

Test Plan and Test Results for TPA SCR # 610

Test Plan Name: DRIFTFAIL

Tested By: George Adams

Date: April 7, 2006

Host Machine: tpa

Host OS: Windows (tpa),
UNIX (spock)

Baseline Version: TPA 5.0.2h

Test Version: TPA 5.0.2q(modified)

Version 5.0.2q of the tpa code was modified to use updated driftfail.f and driftdrive.f files. Process level tests pl-1 through pl-6 were executed using these updated files. The build for these process level tests is identified as tpa502qmod1. Subsequent to these tests, driftfail.f and driftdrive.f files were updated again. Tests pl-7 and pl-8 were run with a new version of these files. The build for these process level tests is identified as tpa502qmod2. Version tpa502qmod2 was used for all of the UNIX tests to compare tests on machine "spock" to those run on the Windows machine "tpa."

Process Level Tests

The process level tests are designed to verify the standalone module results against spreadsheet calculations.

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
`SeismicDisruptiveScenarioFlag(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 calculated values.

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 calculated values to within 1%.

9.0 Test Results

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

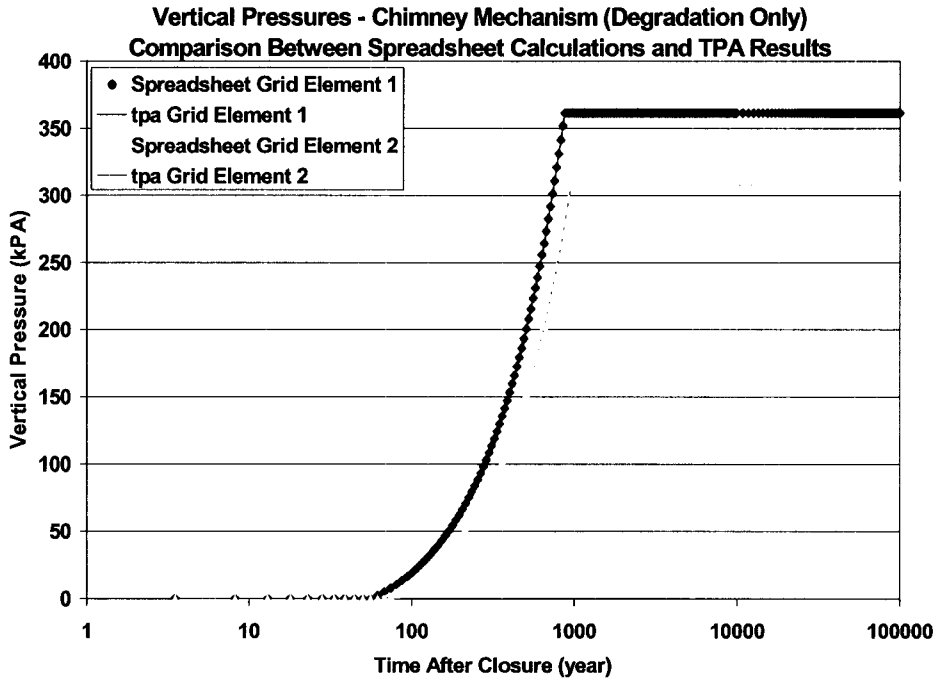
9.2 Criterion 1: Code generated and spreadsheet calculated values agree to within 1%.

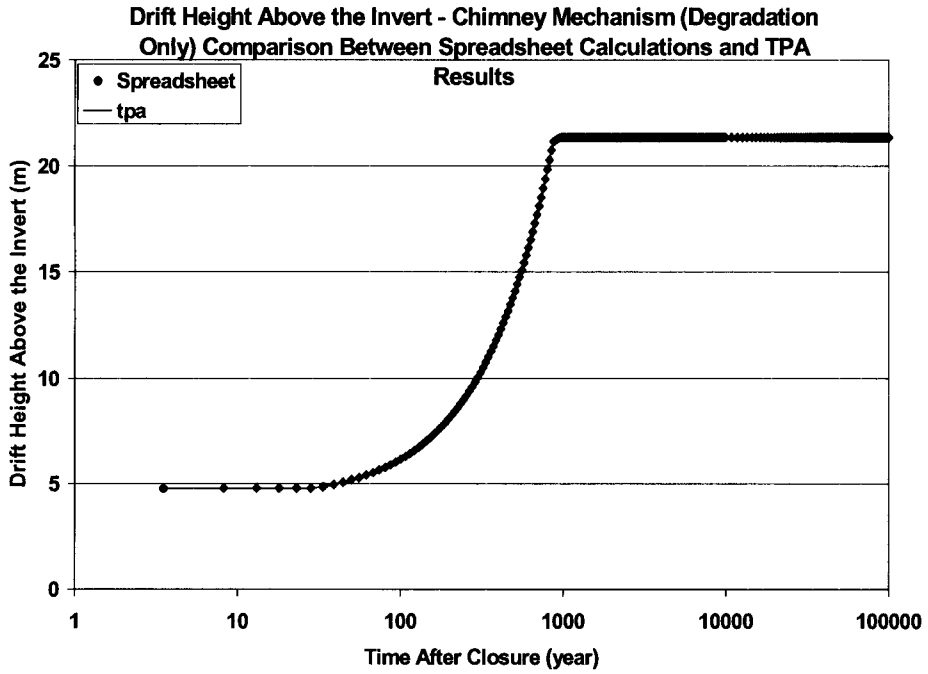
9.3 Overall Test Status:

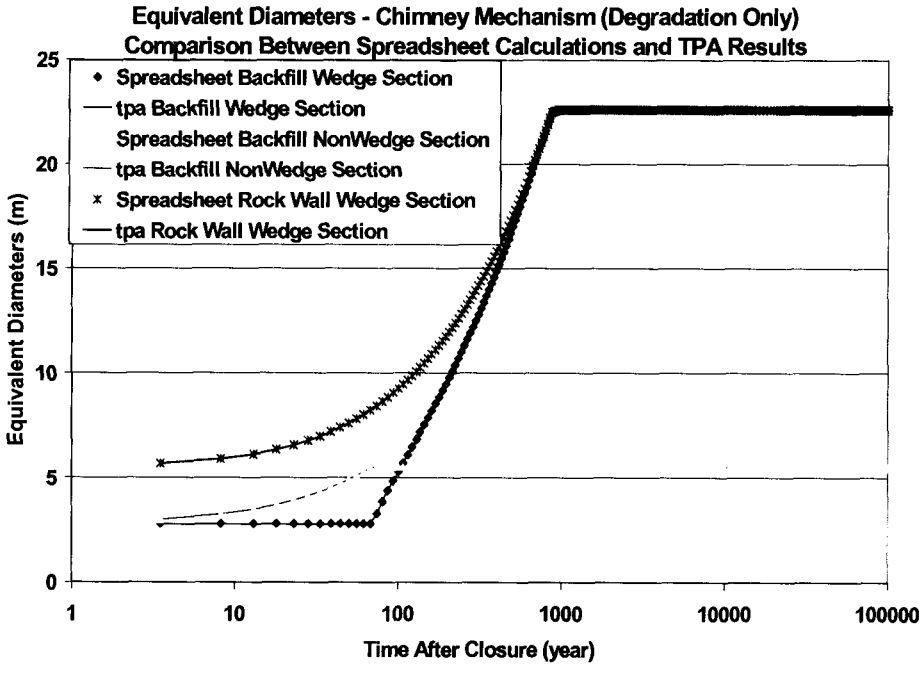
This test **PASSED** the criterion above for test PL-1 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

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.






Equivalent Diameters - Chimney Mechanism (Degradation 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)
25
20
15
10
5
0
1
10
100
1000
10000
100000
Time After Closure (year)

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
```

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 calculated values.

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 calculated values to within 1%.

9.0 Test Results

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

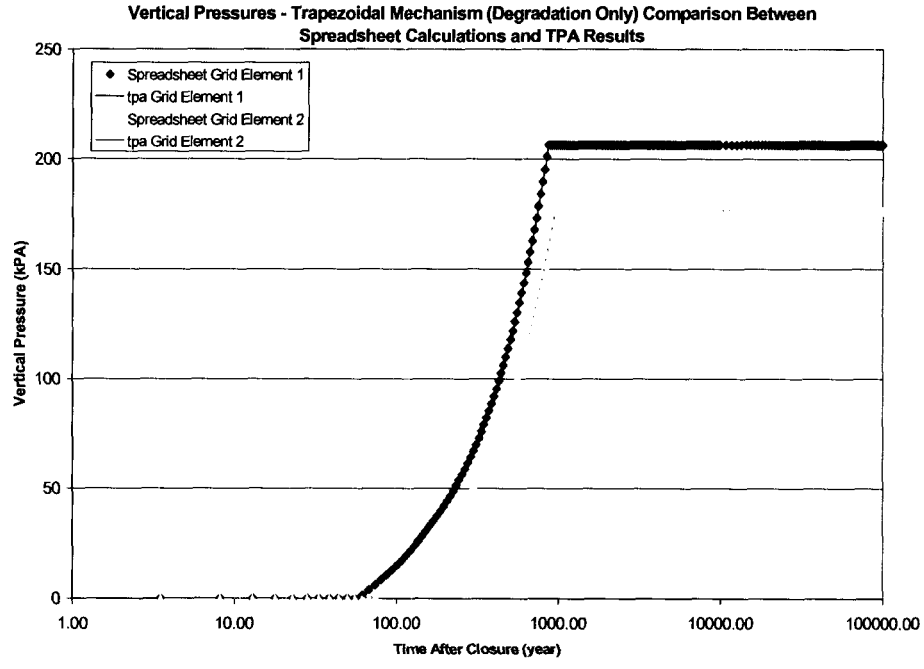
9.2 Criterion 1: Code generated and spreadsheet calculated values agree to within 1%.

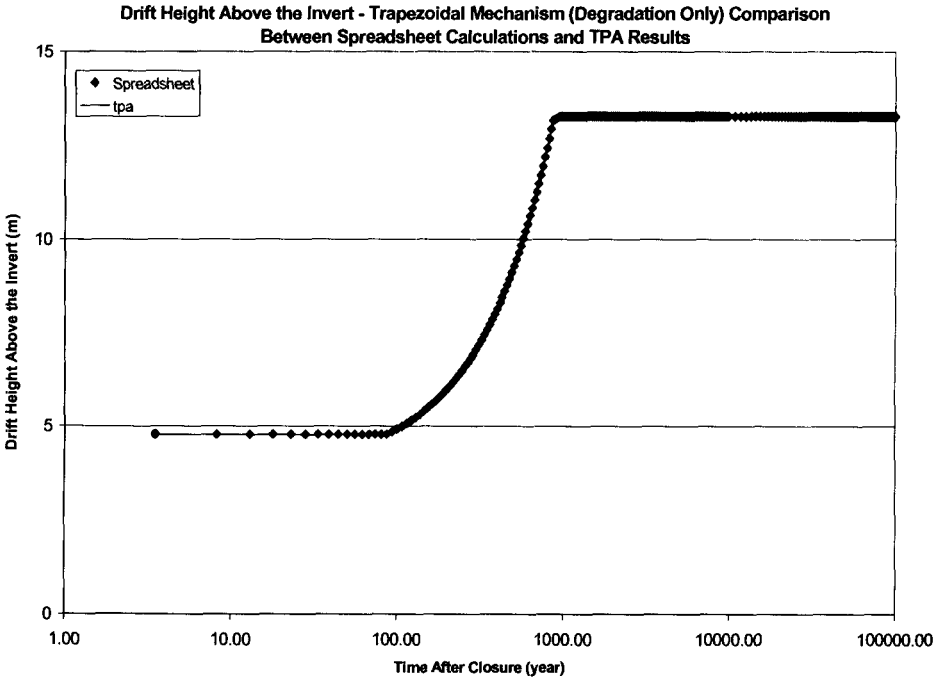
9.3 Overall Test Status:

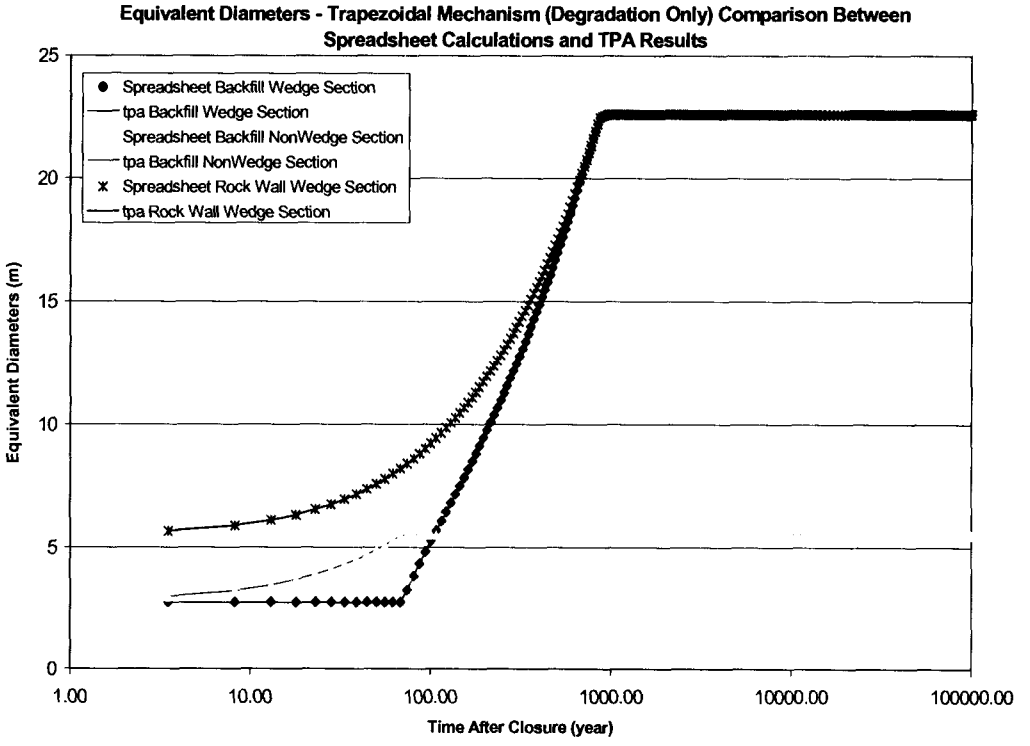
This test **PASSED** the criterion above for test PL-2 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

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.






Equivalent Diameters - Trapezoidal Mechanism (Degradation 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)
25
20
15
10
5
0
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.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
```

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 calculated values.

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 calculated values to within 1%.

