Software Release Notice
Developed or Modified Software

1. Software Name and Project Number:: TPA (Total-System Performance Assessment) — Version: 5.1a

2. Software Function: Conduct post-closure performance calculations of the potential geologic repository at Yucca Mountain, Nevada, as an aid to developing risk insights.

3. Summary of Actions:
❑ New Software ☒ Update to Existing Software ❑ Software Retirement

4. Software Development

4a. Software Requirements Description (SRD) Date Approved: ___June 11, 2007 __
4b. Software Development Plan (SDP) Date Approved: ___May 10, 2005 ____
4c. Software Change Report (SCR) Nos: _ 695______________________
4d. User's Guide Date Date Approved___ July 27, 2007 __________
4e. Enclosed: ☒ Copy of Program Title Block ☒ Sample Source Code Header Block

Developer: R. Janetzke	Date: Sep 22, 2007

Remarks:

5. Software Installation

5a. Computer Platform(s):	5b. Operating System(s):	5c. Programming Language(s):
Personal Computer	Windows/XP	Lahey Fortran LF95

5d. Installation Testing: ☒ Passed Testing Performed on: Sep 19, 2007
Description of Testing Performed:

5e. Archive Copy: ☒ Enclosed ❑ Not Available, Why:

Installation Performed by: R. Janetzke	Date: Sep 19,2007

Remarks: Installed on ALBY (Windows XP / Lahey LF95)

6. Software Assessment

6a. Acceptance Testing:
❑ Enclosed ❑ Documented in Scientific Notebook No. __________
☒ Documented in SCRs (see above)______________

6b. Validation Status:
☒ Full Validation ❑ Limited Validation
❑ Not Validated, Explain:
Date of Validation: Jun 20, 2007 (Regression testing completed on Sep 23, 2007 for SCR695)

Software Developer: R. Janetzke	Date: 9-24-07

Remarks: Validation regression test set was based on the full validation performed for TPA 5.1.

7. Approval

Manager: J. Winterle [signature]	Date 9/25/07

Remarks: Note validation regression testing is part of SCR 695 documentation

7. QA Verification

SRN Number: 433

Software Custodian [signature]	Date: 9/25/2007

Remarks:

TOP-6-2 (12/2004)