9.0 Test Results

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

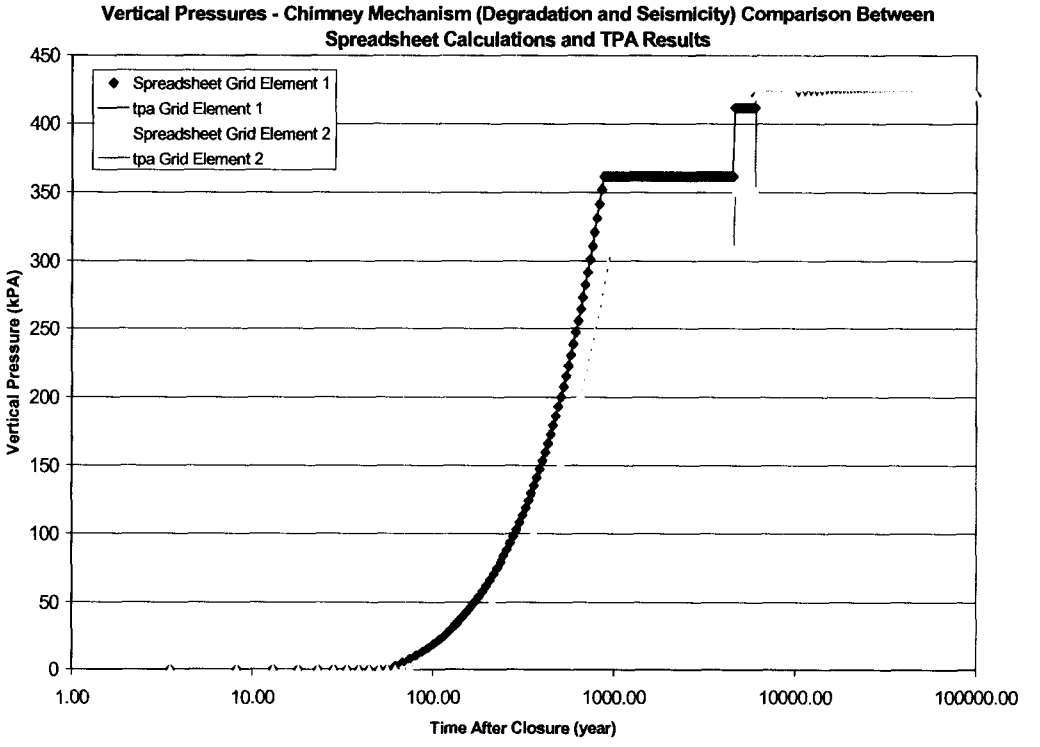
9.2 Criterion 1: Code generated and spreadsheet calculated values agree to within 1%.

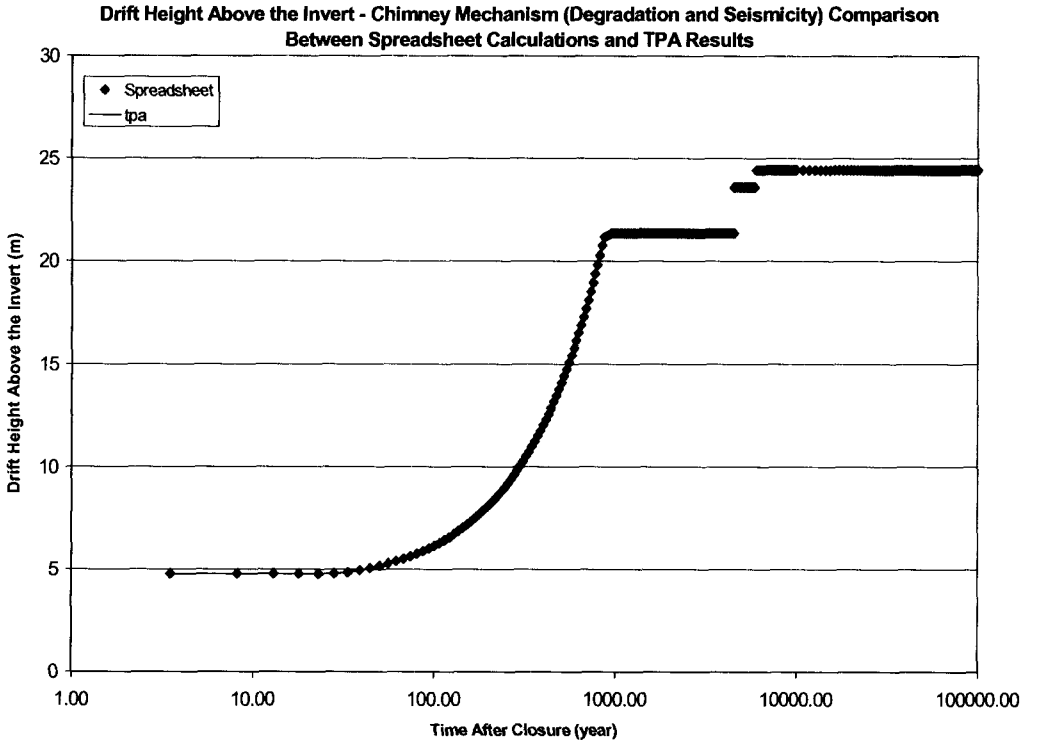
9.3 Overall Test Status:

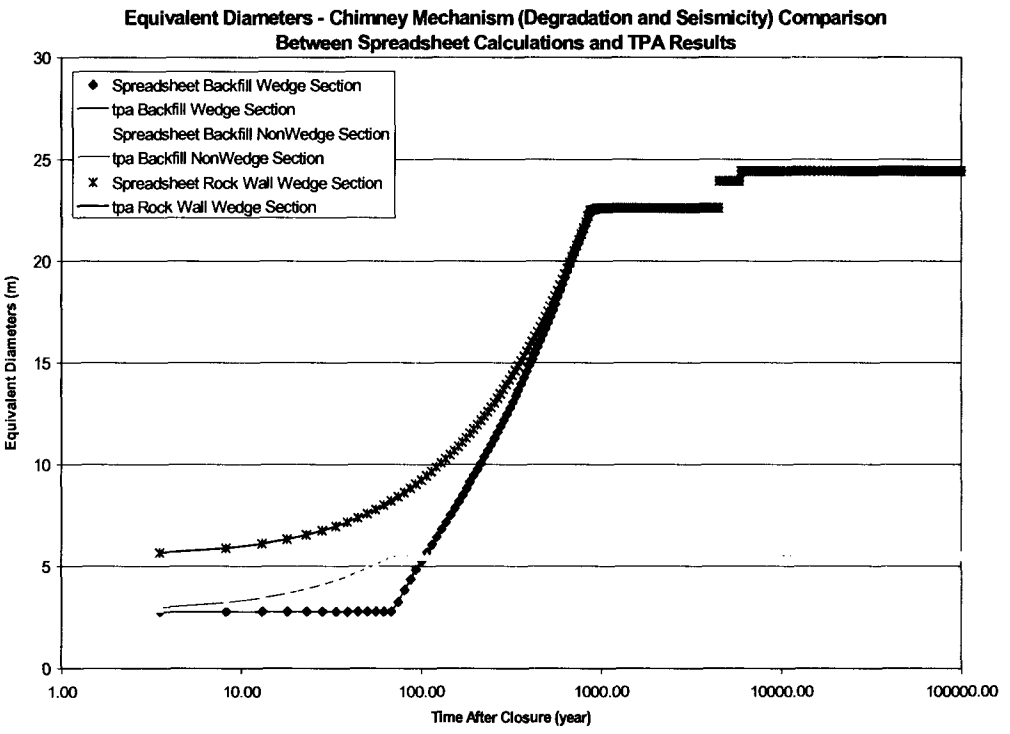
This test **PASSED** the criterion above for test PL-3 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

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.






Equivalent Diameters - Chimney 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)
30
25
20
15
10
5
0
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.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
```

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 calculated values.

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 calculated values to within 1%.

9.0 Test Results

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

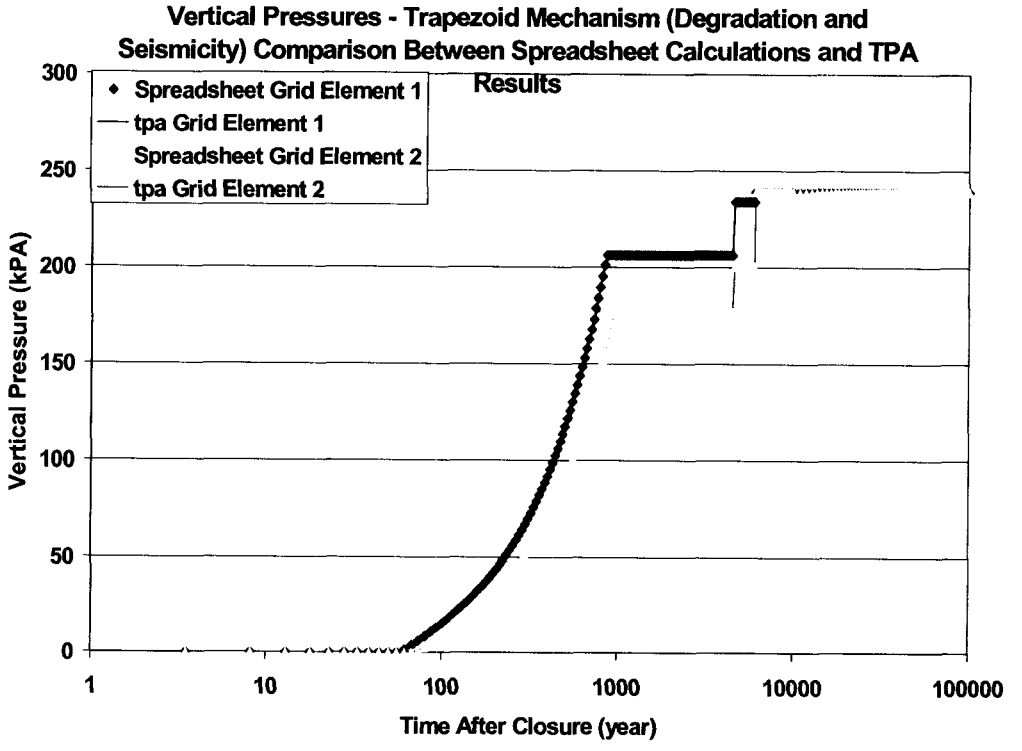
9.2 Criterion 1: Code generated and spreadsheet calculated values agree to within 1%.

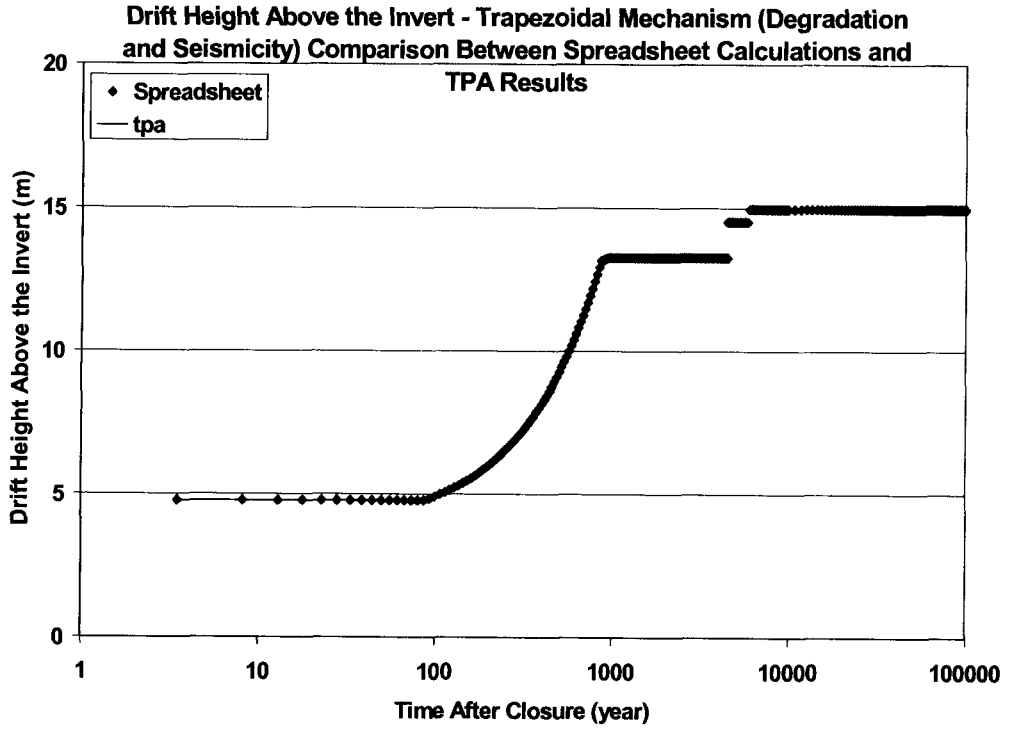
9.3 Overall Test Status:

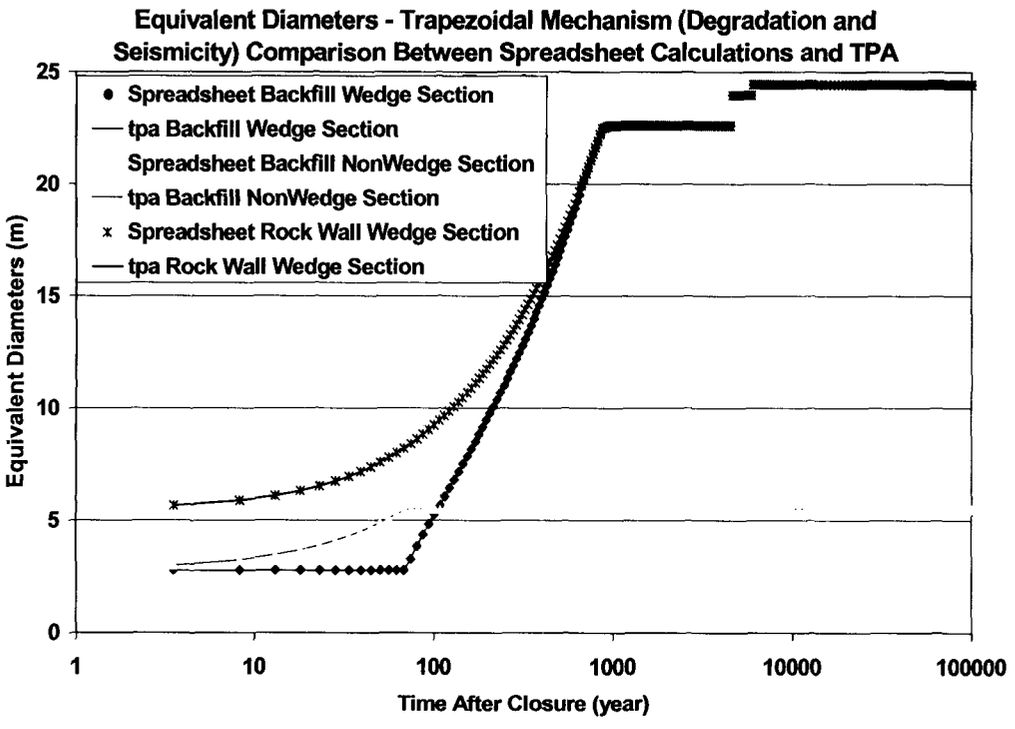
This test **PASSED** the criterion above for test PL-4 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

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.






Equivalent Diameters - Trapezoidal Mechanism (Degradation and Seismicity) Comparison Between Spreadsheet Calculations and TPA
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)
25
20
15
10
5
0
1
10
100
1000
10000
100000
Time After Closure (year)

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
```

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 calculated values.

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 calculated values to within 1%.

9.0 Test Results

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

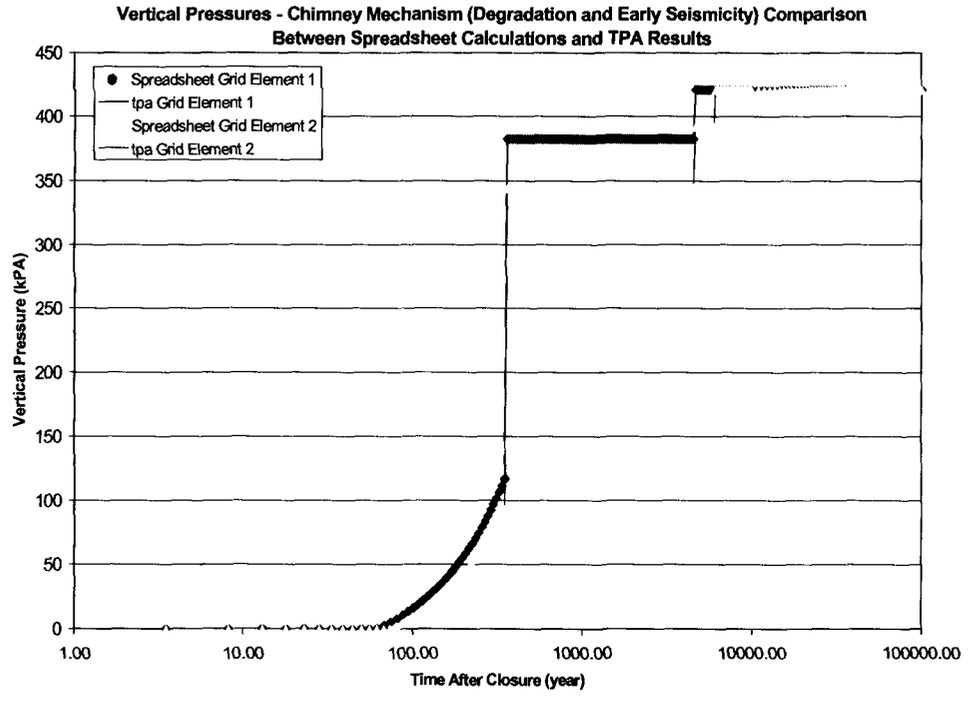
9.2 Criterion 1: Code generated and spreadsheet calculated values agree to within 1%.

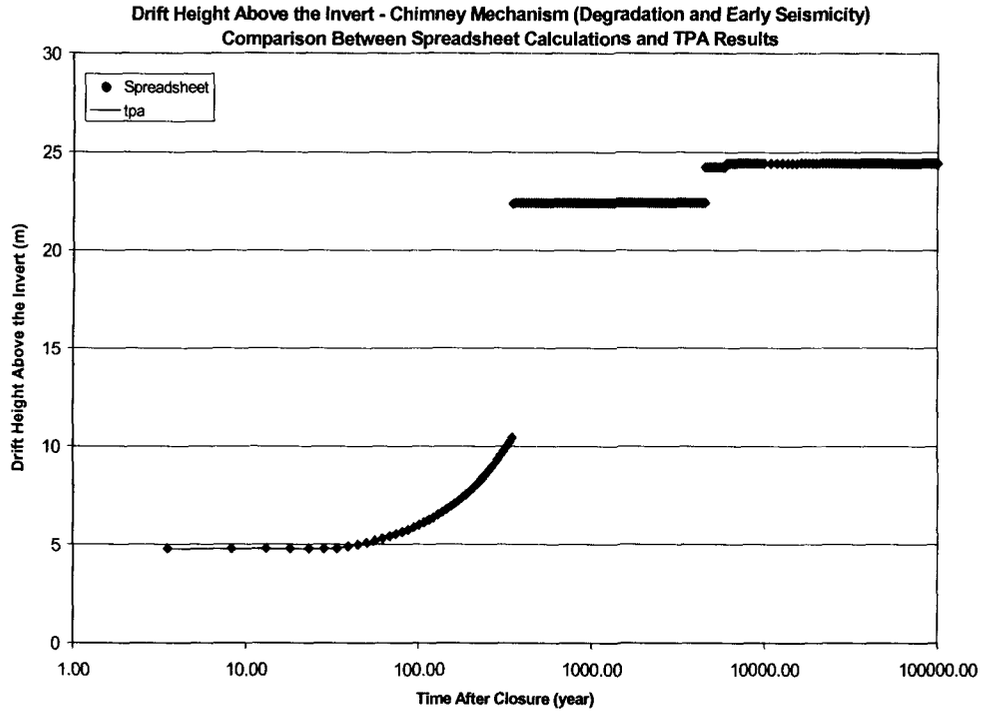
9.3 Overall Test Status:

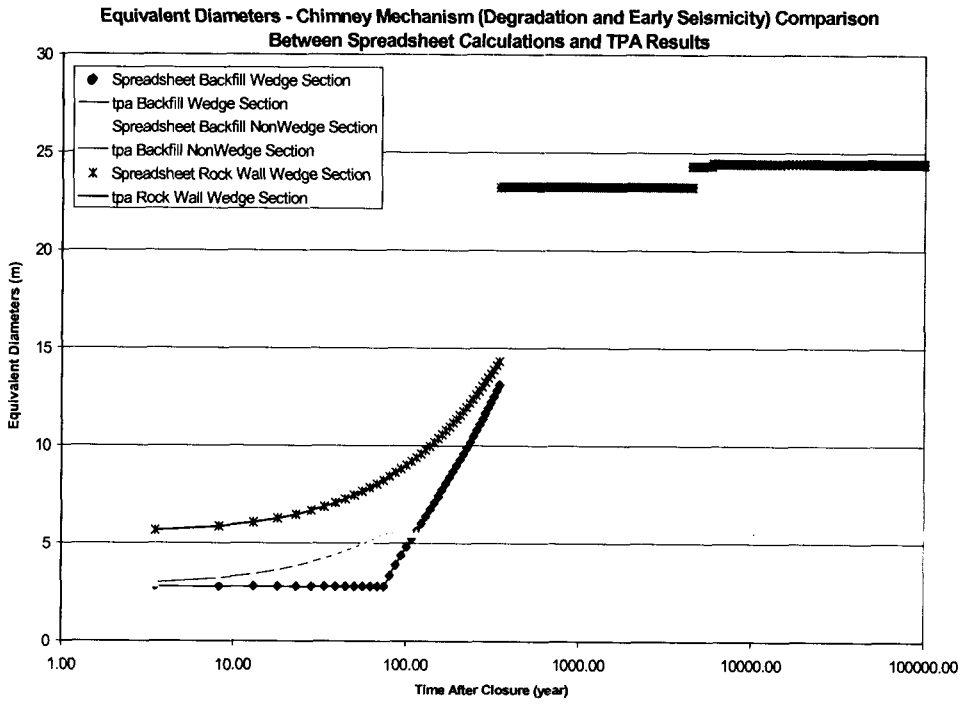
This test **PASSED** the criterion above for test PL-5 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

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.






Equivalent Diameters - Chimney Mechanism (Degradation and Early 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)
30
25
20
15
10
5
0
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 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
```

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 calculated values.

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 calculated values to within 1%.

9.0 Test Results

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

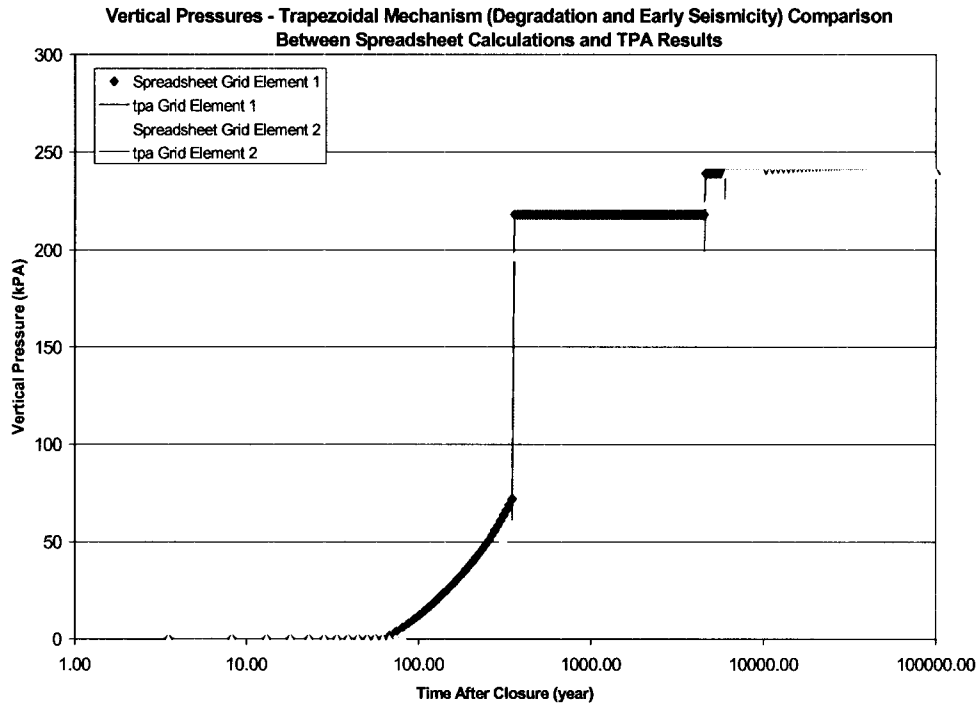
9.2 Criterion 1: Code generated and spreadsheet calculated values agree to within 1%.

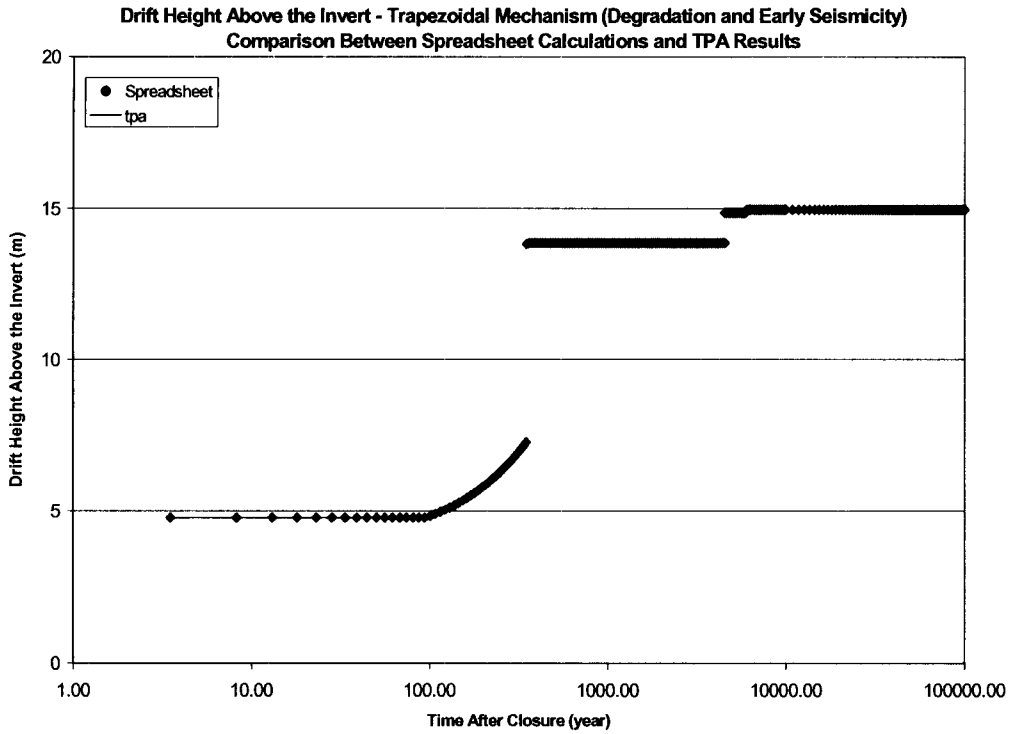
9.3 Overall Test Status:

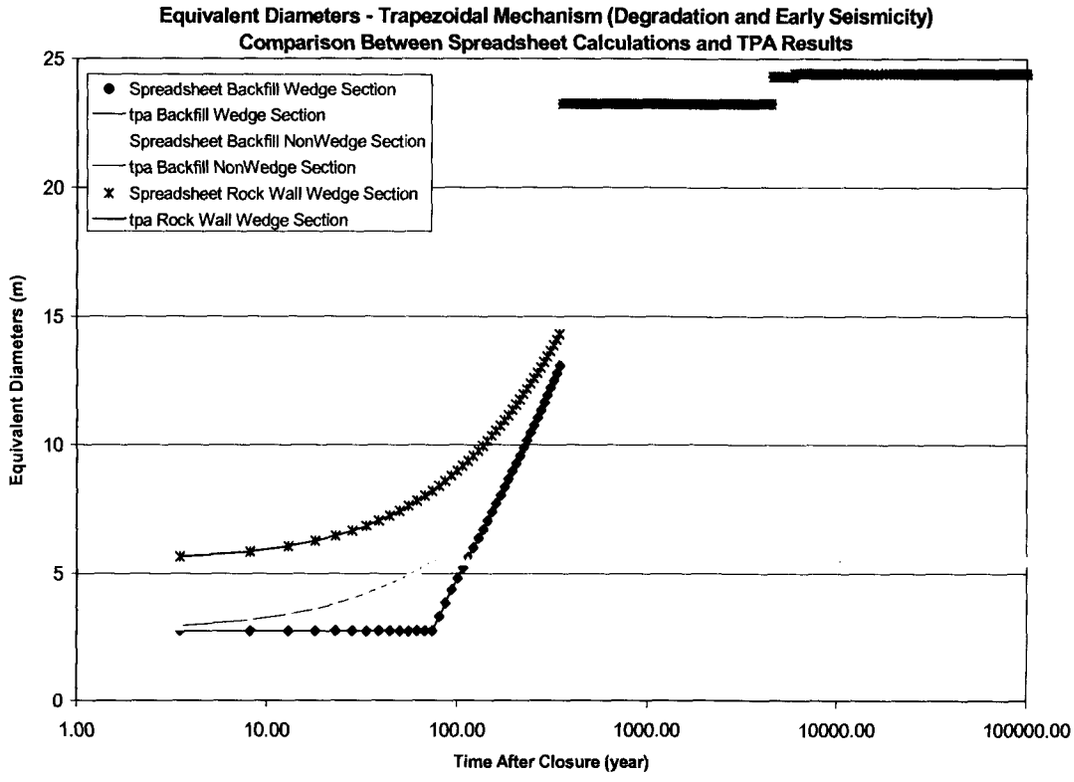
This test **PASSED** the criterion above for test PL-6 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

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.






Equivalent Diameters - Trapezoidal Mechanism (Degradation and Early 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)
25
20
15
10
5
0
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 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
```

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 calculated values.

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 calculated values to within 1%.