INSTALLATION TEST OUTPUT

```
=======================================================================
         exec: Welcome to TPA Version 5.1a
       Job started: Wed Sep 19 15:23:37 2007
=======================================================================
REPOSITORY DESIGN INFORMATION
Subarea   Area      Waste   Number of WP
   #     [m^2]      [MTU]
   1    224091.0     3025.5        526
   2    448476.0     6108.4       1062
   3   1241313.5    16703.3       2904
   4    775953.1    10313.0       1793
   5    605892.0     8351.7       1452
   6    152357.0     1972.9        343
   7    318122.0     4003.3        696
   8    439350.0     5355.0        931
   9    305880.0     4158.6        723
  10    747165.5    10048.4       1747

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

Specified Global Parameters:

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

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

The specified path for data  = d:\ronj-\tpa51a\
The specified path for codes = d:\ronj-\tpa51a\

**To modify global parameters or the path, stop code execution using control-C**
-----------------------------------------------------------------------
    subarea   1 of  10           realization    1 of  500
-----------------------------------------------------------------------
exec: calling uzflow
        Mean Annual Infiltration at Start(AAI0):    4.2736E+01
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      435.7  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =      967.4  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     19 at TPA time =    946.9 yr
 *** failed WPs:  19   out of  526  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                 Highest release rates from Sub Area 1
             Am241   4.3208E-01 [Ci/yr/SA] at  1.524E+03 yr
             Tc99    3.8425E-01 [Ci/yr/SA] at  2.044E+03 yr
             Ni59    9.1383E-02 [Ci/yr/SA] at  2.044E+03 yr
             Am243   8.7733E-02 [Ci/yr/SA] at  6.407E+03 yr
             Ja241   2.6108E-02 [Ci/yr/SA] at  1.524E+03 yr
             Cs135   1.8708E-02 [Ci/yr/SA] at  2.044E+03 yr
exec: calling uzft
                     Highest release rates from UZ
             Tc99    3.8187E-01 [Ci/yr/SA] at  2.094E+03 yr
             Ni59    7.5332E-02 [Ci/yr/SA] at  4.499E+03 yr
             Am243   4.5761E-02 [Ci/yr/SA] at  1.000E+04 yr
             Cs135   1.8354E-02 [Ci/yr/SA] at  2.251E+03 yr
             Pu239   8.0191E-03 [Ci/yr/SA] at  1.000E+04 yr
             Ja241   5.5316E-03 [Ci/yr/SA] at  1.641E+03 yr
exec: calling szft
                     Highest release rates from SZ
             Tc99    1.2829E-01 [Ci/yr/SA] at  5.832E+03 yr
```

```
           Se79    5.2948E-04 [Ci/yr/SA] at  7.730E+03 yr
           I129    2.9618E-04 [Ci/yr/SA] at  5.832E+03 yr
           Cl36    1.2823E-04 [Ci/yr/SA] at  5.696E+03 yr
           Ja241   1.2897E-07 [Ci/yr/SA] at  1.000E+04 yr
           Jc245   1.2496E-07 [Ci/yr/SA] at  1.000E+04 yr
------------------------------------------------------------------------
    subarea   2 of  10          realization    1 of  500
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      315.6  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  1062  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
------------------------------------------------------------------------
    subarea   3 of  10          realization    1 of  500
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      854.4  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  2904  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
------------------------------------------------------------------------
    subarea   4 of  10          realization    1 of  500
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =     1219.1  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  1793  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
------------------------------------------------------------------------
    subarea   5 of  10          realization    1 of  500
------------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
```

```
     exec: time of drip shield mechanical failure =      711.9  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  1452  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
----------------------------------------------------------------------
    subarea   6 of  10           realization    1 of  500
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      366.5  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  343  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
----------------------------------------------------------------------
    subarea   7 of  10           realization    1 of  500
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      315.6  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  696  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
----------------------------------------------------------------------
    subarea   8 of  10           realization    1 of  500
----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      270.4  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  931  ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
```

```
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
-----------------------------------------------------------------------
    subarea   9 of  10          realization    1 of  500
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      435.7  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: time of corrosion breach on welded areas =     1195.7  yr
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
exec: failed WPs from LOC CORR   event =     27 at TPA time =   1189.0 yr
 *** failed WPs:  27   out of  723   ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
               Highest release rates from Sub Area 9
           Tc99    4.7233E-01 [Ci/yr/SA] at  2.094E+03 yr
           Am241   3.5243E-01 [Ci/yr/SA] at  1.810E+03 yr
           Ni59    1.1103E-01 [Ci/yr/SA] at  2.602E+03 yr
           Am243   9.3393E-02 [Ci/yr/SA] at  5.434E+03 yr