9.0 Test Results

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

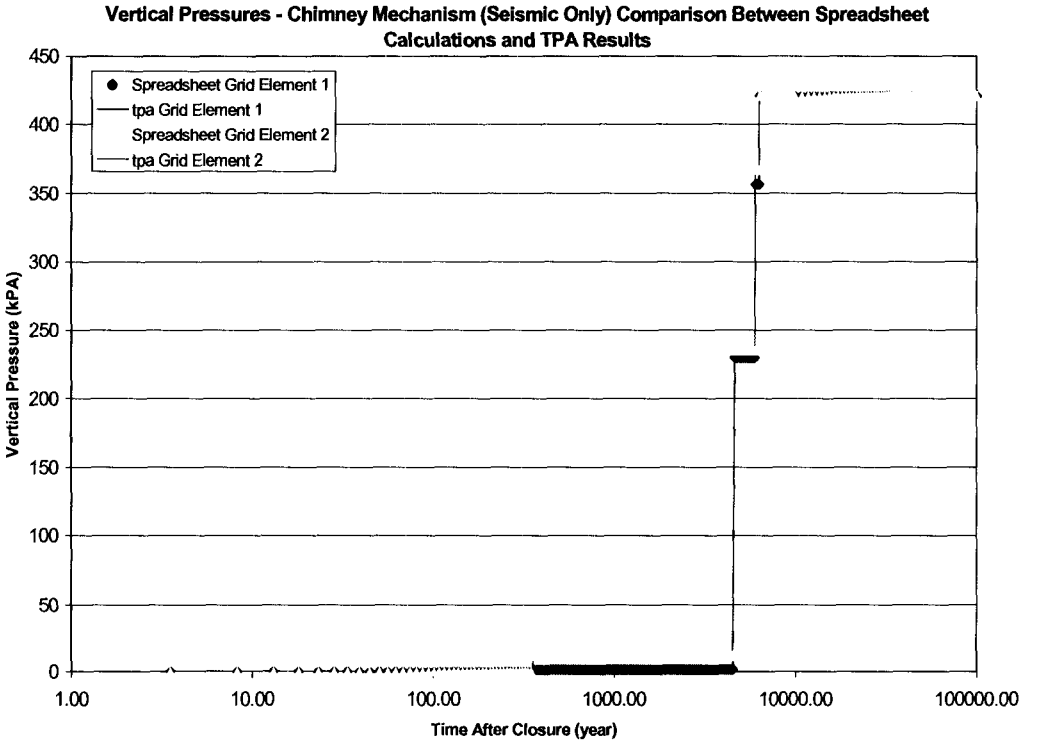
9.2 Criterion 1: Code generated and spreadsheet calculated values agree to within 1%.

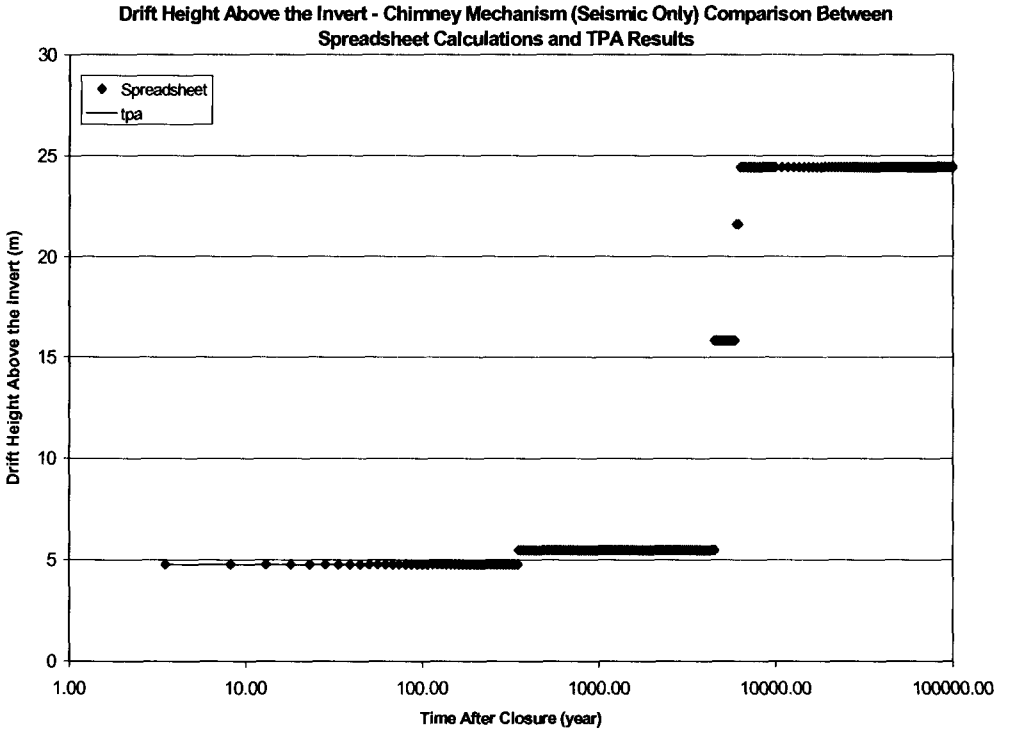
9.3 Overall Test Status:

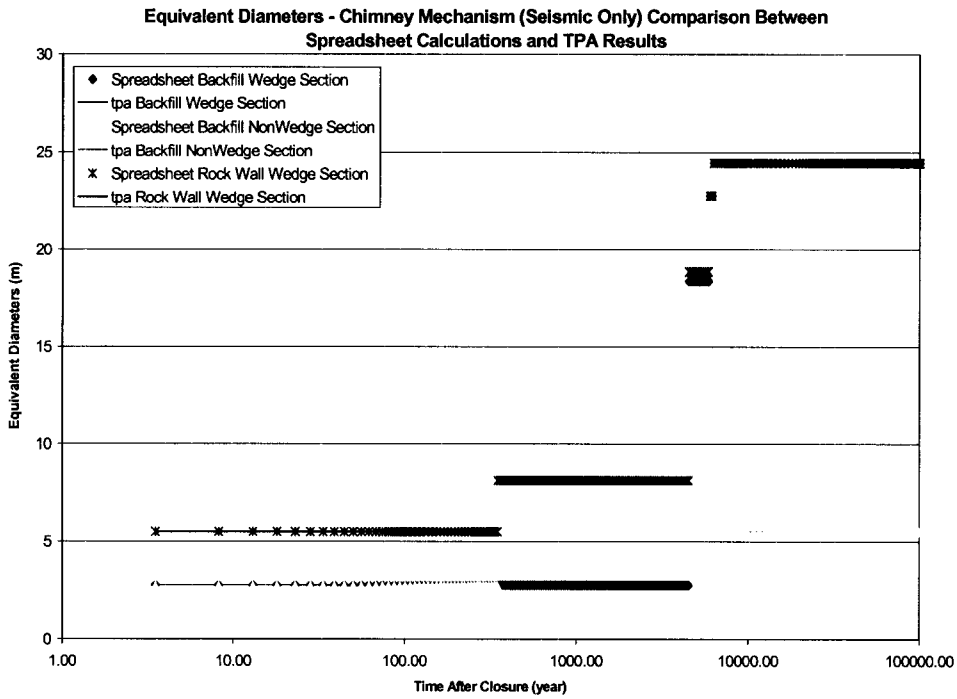
This test **PASSED** the criterion above for test PL-7 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

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.






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)
30
25
20
15
10
5
0
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
```

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 calculated values.

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 calculated values to within 1%.

9.0 Test Results

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

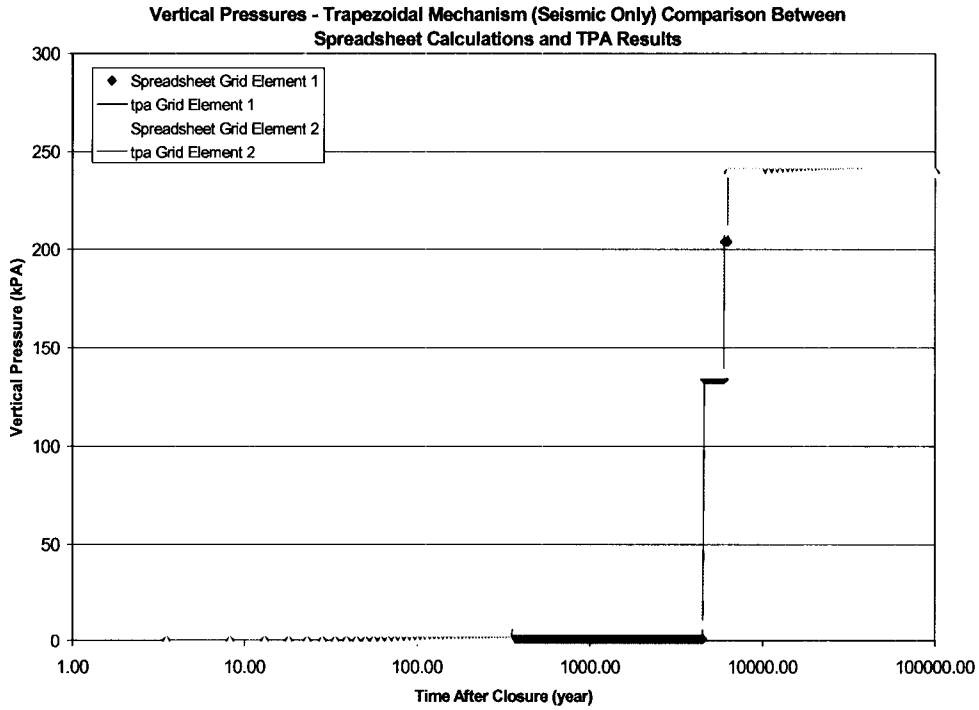
9.2 Criterion 1: Code generated and spreadsheet calculated values agree to within 1%.

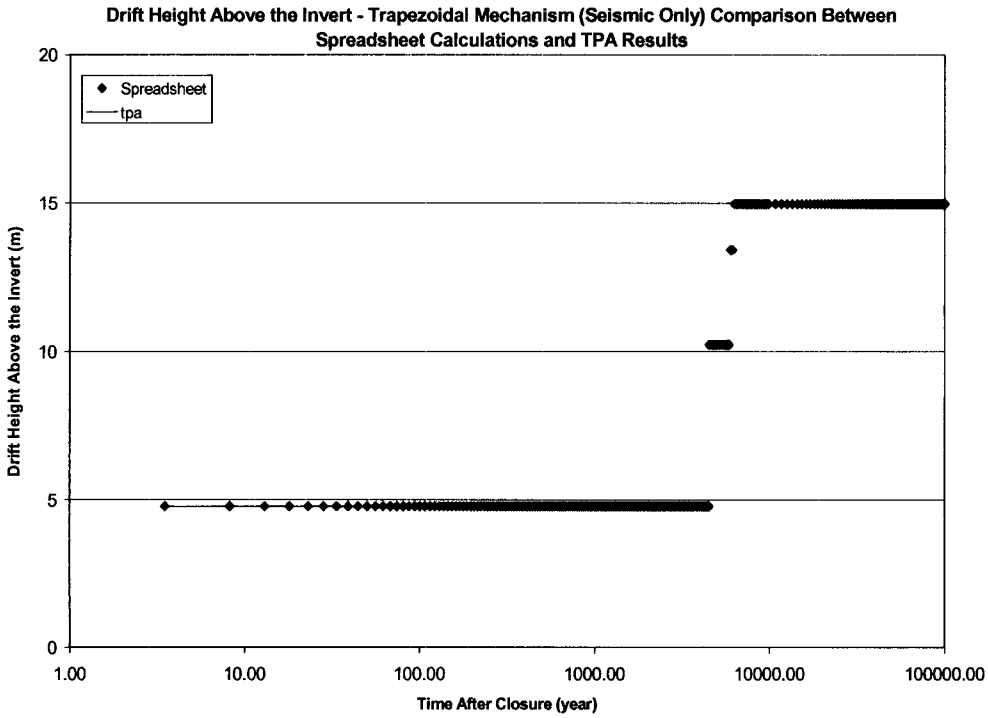
9.3 Overall Test Status:

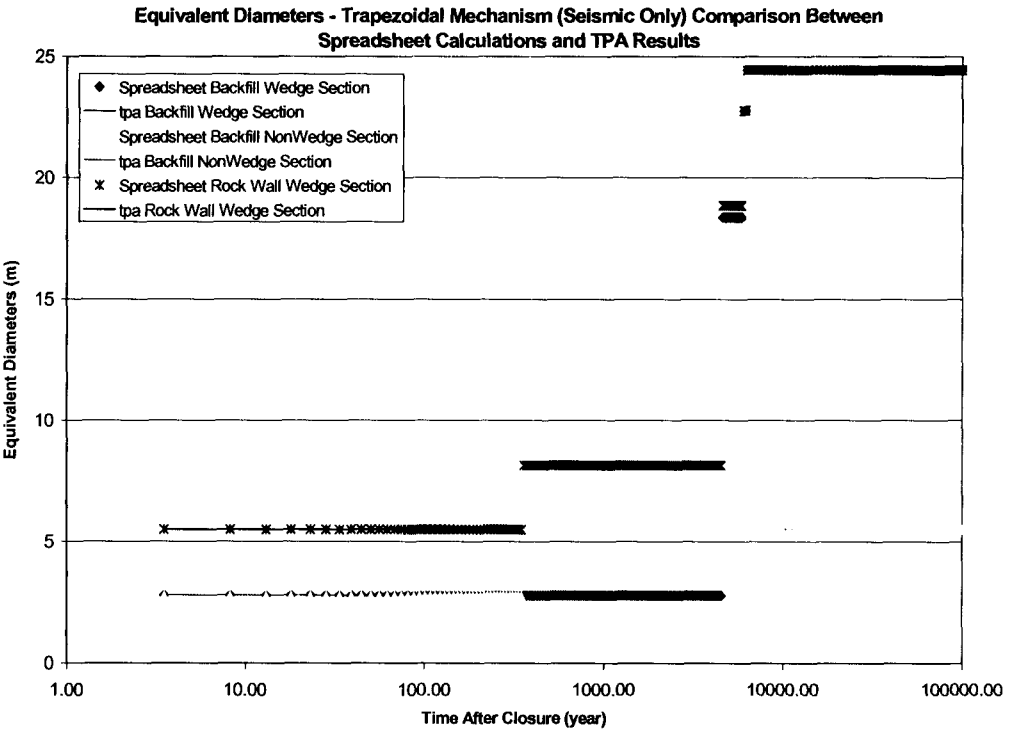
This test **PASSED** the criterion above for test PL-8 for the Windows execution on machine tpa because tpa generated values agreed with spreadsheet calculations to within 1%.

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.






Equivalent Diameters - Trapezoidal 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)
25
20
15
10
5
0
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 15:33:24 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
```

System Level Tests

The system level test is designed to verify the results obtained from multiple realizations for drift degradation times and vertical pressures.

SL-1 Verify Drift Degradation Time

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\sl1

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 Set the values in TPA.INP in accordance with the following table:

Test Case 1 (Degradation Only)

Parameter	**Value**
MaximumTime[yr]	1.0E5
NumberOfRealizations	50
StartAtSubarea	3
StopAtSubarea	3
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
OutputMode(0=None,1=All,2=UserDefined)	1
SelectAppendFiles	4
DegradationTimeRockTypeOneSubarea_3[yr]	lognormal {369.32, 1523.05}
DegradationTimeRockTypeTwoSubarea_3[yr]	lognormal {369.32, 1523.05}

Test Case 2 (Degradation and Seismicity)

Parameter	**Value**
MaximumTime[yr]	1.0E5
NumberOfRealizations	50
StartAtSubarea	3

StopAtSubarea	3
OutputMode(0=None,1=All,2=UserDefined)	1
SelectAppendFiles	4
DegradationTimeRockTypeOneSubarea_3[yr]	lognormal {369.32, 1523.05}
DegradationTimeRockTypeTwoSubarea_3[yr]	lognormal {369.32, 1523.05}

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used

6.1 Input files are modified in accordance with Section 4.0.

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 degradation times generated agree with the input distribution degradation times and that the degradation time shifts to lower values when seismicity is included.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.ech, driftfail.rlt, dsfail.res

8.5 Procedure:

1. At the command prompt from the <<Run Directory>>, type the following: "tpa.exe > sl1_A.out." for Test Case A and "tpa.exe > sl1_B.out" for Test Case B.

2. Plot the drift failure data against the input degradation time distribution.

8.6 Pass/Fail Criteria: For the degradation only case, the times for drift degradation agree with the input distribution times.

9.0 Test Results

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

9.2 Criterion 1: The drift degradation times agree with the input distribution times.

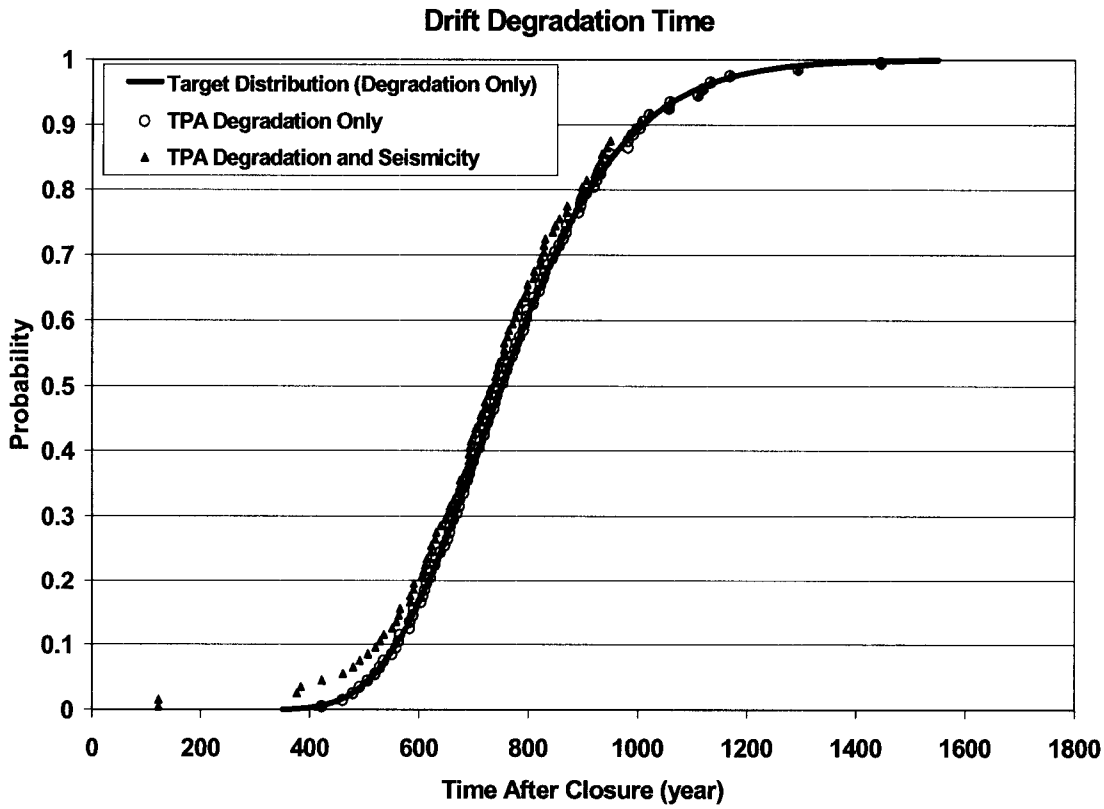
9.3 Criterion 2: The drift degradation distribution shifts to lower values when seismicity is included.

9.4 Overall Test Status:

This test **PASSED** the criterion above for test SL-1 for the Windows execution on machine tpa because tpa generated degradation times follow the input distribution and when seismicity is included, the distribution shifts to lower values.

This test **PASSED** the criterion above for test SL-1 for the UNIX execution because the output files were checked by the diff command with the PC generated output files. The output from the UNIX execution differed as shown in the following pages; however, the differences were minor between the files.

Test result from machine tpa showing degradation times fall on the input distribution for the degradation only scenario and the times shift to the left (earlier times) when seismicity is included.



Output files for test SL1-A from machine spock checked against output files from machine tpa.

DRIFTFAIL.ECH (Differences in pga values)

```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 17:53:50 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 16:15:10 2006
862c862
<     6    7.68814E+04    1.82821E-05    9.12784E-01    5.33553E+00    1.00741E-01
---
>     6    7.68814E+04    1.82821E-05    9.12784E-01    5.33552E+00    1.00741E-01
1115c1115
<     7    5.66011E+04    7.16657E-06    1.26822E+00    5.71565E+00    2.09949E-01
---
>     7    5.66011E+04    7.16657E-06    1.26822E+00    5.71564E+00    2.09949E-01
1120c1120
<    12    9.93307E+04    8.95963E-05    4.98626E-01    2.51899E-01    1.96193E-01
---
>    12    9.93307E+04    8.95963E-05    4.98626E-01    2.51900E-01    1.96193E-01
1278c1278
<     9    5.21915E+04    6.88783E-05    5.67151E-01    2.78119E-01    1.98799E-01
---
>     9    5.21915E+04    6.88783E-05    5.67151E-01    2.78120E-01    1.98799E-01
1298,1299c1298,1299
<     5    4.00863E+04    6.38940E-05    5.86724E-01    3.83414E-01    1.95579E-01
<     6    4.64639E+04    4.60096E-05    6.72291E-01    2.70573E+00    1.01949E-01
---
>     5    4.00863E+04    6.38940E-05    5.86724E-01    3.83415E-01    1.95579E-01
>     6    4.64639E+04    4.60096E-05    6.72291E-01    2.70572E+00    1.01949E-01
```

DRIFTFAIL.RLT (Differences in vertical pressures for rock type 1 and rock type failure time)

```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 17:53:50 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 16:15:10 2006
9088c9088
<    3.55820E+02   1.38659E+01   5.50000E+00   1.24118E+01   5.50000E+00   9.97270E+00
1.10062E+02   5.89141E+01
---
>    3.55820E+02   1.38659E+01   5.50000E+00   1.24118E+01   5.50000E+00   9.97270E+00
1.10063E+02   5.89141E+01
17314c17314
< Rock Type Two Failure Time:                1.03312E+03
---
> Rock Type Two Failure Time:                1.03313E+03
```

DSFAIL.RES (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Thu Apr  6 17:53:50 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 16:15:10 2006
```

Output files for test SL1-B from machine spock checked against output files from machine tpa.

DRIFTFAIL.ECH (Differences in pga values)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 07:59:49 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 16:26:33 2006
862c862
<     6    7.68814E+04    1.82821E-05    9.12784E-01    5.33553E+00    1.00741E-01
---
>     6    7.68814E+04    1.82821E-05    9.12784E-01    5.33552E+00    1.00741E-01
1115c1115
<     7    5.66011E+04    7.16657E-06    1.26822E+00    5.71565E+00    2.09949E-01
---
>     7    5.66011E+04    7.16657E-06    1.26822E+00    5.71564E+00    2.09949E-01
1120c1120
<    12    9.93307E+04    8.95963E-05    4.98626E-01    2.51899E-01    1.96193E-01
---
>    12    9.93307E+04    8.95963E-05    4.98626E-01    2.51900E-01    1.96193E-01
1278c1278
<     9    5.21915E+04    6.88783E-05    5.67151E-01    2.78119E-01    1.98799E-01
---
>     9    5.21915E+04    6.88783E-05    5.67151E-01    2.78120E-01    1.98799E-01
1298,1299c1298,1299
<     5    4.00863E+04    6.38940E-05    5.86724E-01    3.83414E-01    1.95579E-01
<     6    4.64639E+04    4.60096E-05    6.72291E-01    2.70573E+00    1.01949E-01
---
>     5    4.00863E+04    6.38940E-05    5.86724E-01    3.83415E-01    1.95579E-01
>     6    4.64639E+04    4.60096E-05    6.72291E-01    2.70572E+00    1.01949E-01
```

DRIFTFAIL.RLT (Differences in vertical pressures for rock type 1 and rock type failure time)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 07:59:49 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 16:26:33 2006
9088c9088
<    3.55820E+02   1.38659E+01   5.50000E+00   1.24118E+01   5.50000E+00   9.97270E+00
1.10062E+02   5.89141E+01
---
>    3.55820E+02   1.38659E+01   5.50000E+00   1.24118E+01   5.50000E+00   9.97270E+00
1.10063E+02   5.89141E+01
17314c17314
< Rock Type Two Failure Time:                1.03312E+03
---
> Rock Type Two Failure Time:                1.03313E+03
```

DSFAIL.RES (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 07:59:49 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 16:26:33 2006
```

SL-2 Verify Vertical Pressures

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\sl2

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 Set the values in TPA.INP in accordance with the following table:

Parameter	**Value**
MaximumTime[yr]	1.0E5
NumberOfRealizations	10
StartAtSubarea	3
StopAtSubarea	3
`SeismicDisruptiveScenarioFlag(yes=1,no=0)`	0
OutputMode(0=None,1=All,2=UserDefined)	1
SelectAppendFiles	4
DriftDegradationMethodSelectionValue	{For chimney: 0.0, 0.5; For Trapezoid: 0.8, 1.0}

4.2 Increase the trapezoid base angle (`TrapezoidBaseAngle`) as follows: Case 1 = 50.7, Case 2 = 75.0 degrees, Case 3 = 87.0 degrees, Case 4 = 90.0 degrees.

5.0 Special Diagnostic Code Modifications Required: None

6.0 Program Modes to be Used

6.1 Input files are modified in accordance with Section 4.0.

7.0 Utility Scripts Needed to Perform the Test

readsp2: Used to read bulking factors for the 10 realizations. Output bulking factors captured to readsp2.out.

8.0 Test Description

8.1 Objective: This test is designed to verify that the vertical pressures generated for the trapezoid drift degradation mechanism approach those of the chimney mechanism as the trapezoid base angle is increased to 90 degrees.

8.2 Assumptions: none

8.3 Constraints: none

8.4 Output Files: driftfail.ech, driftfail.rlt

8.5 Procedure:

1. At the command prompt from the <<Run Directory>>, type the following: "tpa.exe > sl2_base.out," "tpa.exe > sl2_chim.out," "tpa.exe > sl2_case1.out," "tpa.exe > sl2_case2.out," "tpa.exe > sl2_case3.out," and "tpa.exe > sl2_case4.out" for the base case, chimney, and trapezoid cases 1, 2, 3, and 4 respectively.

2. For the test cases, the trapezoid base angle is increased to 90 degrees.

8.6 Pass/Fail Criteria: The vertical pressures for the trapezoid drift degradation mechanism approach those for the chimney mechanism as the trapezoid base angle is increased to 90 degrees.

9.0 Test Results

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

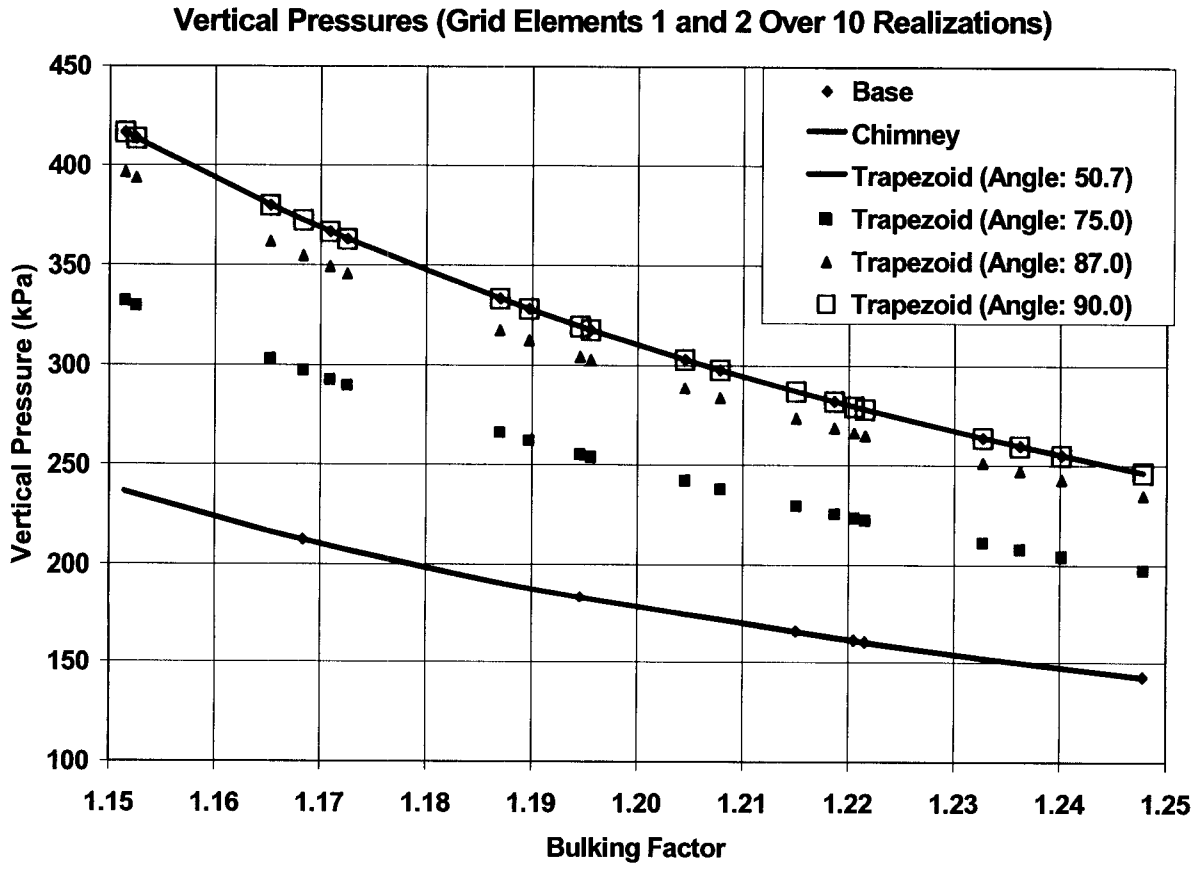
9.3 Criterion 2: The vertical pressures for the trapezoid mechanism approach those of the chimney mechanism as the trapezoid base angle is increased to 90 degrees.