           Cs135   2.2646E-02 [Ci/yr/SA] at  2.540E+03 yr
           Ja241   2.1934E-02 [Ci/yr/SA] at  1.766E+03 yr
exec: calling uzft
                   Highest release rates from UZ
           Tc99    4.6982E-01 [Ci/yr/SA] at  2.251E+03 yr
           Cs135   2.0921E-02 [Ci/yr/SA] at  4.093E+03 yr
           Se79    2.9814E-03 [Ci/yr/SA] at  2.363E+03 yr
           Ja241   1.9674E-03 [Ci/yr/SA] at  2.540E+03 yr
           Ja243   1.7792E-03 [Ci/yr/SA] at  1.000E+04 yr
           I129    1.0360E-03 [Ci/yr/SA] at  2.665E+03 yr
exec: calling szft
                   Highest release rates from SZ
           Tc99    2.0200E-01 [Ci/yr/SA] at  6.113E+03 yr
           Se79    8.5439E-04 [Ci/yr/SA] at  8.101E+03 yr
           I129    4.6206E-04 [Ci/yr/SA] at  6.113E+03 yr
           Cl36    1.9878E-04 [Ci/yr/SA] at  6.113E+03 yr
           Ja241   8.7469E-08 [Ci/yr/SA] at  1.000E+04 yr
           Jc245   8.1564E-08 [Ci/yr/SA] at  1.000E+04 yr
-----------------------------------------------------------------------
    subarea  10 of  10          realization    1 of  500
-----------------------------------------------------------------------
exec: calling uzflow
exec: calling driftdriver
exec: calling nfenvFl
exec: calling dsfail
exec: calling mechdriver (drip shield)
     exec: time of drip shield mechanical failure =      411.6  yr
     *** No Drip Shield Failure by General Corrosion ***
exec: calling  nfenv
exec: calling ebsfail
     ebsfail: No Corrosion Breach on WP Welded Areas
     *** No Localized Corrosion Breach on the Mill-Annealed WP Body ***
     *** No WP Breach by General Corrosion ***
exec: calling mechdriver (waste package)
 *** failed WPs:  0   out of  1747   ***
exec: calling ebsrel
      ebsrel: running spent fuel waste form
      ebsrel: running glass waste form
                        There is no EBS release
exec: calling uzft
                        There is no UZ release
exec: calling szft
                        There is no SZ release
exec: calling dcagw
                   Highest annual dose GW pathway
           Tc99    2.7756E-01 [mrem/yr]  at  5.971E+03 yr
           I129    8.3361E-02 [mrem/yr]  at  6.113E+03 yr
           Se79    3.9285E-03 [mrem/yr]  at  7.914E+03 yr
           Cl36    4.4006E-04 [mrem/yr]  at  5.971E+03 yr
           Cm245   4.0269E-05 [mrem/yr]  at  1.000E+04 yr
           Am241   3.9109E-05 [mrem/yr]  at  1.000E+04 yr
         At end of TPI, annual dose GW pathway
           Tc99    1.8681E-01 [mrem/yr]
           I129    5.7626E-02 [mrem/yr]
           Se79    3.7084E-03 [mrem/yr]
           Cl36    2.9545E-04 [mrem/yr]
           Cm245   4.0269E-05 [mrem/yr]
           Am241   3.9109E-05 [mrem/yr]
```

```
                sum  2.4853E-01 [mrem/yr]
exec: end realizations

exec: Peak Mean Dose is 3.64640E-04 rem/yr at     5970.9 yr, based on      1 realizations.

exec:  Run Successfully Completed
```

```
C Program Name:         TPA - Total-System Performance Assessment Code
C File Name:            %M%
C File Date:            %G%
C Release Version:      5.1a
C
C Client Name:          USNRC
C                       U. S. Nuclear Regulatory Commission
C                       NRC Office of Nuclear Material Safety and Safeguards
C                       Division of High Level Waste Repository Safety
C
C Contract Number:      NRC 02-02-012
C
C NRC Contact:          Chris Grossman (301) 492-3177
C
C CNWRA Contact:        Ron Janetzke (210) 522-3318
C                       Center for Nuclear Waste Regulatory Analyses
C                       San Antonio, Texas 78238-5166
C
C Documentation:        "Total-System Performance Assessment (TPA)
C                       Version 5.1 User Guide",
C                       Center for Nuclear Waste Regulatory Analyses
C
C NUREG-Series Designator: N/A
C
C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
C
C                         D I S C L A I M E R
C
C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
C
C     "This computer code/material was prepared as an account of work
C performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA)
C for the Division of High Level Waste Repository Safety of the Nuclear
C Regulatory Commission (NRC), an independent agency of the United States
C Government.  Neither the developer(s) of the code nor any of their
C sponsors make any warranty, expressed or implied, or assume any legal
C liability or responsibility for the accuracy, completeness, or
C usefulness of any information, apparatus, product or process
C disclosed, or represent that its use would not infringe on privately-
C owned rights."
C
C     "In no event unless required by applicable law will the sponsors
C or those who have written or modified this code, be liable for
C damages, including any lost profits, lost monies, or other special,
C incidental or consequential damages arising out of the use or
C inability to use the program (including but not limited to loss of
C data or data being rendered inaccurate or losses sustained by third
C parties or a failure of the program to operate with other programs),
C even if you have been advised of the possibility of such damages or
C for any claim by any other party."
C
C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
```

```
C = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = = =
c
c     CONTENTS:
c              function tempgl( t )
c              subroutine cond3dxyzt
c              subroutine xgauleg(func,a,b,n,ss)
c     HISTORY:
c             by Randall D. Manteufel (previous version)
c             Modified by S. Mohanty, R. W. Rice (2/14/2000)
c             6-28-03  blw   SCR453; Reformat headers for automated tests.
c             2-04-05 GADAMS SCR553
c             6-04-05 GADAMS SCR604
c
c             3-23-06 jmm SCR599; Bug fix for tend = tpa time step.
c
c             function tempgl solution from:
c             J. Claesson, T. Probert
c             Depts. of Building Physics and Mathematical Physics
c             Lund University,
c             Lund Sweden
c             SKB Technical Report 96-12
c             January 1996
c
c========================================================================
```