9.3 Overall Test Status:

This test **PASSED** the criterion above for test SL-2 for the Windows execution on machine tpa because tpa generated vertical pressures for the trapezoid mechanism approach those of the chimney mechanism as the trapezoid base angle is increased to 90 degrees.

This test **PASSED** the criterion above for test SL-2 for the UNIX execution because the output files were checked by the diff command with the PC generated output files. The output from the UNIX execution differed as shown in the following pages; however, the differences were minor between the files.

Test results from machine tpa showing the vertical pressures for the trapezoid drift failure mechanism approach those for the chimney mechanism as the trapezoid base angle is increased to 90 degrees.



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

BASE Case:

DRIFTFAIL.ECH (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 09:08:22 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 17:45:28 2006
```

DRIFTFAIL.RLT

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 09:08:22 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 17:45:28 2006
```

Chimney

DRIFTFAIL.ECH (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 09:21:35 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:09:03 2006
```

DRIFTFAIL.RLT (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 09:21:35 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:09:03 2006
```

Trapezoid (Angle = 50.7; Case 1)

DRIFTFAIL.ECH (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 09:37:09 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:35:06 2006
```

DRIFTFAIL.RLT (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 09:37:09 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:35:06 2006
```

Trapezoid (Angle = 75.0; Case 2)

DRIFTFAIL.ECH (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 09:50:30 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:39:35 2006
```

DRIFTFAIL.RLT (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 09:50:30 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:39:35 2006
```

Trapezoid (Angle = 87.0; Case 3)

DRIFTFAIL.ECH (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 10:05:39 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:50:28 2006
```

DRIFTFAIL.RLT (Difference in vertical pressure for rock type 1 and date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 10:05:39 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:50:28 2006
120c120
<    5.01299E+02   1.95079E+01   5.50000E+00   1.93205E+01   5.50000E+00   1.60330E+01
2.56812E+02   1.37768E+02
---
>    5.01299E+02   1.95079E+01   5.50000E+00   1.93205E+01   5.50000E+00   1.60330E+01
2.56813E+02   1.37768E+02
```

Trapezoid (Angle = 90.0; Case 4)

DRIFTFAIL.ECH (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 10:17:28 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:54:51 2006
```

DRIFTFAIL.RLT (Differences in date/time stamp)

```
3c3
<  TPA 5.0.2q, Job started: Fri Apr  7 10:17:28 2006
---
>  TPA 5.0.2q, Job started: Tue Apr 04 18:54:51 2006
```

SOFTWARE CHANGE REPORT (SCR)

1. SCR No. (*Software Developer Assigns*): SCR 611	2. Software Title and Version: TPA 5.1h	3. Project No: 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *ebsrel.f, releaset.f, exec.f, tpa.inp, tpanames.dbs, calc_Concentrations.h, calc_EffectiveSolLimit.h, ebsre-cld.i, set_Colloid.h*

The current abstraction accounts for the release of irreversibly attached colloids by raising the solubility limit by a factor that is a function of a constant colloid release factor. This assures that the dissolved radionuclides are released at solubility limit. However, this abstraction could result in an overestimation of irreversible colloid release.

5. Change Requested by:	6. Change Authorized by (*Software Developer*):
O. Osidele, S. Painter Date: 11-4-2005	R. Janetzke Date:11-4-05

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

See Attachment A for a more detailed discussion of the modified colloid model, and Attachment B for the description of the changes made to the code.

8. Implemented by:	Date:
C. Scherer	2/24/06

9. Description of Acceptance Tests:

See Attachment C for PC Acceptance Testing and Attachment D for UNIX Acceptance Testing. Three process-level tests were conducted, one for each of the three new subroutines described in Attachment B.

10. Tested by: O. Osidele	Date: 3/10/06

CNWRA Form TOP-5 (05/2000)

UPDATE REQUIREMENTS for TPA.INP

SCR 611

Status (*ADD, DELETE, MODIFY TO, MODIFY FROM*)	**Module**	**Parameter Name**	**Description** (*Definition of parameter in terms of its function in TPA code; calculated from . . ., used for calculating . . ., used to relate . . ., etc.*)	**Distribution**	**Range**	**Justification** *1. Site references (journals, scientific notebooks, publications). 2. Indicate level of uncertainty covered by the distribution / range. 3. Explain why you chose this range / distribution vs. other possible values / methods / distributions.*	**Source**
DELETE	EBSFILT	ColloidReleaseFactor_Jc246[]					Scott Painter
DELETE	EBSFILT	ColloidReleaseFactor_Jt230[]					Scott Painter
DELETE	EBSFILT	ColloidReleaseFactor_Jp239[]					Scott Painter

DELETE	EBSFILT	ColloidReleaseFactor_Ja243[]					Scott Painter
DELETE	EBSFILT	ColloidReleaseFactor_Jc245[]					Scott Painter
DELETE	EBSFILT	ColloidReleaseFactor_Ja241[]					Scott Painter
DELETE	EBSFILT	ColloidReleaseFactor_Jp240[]					Scott Painter
DELETE	EBSFILT	ColloidReleaseFactor_Jt229[]					Scott Painter
ADD	EBSREL	SorptionCapacity[moles/m3]		usersuppliedpwisecdf	14 3.9312e-6, 0.0 1.1665e-4, 0.05 2.2018e-4, 0.1 4.6261e-4, 0.2 8.1722e-4, 0.3 1.4278e-3, 0.4 2.5857e-3, 0.5 4.6258e-3, 0.6 8.5846e-3, 0.7 1.6488e-2, 0.8 3.4794e-2, 0.9 5.3952e-2, 0.95 9.38e-2, 0.99 1.44244e-1, 1.0		Scott Painter

ADD	EBSREL	AffinityFactorAm		uniform	5.0, 15.0		Scott Painter
ADD	EBSREL	AffinityFactorCm		uniform	5.0, 15.0		Scott Painter
ADD	EBSREL	AffinityFactorTh		uniform	5.0, 15.0		Scott Painter
ADD	EBSREL	AffinityFactor_U		loguniform	0.005, 0.05		Scott Painter

ATTACHMENT A

Proposed Refinement for Irreversible Colloids Abstraction in TPA

Scott Painter
8/16/2005 (rev. 11/8/2005)

Overview of the abstraction:

Consider iron-oxide type corrosion products as dominant in waste package. Focus on release abstraction – transport model remains unchanged.

Physical picture is fast irreversible sorption with competition until all sorption sites on colloids are filled.

Pu, Am, Th, and Cm compete for available sorption sites on colloids. U also competes. Evaluate later whether U needs to be tracked as a colloidal species.

Assign radionuclide mass to colloids until *finite sorption capacity* is reached.

Remainder of radionuclide mass is dissolved (limited by solubility or dissolution rate).

Abstraction is conservative. Additional competition with stationary corrosion products may reduce releases, but this will require more detailed model and technical basis is more difficult to develop.

Dataflow:

(1) Before calling RELEASET, sample sorption capacity (colloid concentration * specific surface area * number sites per unit area). This is a new parameter S_X. Convert S_X from moles/m^3 to kg/m^3 by multiplying S_X by 240/1000, where 240 is a rough average atomic weight and 1000 is number of grams in 1 kg.

(2) For each of the five elements, sample *relative affinity* γ for corrosion product colloid. A Kd for sorption on hematite is adequate here. [γ_{Pu} = 1.0d0]

(3) Sample solubility limit C_S for each radioelement.

(4) Calculate an *effective solubility limit* (kg/m^3) by assuming that Pu, Am, U are solubility limited and that sorption is described by a competitive Langmuir-like sorption model. Effective solubility limit is then

$$C_{seff,\,Pu} = C_{S,Pu} + S_X \frac{\gamma_{Pu}\, C_{S,Pu}}{\gamma_{Pu}\, C_{S,Pu} + \gamma_{Am}\, C_{S,Am} + \gamma_U\, C_{S,U}}$$ and similar for Am and U.

Solubility for Th and Cm are unchanged.

(5) Call RELEASET with the effective solubility limits.

(6) Convert release rate to concentration:

$$C_j[kg/m^3] = 2.795e\text{-}9 * \frac{Release[ci/yr] * t_{1/2}[yr]}{Q_{out}[m^3/yr]} * A[AMU]$$

where Release is the total release rate, A is atomic weight [g/mol], Q_{out} is the total flow rate for all waste packages [$Q_{out} = Q_{in}$ (for bathtub model , Q_{in} after bathtub filles, 0 before)] and $t_{1/2}$ is the halflife; the constant 2.795e-9 is a unit conversion factor for converting from curies to moles and is calculated by (3.7e10 [Bq/Ci]) * (365 * 24 * 3600 [sec/yr]) / ((6.022e23 [particles/mole] * (1000 g/kg) * Ln(2)), where Ln(2) is there to convert from decay constant to half-life

(7) Using concentrations C_j as calculated above in (6), set the "J" species concentrations:

$$C_{JPu} = S_X * \frac{\gamma_{Pu} Min(C_{Pu}, C_{S,Pu})}{\sum \gamma_j Min(C_j, C_{S,j})}$$ where sum is over Pu, Am, Th, Cm, and U.

(8) $C_{JPu} = Min(C_{Pu}, C_{JPu})$

(9) Dissolved concentration in water leaving waste package is the C_{Pu} - C_{JPu}.

(10) Convert from concentration back to release rate before written to output files.

Notes:

Final dissolved concentrations may be slightly above true solubility limit, but this is relatively unimportant.

At later times, when releases from waste package are limited by dissolution rate, colloids may take all released Pu. This is consistent with Los Alamos sorption experiments that show strong uptake and little desorption of Pu and Am and is not important for performance.

Required TPA modifications are minor.

Work needed on two parameter distributions, but we have distributions for other parameters. Need to look at possible correlations in Kd values.

ATTACHMENT B

Description of Change(s) or Problem Resolution

Several new parameters were added to *tpa.inp* (see table above) and colloid release factors were eliminated. The subroutine get_colloidreleasefactor is no longer needed and was commented out. Three new subroutines were created to do the following:

- calc_EffectiveSolLimit - calculates effective solubility limit for Am, Pu and U
- calc_Concentrations - reads ebsnef.dat file and calculates values based on summing affinity factor and solubility products across nuclides per time step to be used in calculating colloid portion of release
- set_Colloid - converts release for current nuclide to concentration; calculates colloid portion for current nuclide, if any; reduces amount of aqueous release accordingly; converts concentrations back to release

A new include file, *ebsrel-cld.i* was created. It contains the common block colloidvalues and other parameters used in the new calculations.

In addition, the following changes were made to the files *ebsrel.f* and *releaset.f*.

ebsrel.f (diff modified *ebsrel.f* and **TPA** 5.0.2h *ebsrel.f*)

```
3c3
< c File Date:           07/15/05
---
> c File Date:           02/11/06
1393,1394d1392
<
<       close( unit=iebsrelinp)
1395a1394,1395
>       close( unit=iebsrelinp )
>
1414c1414
<
---
>
1571d1570
< c css 12-19-05; SCR611:  limited sorption capacity for colloids
1575,1581c1574,1576
< cc            call get_colloidreleasefactor(names(ii),
< cc     &                    colrelfac)
< cc            sol = (1 + (colrelfac / (1-colrelfac))) * sol
<             if (icldmod .eq. 1)  then
<                call calc_EffectiveSolLimit(ir, names(ii), sol, effsol)
<                sol = effsol
<             endif
---
```

```
>             call get_colloidreleasefactor(names(ii),
>      &                  colrelfac)
>             sol = (1 + (colrelfac / (1-colrelfac))) * sol
1583d1577
< c end change:  SCR611
1696,1697c1690,1691
< cc rwj 2-11-06; scr602; temporary values pending new seepage code.
<      &      ,sawetnew(it),1.d0, 1.d0,1.d0
---
> cc rwj 2-11-06; scr602 ; temporary values pending new seepage code.
>      &      ,sawetnew(it),1.d0,1.d0,1.d0
2053,2058d2046
< c css 12/30/05; SCR611:  calculate colloid concentrations (new model)
< c    write new columns in ebsnef.dat - contains qout & concentration
<       double precision qout1
<       double precision qout2
< c end change:  SCR611
<
2095,2096d2082
< c css 12/30/05; SCR611:  calculate colloid concentrations (new model)
< c    write new columns in ebsnef.dat - contains qout
2098,2109c2084,2087
<           read (iebssfdat,   *,err=901) ajtim1, ajval1,
<      &                                  i_affected_flag1, qout1
<           read (iebsglassdat,*,err=902) ajtim2, ajval2,
<      &                                  i_affected_flag2, qout2
<           write (iebsnefdat,  '(1x, 1pe12.4, 1x, 1pe12.4, 1x, i4,
<      &                           1pe12.4)')
<      &          ajtim2, ajval1 + ajval2, i_affected_flag1,
<      &          qout1 + qout2
< c          read (iebssfdat,   *,err=901) ajtim1, ajval1, i_affected_flag1
< c          read (iebsglassdat,*,err=902) ajtim2, ajval2, i_affected_flag2
< c          write (iebsnefdat,  '(1x, 1pe12.4, 1x, 1pe12.4, 1x, i4)')
< c     &          ajtim2, ajval1 + ajval2, i_affected_flag1
---
>           read (iebssfdat,   *,err=901) ajtim1, ajval1, i_affected_flag1
>           read (iebsglassdat,*,err=902) ajtim2, ajval2, i_affected_flag2
>           write (iebsnefdat,  '(1x, 1pe12.4, 1x, 1pe12.4, 1x, i4)')
>      &          ajtim2, ajval1 + ajval2, i_affected_flag1
2111d2088
< c end change:  SCR611
2154,2155c2131,2133
< c                 mass is depleted earlier. Aqueous concentrations do not
< c                 exceed the intended solubility limit.  After a portion
---
> c                 mass is depleted earlier, but no reduction in release of
> c                 aqueous nuclides is necessary, and aqueous concentrations
> c                 do not exceed the intended solubility limit.  After a
portion
2190,2192d2167
< c css 12-30-2005; SCR611:  add new model for colloid sorption capacity
<       INCLUDE 'ebsrel-cld.i'
< c end change:  SCR611
2205,2209d2179
< c
< c css 12-30-2005; SCR611:  add new model for colloid sorption capacity
< c ColloidReleaseFactor parameters not used for new model
< cc      dimension cldfac(maxclnuc)
```

```
< cc      dimension icldfac(maxclnuc)
2211,2213c2181,2182
<       double precision qout
<       double precision conc
< cc end change:  SCR611
---
>       dimension cldfac(maxclnuc)
>       dimension icldfac(maxclnuc)
2233,2238c2202,2207
< cc           if (cldnames(i)(1:1) .eq. 'J') then
< cc             name = 'ColloidReleaseFactor_'//cldnames(i)(1:len)//'[]'
< cc             icldfac(i) = ispquery( name )
< cc           else
< cc             icldfac(i) = 0
< cc           end if
---
>           if (cldnames(i)(1:1) .eq. 'J') then
>             name = 'ColloidReleaseFactor_'//cldnames(i)(1:len)//'[]'
>             icldfac(i) = ispquery( name )
>           else
>             icldfac(i) = 0
>           end if
2252,2263c2221,2229
< c css 12/30/2005; SCR611 - new colloid sorption calculations
< c   ColloidReleaseFactor parameters not used in new model
< ccc   Get sampled colloid release factor.
< cc      do i = 1, numclnuc
< ccc   Set factors for solute nuclides in colloid chains to 0.
< cc          if (cldnames(i)(1:1) .eq. 'J') then
< cc            cldfac(i) = valuesp(icldfac(i))
< cc          else
< cc            cldfac(i) = 0.0d0
< cc          end if
< cc      end do
< c end change:  SCR611
---
> c   Get sampled colloid release factor.
>       do i = 1, numclnuc
> c   Set factors for solute nuclides in colloid chains to 0.
>           if (cldnames(i)(1:1) .eq. 'J') then
>             cldfac(i) = valuesp(icldfac(i))
>           else
>             cldfac(i) = 0.0d0
>           end if
>       end do
2265,2269d2230
< c css 12/30/2005; SCR611 - new colloid sorption calculations
< cc call new routine w/ isotope loop to sum info to use below
<         call calc_Concentrations(iebsnefdat)
< c end change:  SCR611
<
2306,2308c2267
< c css 12-30-2005; SCR611:  don't need ColloidReleaseFactor anymore
< cc              colloidfactor = cldfac(j)
< c end change:  SCR611
---
>               colloidfactor = cldfac(j)
2316,2320c2275
```

```
< c css 12-19-2005; SCR611 - calculate colloid concentrations (new model)
< c    new column in ebsnef.dat contains qout
< c             read(iebsnefdat,*,err=9078) ajtim, ajval, i_affected_flag
<              read(iebsnefdat,*,err=9078) ajtim, ajval, i_affected_flag,
<      &                                   qout
---
>              read(iebsnefdat,*,err=9078) ajtim, ajval, i_affected_flag
2322,2325c2277,2278
< c             write(iebsnefout,'(1p2e13.4,i4)',err=9078) ajtim, ajval,
< c     &             i_affected_flag
<              write(iebsnefout,'(1p2e13.4,i4,1x,e13.4)',err=9078)
<      &            ajtim, ajval, i_affected_flag, qout, ajconc(is,it)
---
>              write(iebsnefout,'(1p2e13.4,i4)',err=9078) ajtim, ajval,
>      &             i_affected_flag
2330,2334c2283
< c css 12-19-2005; SCR611 - calculate colloid concentrations (new model)
< c                & convert to release rate; decrease aqueous value
< c             read(iebsnefdat,*,err=9078) ajtim, ajval, i_affected_flag
<              read(iebsnefdat,*,err=9078) ajtim, ajval, i_affected_flag,
<      &                                   qout
---
>              read(iebsnefdat,*,err=9078) ajtim, ajval, i_affected_flag
2336,2341c2285,2288
< cc              cldval= ajval* colloidfactor
<              call set_Colloid(nameisoebspac, ljustify, qout, is,
<      &                        it, ajval, cldval, conc)
< ccc css 07-06-2005; SCR567 - reduce aqueous value by amount assigned to
< ccc             colloidal value
< cc              ajval = ajval * (1 - colloidfactor)
---
>              cldval= ajval* colloidfactor
> c css 07-06-2005; SCR567 - reduce aqueous value by amount assigned to
> c             colloidal value
>              ajval = ajval * (1 - colloidfactor)
2343,2352c2290,2293
< c    write new columns in ebsnef.dat contains qout & colloid concentration
<              write(iebsnefout,'(1p2e13.4,i4,1p2e13.4)',err=9078) ajtim,
<      &          ajval, i_affected_flag, qout, ajconc(is,it)
<              write(iebsnefcld,'(1p2e13.4,i4,1p2e13.4)',err=9078) ajtim,
<      &          cldval, i_affected_flag, qout, conc
< c             write(iebsnefout,'(1p2e13.4,i4)',err=9078) ajtim,
< c     &                            ajval, i_affected_flag
< c             write(iebsnefcld,'(1p2e13.4,i4)',err=9078) ajtim,
< c     &                            cldval, i_affected_flag
< c end change:  SCR611
---
>              write(iebsnefout,'(1p2e13.4,i4)',err=9078) ajtim,
>      &                           ajval, i_affected_flag
>              write(iebsnefcld,'(1p2e13.4,i4)',err=9078) ajtim,
>      &                           cldval, i_affected_flag
2388,2397c2329,2331
< c css 12/30/05; SCR611:  calculate colloid concentrations (new model)
< c    write new columns in ebsnef.dat contains qout & colloid concentration
<           read(iebsnefout,*,err=9078) ajtim, ajval, i_affected_flag,
<      &                                qout, conc
<           write(iebsnefdat,'(1p2e13.4,i4,1p2e13.4)',err=9078)
<      &       ajtim, ajval, i_affected_flag, qout, conc
```

```
< c          read(iebsnefout,*,err=9078) ajtim, ajval, i_affected_flag
< c          write(iebsnefdat,'(1p2e13.4,i4)',err=9078) ajtim, ajval,
< c     &                                 i_affected_flag
< c end change:  SCR611
---
>           read(iebsnefout,*,err=9078) ajtim, ajval, i_affected_flag
>           write(iebsnefdat,'(1p2e13.4,i4)',err=9078) ajtim, ajval,
>      &                                 i_affected_flag
2402,2403d2335
< c css 12/30/05; SCR611:  calculate colloid concentrations (new model)
< c    write new columns in ebsnef.dat contains qout & colloid concentration
2408,2414c2340,2342
<           read(iebsnefcld,*,err=9078) ajtim, ajval, i_affected_flag,
<      &                                qout, conc
<           write(iebsnefdat,'(1p2e13.4,i4,1p2e13.4)',err=9078)
<      &        ajtim, ajval, i_affected_flag, qout, conc
< cc          read(iebsnefcld,*,err=9078) ajtim, ajval, i_affected_flag
< cc          write(iebsnefdat,'(1p2e13.4,i4)',err=9078) ajtim, ajval,
< cc     &                 i_affected_flag
---
>           read(iebsnefcld,*,err=9078) ajtim, ajval, i_affected_flag
>           write(iebsnefdat,'(1p2e13.4,i4)',err=9078) ajtim, ajval,
>      &                 i_affected_flag
2417d2344
< c end change:  SCR611
```

releaset.f (diff modified *releaset.f* and **TPA** 5.0.2h *releaset.f*)

```
309,315d308
< c
< c css 1/31/06 - SCR611; save total flowrate_out (qout) for each WP
< c                       failure type per time step
<         real*8  totqoutbyWPfailtype(9, maxntime)
<         integer j, lc
< c end change; SCR611
<
866,870d858
< c css 1/31/06 - SCR611; initialize totqoutbyWPfailtype array
<           do lc=1,9
<              totqoutbyWPfailtype(lc,k) = 0.0
<           end do
< c end change:  SCR611
940,953d927
< c
< c css 1/31/06 - SCR611; qout (flowrate_out) needed for colloid
< c                       computations in ebsrel
< c       save flowrate_out per WP failure type;
< c       multiply by number of waste packages of current failure type
< c       since releaset works on only one representative waste package;
< c       sum total qout per time step across all WP failure types
< c
<           do j=1,ntemp
<              totqoutbyWPfailtype(itype,j) = flowrate_out(j) * numwp
<              totqoutbyWPfailtype(9,j) = totqoutbyWPfailtype(9,j) +
<      &                                  totqoutbyWPfailtype(itype,j)
<           end do
< c end change; SCR611
```

```
1178d1151
< c css 12-30-2005; SCR611 write qout=flowrate_out to ebsnef.dat
1180,1184c1153
<      &          affected_nuclide(k, i, itim),
<      &          totqoutbyWPfailtype(9,itim)
< c end change:  SCR611
< cc              write (20, 9003) tregular(itim), fracre(k, i, itim),
< cc     &          affected_nuclide(k, i, itim)
---
>      &          affected_nuclide(k, i, itim)
1300,1304c1269,1270
< c
< c css 12-30-2005; SCR611:  write out flowrate_out = qout to ebsnef.dat
<  9003   format (2(1x, 1pe12.4), I4, 1x, e12.4)
< cc  9003   format (2(1x, 1pe12.4), I4)
< c end change:  SCR611
---
>
>  9003   format (2(1x, 1pe12.4), I4)
```

ATTACHMENT C

PC Acceptance Testing

Test Plan for TPA SCR 611

Test Plan Name: PC Testing of Release of Irreversibly Attached Colloids

Tested By: O. Osidele **Date:** March 10, 2006

Host Machine: TPA **Host OS:** XP Professional

Baseline Version: 5.1h **Test Version:** 5.0.2j

Process Level (PL) Tests

PL-1. Name: Effective Solubility Limits for Am, Pu, and U

Path for run directory: d:\oosidele\run_tpa502j

Path for archive of results: \scr611_test\PC\run_tpa502j
(archived on CD named "Test Plan for SCR 611")

Environment variables: TPA_TEST=d:\oosidele\tpa502j
TPA_DATA=d:\oosidele\tpa502j

Special input files or modifications to input files required: *tpa.inp*
(run one realization for Subarea 2 only)

Special diagnostic code modifications required : Print statements added to *ebsrel.f* to display the solubility for each radionuclide before (`sol`) and after (`effsol`) executing the `calc_EffectiveSolLimit` subroutine.

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

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

Test description: Calculation of effective solubility limits for Am, Pu, and U is examined.

- Objective: Verify by spreadsheet calculation the values calculated by the test code.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** Screen print (*tpa.out)*

- **Step by step test procedure to be used:**
  1. Execute the test code with the specified modifications using the basecase *tpa.inp* file (for Subarea 2 only) and capture the screenprint in the *tpa.out* file.
  2. Extract the sampled values for sorption capacity and relative affinity. Calculate the equation for effective solubility limit (given in Section 4 of Attachment A) in a spreadsheet.
  3. Compare the spreadsheet calculation with the screenprint.

- **Pass/Fail criteria:**
  The screenprint should give the same value of effective solubility limit for each radionuclide as the spreasheet calculations.

Test Results:

Files on the CD in the *\scr611_test\PC\run_tpa502j* subdirectory contain results for this test run. Spreadsheet calculations are in *\scr611_test\scr611_calcs.xls*. Cells E10...O10 give the calculated effective solubility limits, summarized as follows:

	Rel. Affinity	Solubility Limit	affinity*solubility limit	Eff. Solubility Limit
CM246	5.1030	1.556E-04		1.556E-04
U238	0.0074	7.109E-03	5.236E-05	7.191E-03
CM245	5.1030	1.556E-04		1.556E-04
AM241	9.9035	1.026E-04	1.016E-03	1.705E-03
U233	0.0074	7.109E-03	5.236E-05	7.191E-03
TH229	9.6726	1.065E-05		1.065E-05
AM243	9.9035	1.026E-04	1.016E-03	1.705E-03
PU239	1.0000	2.283E-04	2.283E-04	5.882E-04
PU240	1.0000	2.283E-04	2.283E-04	5.882E-04
U234	0.0074	7.109E-03	5.236E-05	7.191E-03
TH230	9.6726	1.065E-05		1.065E-05

The relevant parts of the screenprint (*tpa.out*) are as follows:

```
exec: calling ebsrel
Cm246
 sol = 1.555636000000000E-04
 effsol = 1.555636000000000E-04
U238
 sol = 7.108610000000000E-03
 effsol = 7.191152445173715E-03
Am241
```

```
 sol = 1.026389000000000E-04
 effsol = 1.705094393640583E-03
Th229
 sol = 1.064574000000000E-05
 effsol = 1.064574000000000E-05
Pu239
 sol = 2.282897000000000E-04
 effsol = 5.881800811857019E-04
```

The calculated value for each unique radionuclide is the same as the screenprint from the code run.

Test status: PASS

PL-2. Name: Release Concentrations and Affinity-weighted Concentrations

Path for run directory: d:\oosidele\run_tpa502j

Path for archive of results: \scr611_test\PC\run_tpa502j
(archived on CD named "Test Plan for SCR 611")

Environment variables: TPA_TEST=d:\oosidele\tpa502j
TPA_DATA=d:\oosidele\tpa502j

Special input files or modifications to input files required: *tpa.inp*
(run one realization for Subarea 2 only)

Special diagnostic code modifications required : Statements added to *ebsrel.f* to save a copy of *ebsnef.dat* to *ebsnef_int.dat* immediately after running the *releaset* standalone code .

Print statements 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`). Only the results for the last timestep are displayed.

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

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

Test description: Calculation of release concentrations and affinity-weighted concentrations for Pu, Am, Th, Cm and U is examined.

- **Objective:** Verify by spreadsheet calculation the values calculated by the test code.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** Screen print (*tpa.out*)

- **Step by step test procedure to be used:**

1. Execute the test code with the specified modifications using the basecase *tpa.inp* file (for Subarea 2 only) and capture the screenprint in the *tpa.out* file.

2. Extract the values for radionuclide half-life and atomic weight from *nuclides.dat*. Extract values for flow and release from *ebsnef_int.dat* into a spreadsheet. Convert release to concentration using the equation in Section 6 of Attachment A.
3. Calculate the total affinity-weighted concentration using the denominator of the equation in Section 7 of Attachment A.
4. Compare the spreadsheet calculations in steps 3 and 4 with the screenprint.

- Pass/Fail criteria:

The screenprint should give the same value of concentration and total affinity-weighted concentration.

Test Results:

Files on the CD in the *\scr611_test\PC\run_tpa502j* subdirectory contain results for this test run. Spreadsheet calculations are in *\scr611_test\scr611_calcs.xls*. Cells Q19...AA218 give the calculated concentrations and cells AC19...AM218 give the calculated affinity-weighted concentrations. Cells AN19...AN218 give the total affinity-weighted concentrations for Pu, Am, Th, Cm and U for all timesteps. For the last timestep, the calculated concentrations, affinity-weighted concentrations, and cumulative affinity-weighted concentrations are summarized as follows:

	Concentration	Affinity-weighted concentration	Cumulative Affinity-weighted concentration
CM246	1.17E-08	5.96E-08	5.96E-08
U238	2.20E-01	5.24E-05	5.24E-05
CM245	1.16E-07	5.93E-07	5.30E-05
AM241	6.13E-09	6.07E-08	5.31E-05
U233	1.20E-05	8.83E-08	5.32E-05
TH229	3.86E-06	3.73E-05	9.05E-05
AM243	4.74E-06	4.69E-05	1.37E-04
PU239	3.72E-04	2.28E-04	3.66E-04
PU240	7.00E-05	7.00E-05	4.36E-04
U234	3.01E-05	2.22E-07	4.36E-04
TH230	3.59E-06	3.47E-05	4.71E-04

The screenprint (*tpa.out*) displays the concentration and cumulative affinity-weighted concentrations. The relevant parts are as follows:

```
CM246
concentration = 1.167197557161357E-08
totalAffCon = 5.956190459033489E-08
U238
concentration = 0.2195759830458385
totalAffCon = 5.241881080669033E-05
CM245
concentration = 1.161809405095729E-07
totalAffCon = 5.301168028721564E-05
```