SOFTWARE CHANGE REPORT (SCR)

1. **SCR No.** (*Software Developer Assigns*): SCR 695	**2. Software Title and Version:** TPA 5.1	**3. Project No:** 20.06002.01.354

4. Affected Software Module(s), Description of Problem(s): *failt.f, szft.f, tpa.inp.*

1. It is necessary to change the logic in the FAILT code to accurately represent the description in the user guide. The minimal failure time among weld corrosion, localized corrosion of the waste package body, and general corrosion of the waste package body, should be selected to define the initial release time. As is now, the localized corrosion failure time, although correctly computed in FAILT, is ignored in RELEASET.

2. The SZFT module calculates R values for actinides using a grain density value, but should be using the bulk density. See Attachment A for details.

3. *tpa.inp* values for PGA in seismic curve are mean values versus median . Mean values are specified, but code is based on median. Attachment B contains the new seismic hazard curve values.

4. EBSREL calculates Fmult using a natural log function but the input parameters, BfmultCoefficient and X0fmultCoefficient are based on Log-10.

5. Change Requested by:
1) R. Rice
2) J. McMurry
3) J. Mancillas
4) C. Manepally

Date: 8-23-2007

6. Change Authorized by (*Software Developer*): R. Janetzke [signature]

Date: 8-23-2007

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

See Attachment C for details.

8. Implemented by: R. Janetzke [signature]

Date: 8-27-2007

9. Code Review Needed (see TOP-018, 5.4.7) Yes ☐ No ☒
(Determined by Software Developer. Code reviews should be performed for modifications with significant risks of code errors. Indicate selection with ☒).
Describe any errors detected and their resolution *(If no errors are found, indicate with "**None**".)*:

Code review accomplished by: N/A

Date: N/A

10. Description of Acceptance Tests:

See Attachment D for a description of the tests.

See attached CD labeled 'SCR695 Test Results' for the test result files.

11. Tested by: O. Pensado [signature]

Date: 8-31-2007

Form TOP-5 (10/2006)

UPDATE REQUIREMENTS for *TPA.INP*

SCR 695

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	EBSREL	BfmultCoefficient		constant	0.22		C. Manepally
MODIFY TO	EBSREL	BfmultCoefficient		constant	0.5		C. Manepally
MODIFY FROM	EBSREL	X0FmultCoefficient		triangular	1.0, 1.47, 2.0		C. Manepally
MODIFY TO	EBSREL	X0FmultCoefficient		triangular	2.3, 3.4, 4.6		C. Manepally

MODIFY FROM	MECHFAIL	Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax [1/yr,m/s,m/s2,_,_,_]	Seismic hazard curve for mean annual probability of exceedance, peak ground velocity, median peak ground acceleration, standard deviation peak ground acceleration, minimum compaction factor, and maximum compaction factor.	hazardcurve	5 1.0e-4 0.47 0.47 0.64 0.10 0.20 1.0e-5 1.05 2.27 0.64 0.20 0.40 1.0e-6 2.44 4.75 0.53 0.30 0.60 1.0e-7 5.35 12.7 0.53 0.40 0.60 1.0e-8 5.35 12.7 0.53 0.40 0.60		O. Pensado

MODIFY TO	MECHFAIL	Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax [1/yr,m/s,m/s2,_,_,_]		hazardcurve	5 1.0e-4 0.47 0.38 0.64 0.10 0.20 1.0e-5 1.05 1.85 0.64 0.20 0.40 1.0e-6 2.44 4.13 0.53 0.30 0.60 1.0e-7 5.35 11.04 0.53 0.40 0.60 1.0e-8 5.35 11.04 0.53 0.40 0.60		O. Pensado

Attachment A

In SZFT, there are two places where the following line of code occurs:

```
ssarea = 3.0d0*porosity / (density*poreradius)
```

those lines need to be replaced by the following:

```
ssarea = 3.0d0*porosity / (density*(1-porosity)*poreradius)
```

Also, the following comment line needs to be revised:

```
c     3*rock_porosity / (rock_grain_density[kg/m^3]*pore_radius[m])
```

should be revised to

```
c     3*rock_porosity / (rock_grain_density[kg/m^3]*(1-rock_porosity)*pore_radius[m])
```

Attachment B

The following is from O. Pensado.

This is the revised seismic hazard curve to make it consistent with the TPA equations. The 3rd column contains median values.