```
AM241
concentration = 6.133768894329145E-09
totalAffCon = 5.307242625760746E-05
U233
concentration = 1.198451258547017E-05
totalAffCon = 5.316069950335213E-05
TH229
concentration = 3.861260712433000E-06
totalAffCon = 9.050897928126378E-05
AM243
concentration = 4.737919538321684E-06
totalAffCon = 1.374311123045383E-04
PU239
concentration = 3.717536248799794E-04
totalAffCon = 3.657208123045382E-04
PU240
concentration = 7.000500181278676E-05
totalAffCon = 4.357258141173250E-04
U234
concentration = 3.014715401830967E-05
totalAffCon = 4.359478662964338E-04
TH230
concentration = 3.591740032159856E-06
totalAffCon = 4.706891908536420E-04
```

The sum of affinity-weighted concentrations (`totalAffCon`) displays a cumulative sum over the radioclunides Pu, Am, Th, Cm and U. The final value corresponds with the calculated value (in Cell AN218) of `4.71E-04`.

The calculated values are the same as the screenprint from the code run.

Test status: PASS

PL-3. Name: Colloid (J-species) Concentrations

Path for run directory: d:\oosidele\run_tpa502j

Path for archive of results: \scr611_test\PC\run_tpa502j
(archived on CD named "Test Plan for SCR 611")

Environment variables: TPA_TEST=d:\oosidele\tpa502j
TPA_DATA=d:\oosidele\tpa502j

Special input files or modifications to input files required: *tpa.inp*
(run one realization for Subarea 2 only)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

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

Test description: Calculation of the colloid (J-species) concentrations is examined.

- **Objective:** Verify by spreadsheet calculation the values calculated by the test code.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** *ebsnef.dat*

- **Step by step test procedure to be used:**
  1. Execute the test code using the basecase *tpa.inp* file (for Subarea 2 only).
  2. Calculate colloid concentration for the J-species in a spreadsheet using the equations in Sections 7 and 8 of Attachment A.
  3. Calculate dissolved concentration for the J-species in a spreadsheet using the equation in Section 9 of Attachment A.
  4. Convert colloid and dissolved concentrations back to release in a spreadsheet using the equation in Section 10 of Attachment A.
  5. Compare the spreadsheet calculations in steps 2–4 with the concentrations and releases written to *ebsnef.dat.*

- **Pass/Fail criteria:**
  The concentrations and releases calculated for the J-species should be the same as those written by the code to *ebsnef.dat.*

Test Results:

Files on the CD in the *\scr611_test\PC\run_tpa502j* subdirectory contain results for this test run. Spreadsheet calculations are in *\scr611_test\scr611_calcs.xls*. Cells AP19...AZ218 and BB19...BL218 give the calculated colloid concentrations from Step 2. Cells BN19...BX218 give the calculated dissolved concentrations from Step 3. Cells BZ19...CJ218 give the calculated colloid release (Curies) from Step 4. Cells CL19...CV218 give the calculated dissolved release (Curies) from Step 4. The calculated concentrations and releases for the last timestep are summarized as follows:

Colloid Concentration (kg/m3) – J-Species

CM246	1.17E-08
CM245	1.16E-07
AM241	6.13E-09
AM243	4.74E-06
PU239	3.72E-04
PU240	7.00E-05
TH230	3.59E-06

Dissolved Concentration (kg/m3)

CM246	0.00E+00
CM245	0.00E+00
AM241	0.00E+00
AM243	0.00E+00
PU239	0.00E+00
PU240	0.00E+00
TH230	0.00E+00

Colloid Release (Ci/yr) – J-Species

CM246	8.37E-06
CM245	4.66E-05
AM241	4.91E-05
AM243	2.20E-03
PU239	5.39E-02
PU240	3.72E-02
TH230	1.69E-04

Dissolved Release (Ci/yr)

CM246	0.00E+00
CM245	0.00E+00
AM241	0.00E+00
AM243	0.00E+00
PU239	0.00E+00
PU240	0.00E+00
TH230	0.00E+00

These values are the same as the corresponding values in the output file *ebsnef.dat*.

Test status: PASS

ATTACHMENT D

Unix Acceptance Testing

Test Plan for TPA SCR 611

Test Plan Name: Unix Testing of Release of Irreversibly Attached Colloids

Tested By: O. Osidele

Date: March 10, 2006

Host Machine: SPOCK

Host OS: Version 5.9
(sun4u sparc SUNW, Ultra-4)

Baseline Version: 5.1h

Test Version: 5.0.2j

Process Level (PL) Tests

PL-1. Name: Effective Solubility Limits for Am, Pu, and U

Path for run directory: /home/oosidele/runSCR611tpa502j

Path for archive of results: \scr611_test\Unix\runSCR611tpa502j
(archived on CD named "Test Plan for SCR 611")

Environment variables: TPA_TEST=/home/oosidele/tpa502j
TPA_DATA=/home/oosidele/tpa502j

Special input files or modifications to input files required: *tpa.inp*
(run one realization for Subarea 2 only)

Special diagnostic code modifications required : Print statements added to *ebsrel.f* to display the solubility for each radionuclide before (`sol`) and after (`effsol`) executing the `calc_EffectiveSolLimit` subroutine.

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

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

Test description: Calculation of effective solubility limits for Am, Pu, and U is examined.

- **Objective:** Verify by spreadsheet calculation the values calculated by the test code.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** Screen print (*tpa.out*)

- **Step by step test procedure to be used:**
  1. Execute the test code with the specified modifications using the basecase *tpa.inp* file (for Subarea 2 only) and capture the screenprint in the *tpa.out* file.
  2. Extract the sampled values for sorption capacity and relative affinity. Calculate the equation for effective solubility limit (given in Section 4 of Attachment A) in a spreadsheet.
  3. Compare the spreadsheet calculation with the screenprint.

- **Pass/Fail criteria:**
  The screenprint should give the same value of effective solubility limit for each radionuclide as the spreasheet calculations.

Test Results:

Files on the CD in the *\scr611_test\PC\run_tpa502j* subdirectory contain results for this test run. Spreadsheet calculations are in *\scr611_test\scr611_calcs.xls*. Cells E10...O10 give the calculated effective solubility limits, summarized as follows:

	Rel. Affinity	Solubility Limit	affnity*solubility limit	Eff. Solubility Limit
CM246	5.1030	1.556E-04		1.556E-04
U238	0.0074	7.109E-03	5.236E-05	7.191E-03
CM245	5.1030	1.556E-04		1.556E-04
AM241	9.9035	1.026E-04	1.016E-03	1.705E-03
U233	0.0074	7.109E-03	5.236E-05	7.191E-03
TH229	9.6726	1.065E-05		1.065E-05
AM243	9.9035	1.026E-04	1.016E-03	1.705E-03
PU239	1.0000	2.283E-04	2.283E-04	5.882E-04
PU240	1.0000	2.283E-04	2.283E-04	5.882E-04
U234	0.0074	7.109E-03	5.236E-05	7.191E-03
TH230	9.6726	1.065E-05		1.065E-05

The relevant parts of the screenprint (*tpa.out*) are as follows:

```
exec: calling ebsrel
Cm246
 sol = 1.555636000000000E-04
 effsol = 1.555636000000000E-04
```

```
U238
 sol = 7.108610000000000E-03
 effsol = 7.191152445173715E-03
Am241
 sol = 1.026389000000000E-04
 effsol = 1.705094393640583E-03
Th229
 sol = 1.064574000000000E-05
 effsol = 1.064574000000000E-05
Pu239
 sol = 2.282897000000000E-04
 effsol = 5.881800811857019E-04
```

The calculated value for each unique radionuclide is the same as the screenprint from the code run.

Test status: PASS

PL-2. Name: Release Concentrations and Affinity-weighted Concentrations

Path for run directory: /home/oosidele/runSCR611tpa502j

Path for archive of results: \scr611_test\Unix\runSCR611tpa502j
(archived on CD named "Test Plan for SCR 611")

Environment variables: TPA_TEST=/home/oosidele/tpa502j
TPA_DATA=/home/oosidele/tpa502j

Special input files or modifications to input files required: *tpa.inp*
(run one realization for Subarea 2 only)

Special diagnostic code modifications required : Statements added to *ebsrel.f* to save a copy of *ebsnef.dat* to *ebsnef_int.dat* immediately after running the *releaset* standalone code .

Print statements 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`). Only the results for the last timestep are displayed.

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

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

Test description: Calculation of release concentrations and affinity-weighted concentrations for Pu, Am, Th, Cm and U is examined.

- **Objective:** Verify by spreadsheet calculation the values calculated by the test code.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** Screen print (*tpa.out*)

- **Step by step test procedure to be used:**
  1. Execute the test code with the specified modifications using the basecase *tpa.inp* file (for Subarea 2 only) and capture the screenprint in the *tpa.out* file.

2. Extract the values for radionuclide half-life and atomic weight from *nuclides.dat*. Extract values for flow and release from *ebsnef_int.dat* into a spreadsheet. Convert release to concentration using the equation in Section 6 of Attachment A.
3. Calculate the total affinity-weighted concentration using the denominator of the equation in Section 7 of Attachment A.
4. Compare the spreadsheet calculations in steps 3 and 4 with the screenprint.

- Pass/Fail criteria:

The screenprint should give the same value of concentration and total affinity-weighted concentration.

Test Results:

Files on the CD in the *\scr611_test\PC\run_tpa502j* subdirectory contain results for this test run. Spreadsheet calculations are in *\scr611_test\scr611_calcs.xls*. Cells Q19...AA218 give the calculated concentrations and cells AC19...AM218 give the calculated total affinity-weighted concentrations. Cells AN19...AN218 give the total affinity-weighted concentrations for Pu, Am, Th, Cm and U for all timesteps. For the last timestep, the calculated concentrations, affinity-weighted concentrations, and cumulative affinity-weighted concentrations are summarized as follows:

	Concentration	Affinity-weighted concentration	Cumulative Affinity-weighted concentration
CM246	1.17E-08	5.96E-08	5.96E-08
U238	2.20E-01	5.24E-05	5.24E-05
CM245	1.16E-07	5.93E-07	5.30E-05
AM241	6.13E-09	6.07E-08	5.31E-05
U233	1.20E-05	8.83E-08	5.32E-05
TH229	3.86E-06	3.73E-05	9.05E-05
AM243	4.74E-06	4.69E-05	1.37E-04
PU239	3.72E-04	2.28E-04	3.66E-04
PU240	7.00E-05	7.00E-05	4.36E-04
U234	3.01E-05	2.22E-07	4.36E-04
TH230	3.59E-06	3.47E-05	4.71E-04

The screenprint (*tpa.out*) displays the concentration and cumulative affinity-weighted concentrations. The relevant parts are as follows:

```
CM246
concentration = 1.167197557161357E-08
totalAffCon = 5.956190459033489E-08
U238
concentration = 0.2195759830458385
totalAffCon = 5.241881080669033E-05
CM245
concentration = 1.161809405095729E-07
totalAffCon = 5.301168028721564E-05
```

```
AM241
concentration = 6.133768894329145E-09
totalAffCon = 5.307242625760746E-05
U233
concentration = 1.198451258547017E-05
totalAffCon = 5.316069950335213E-05
TH229
concentration = 3.861260712433000E-06
totalAffCon = 9.050897928126378E-05
AM243
concentration = 4.737919538321684E-06
totalAffCon = 1.374311123045383E-04
PU239
concentration = 3.717536248799794E-04
totalAffCon = 3.657208123045382E-04
PU240
concentration = 7.000500181278676E-05
totalAffCon = 4.357258141173250E-04
U234
concentration = 3.014715401830967E-05
totalAffCon = 4.359478662964338E-04
TH230
concentration = 3.591740032159856E-06
totalAffCon = 4.706891908536420E-04
```

The sum of affinity-weighted concentrations (`totalAffCon`) displays a cumulative sum over the radioclunides Pu, Am, Th, Cm and U. The final value corresponds with the calculated value (in Cell AN218) of `4.71E-04`.

The calculated values are the same as the screenprint from the code run.

Test status: PASS

PL-3. Name: Colloid (J-species) Concentrations

Path for run directory: /home/oosidele/runSCR611tpa502j

Path for archive of results: \scr611_test\Unix\runSCR611tpa502j
(archived on CD named "Test Plan for SCR 611")

Environment variables: TPA_TEST=/home/oosidele/tpa502j
TPA_DATA=/home/oosidele/tpa502j

Special input files or modifications to input files required: *tpa.inp*
(run one realization for Subarea 2 only)

Special diagnostic code modifications required : None

Program modes to be used (append flags, scenario/model switches, etc.): None

Utility scripts needed to perform the test: None

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

Test description: Calculation of the colloid (J-species) concentrations is examined.

- **Objective:** Verify by spreadsheet calculation the values calculated by the test code.

- **Assumptions:** None, other than the assumptions made in the TPA code

- **Constraints:** None

- **Output files to compare or examine:** *ebsnef.dat*

- **Step by step test procedure to be used:**
  1. Execute the test code using the basecase *tpa.inp* file (for Subarea 2 only).
  2. Calculate colloid concentration for the J-species in a spreadsheet using the equations in Sections 7 and 8 of Attachment A.
  3. Calculate dissolved concentration for the J-species in a spreadsheet using the equation in Section 9 of Attachment A.
  4. Convert colloid and dissolved concentrations back to release in a spreadsheet using the equation in Section 10 of Attachment A.
  5. Compare the spreadsheet calculations in steps 2–4 with the concentrations and releases written to *ebsnef.dat.*

- **Pass/Fail criteria:**
  The concentrations and releases calculated for the J-species should be the same as those written by the code to *ebsnef.dat.*

Test Results:

Files on the CD in the *\scr611_test\PC\run_tpa502j* subdirectory contains results for this test run. Spreadsheet calculations are in *\scr611_test\scr611_calcs.xls*. Cells AP19...AZ218 and BB19...BL218 give the calculated colloid concentrations from Step 2. Cells BN19...BX218 give the calculated dissolved concentrations from Step 3. Cells BZ19...CJ218 give the calculated colloid release (Curies) from Step 4. Cells CL19...CV218 give the calculated dissolved release (Curies) from Step 4. The calculated concentrations and releases for the last timestep are summarized as follows:

Colloid Concentration (kg/m3) – J-Species

CM246	1.17E-08
CM245	1.16E-07
AM241	6.13E-09
AM243	4.74E-06
PU239	3.72E-04
PU240	7.00E-05
TH230	3.59E-06

Dissolved Concentration (kg/m3)

CM246	0.00E+00
CM245	0.00E+00
AM241	0.00E+00
AM243	0.00E+00
PU239	0.00E+00
PU240	0.00E+00
TH230	0.00E+00

Colloid Release (Ci/yr) – J-Species

CM246	8.37E-06
CM245	4.66E-05
AM241	4.91E-05
AM243	2.20E-03
PU239	5.39E-02
PU240	3.72E-02
TH230	1.69E-04

Dissolved Release (Ci/yr)

CM246	0.00E+00
CM245	0.00E+00
AM241	0.00E+00
AM243	0.00E+00
PU239	0.00E+00
PU240	0.00E+00
TH230	0.00E+00

These values are the same as the corresponding values in the output file *ebsnef.dat*.

Test status: PASS