New:

```
hazardcurve
Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_]
5
1.0e-4 0.47  0.38 0.64 0.10 0.20
1.0e-5 1.05  1.85 0.64 0.20 0.40
1.0e-6 2.44  4.13 0.53 0.30 0.60
1.0e-7 5.35 11.04 0.53 0.40 0.60
1.0e-8 5.35 11.04 0.53 0.40 0.60
```

Old:

```
hazardcurve
Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_]
5
1.0e-4 0.47 0.47 0.64 0.10 0.20
1.0e-5 1.05 2.27 0.64 0.20 0.40
1.0e-6 2.44 4.75 0.53 0.30 0.60
1.0e-7 5.35 12.7 0.53 0.40 0.60
1.0e-8 5.35 12.7 0.53 0.40 0.60
```

The equation to do the transformation is

```
median = Exp[ 0.5*(-Ls^2 + 2*LN[mean])  ] = mean*Exp[-Ls^2 / 2]
```

where Ls is the data on the 4th column.

Attachment C

TPA Version 5.1a

Changes since Version 5.1

1) codes/failt.f: line 361 add clarification of LC type

2) codes/failt.f: line 616 change test from `.gt.` to `.ge.`

3) codes/failt.f: lines 2286 and 2312 - Remove print statements

```
1,4c1,4
< c Program Name:        failt
< c File Name:           failt.f
< c File Date:           06/16/07
< c Release Version:     5.0
---
> C Program Name:        TPA - Total-System Performance Assessment Code
> C File Name:           %M%
> C File Date:           %G%
> C Release Version:     5.1
72a73,74
> c  08-27007 R. Janetzke SCR695; Adjusted sensing localized corrosion time
> c                                and associated screen prints.
358,359c360,362
<       & '!! This section contains corrosion failure data versus time',
<       & '!! for the waste package outer layer only.  Corrosion credit',
---
>       & '!! This section contains corrosion failure data versus time'//
>       & ' for the localized corrosion (LC) type',
>       & '!! for the waste package outer layer only. Corrosion credit',
610c613,616
<            if ( pnt .gt.thicktot .or. ifail.eq.1 ) then
---
> cc rwj 8-27-07; SCR695
> c          if ( pnt .gt.thicktot .or. ifail.eq.1 ) then
>            if ( pnt .ge.thicktot .or. ifail.eq.1 ) then
>
2280,2281c2286,2289
<              PRINT *, "failt: Outer overpack LC initiated at", time,
<       &                " years"
---
> cc rwj 8-27-07; SCR695
> c            PRINT *, "failt: Outer overpack LC initiated at", time,
> c     &                " years"
>
2304,2305c2312,2315
<                 PRINT *, "failt: Inner overpack LC initiated at", time,
<       &                " years"
---
> cc rwj 8-27-07; SCR695
> c               PRINT *, "failt: Inner overpack LC initiated at", time,
> c     &                " years"
>
```

4) szft.f: lines 391 and 509 - use bulk density in equation for ssarea

5) tpa.inp: update BFmultCoefficient to 0.5
   update X0FmultCoefficient to triangular 2.3, 3.4, 4.6
   update hazardcurve

```
Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_]
5
1.0e-4  0.47  0.38  0.64  0.10  0.20
1.0e-5  1.05  1.85  0.64  0.20  0.40
```

```
1.0e-6  2.44  4.13  0.53  0.30  0.60
1.0e-7  5.35 11.04  0.53  0.40  0.60
1.0e-8  5.35 11.04  0.53  0.40  0.60
```

6) exec.f: line 15459 - change toltime to 1.0d-5

Attachment D

Requirement 1. It is necessary to change the logic in the FAILT code to accurately represent the description in the user guide. The minimal failure time among weld corrosion, localized corrosion of the waste package body, and general corrosion of the waste package body, should be selected to define the initial release time. As is now, the localized corrosion failure time, although correctly computed in FAILT, is ignored in RELEASET.

Test 1.1:

I verified that the file failt.out does not include extra print statements.

Run TPA 5.1 and 5.1a with the following changes
Changes to force localized corrosion (WP body and welds):
AA_1_1[C/m2/yr]=1.60e3
EnvironmentII_Wastepackage_DeltaECrit[VSHE]=-2.0
No initially defective WPs: DefectiveFractionOfWPs/cell=0.0
Subarea 3 only, Realization 1

Extract of *failt.out* from version 5.1

```
! SECTION 4 ; WASTE PACKAGE CORROSION FAILURE DATA
!
! This section contains corrosion failure data versus time
! for the waste package outer layer only.  Corrosion credit
! is restricted to the waste package outer layer.
!
! Step                  ; tpa time step
! Time                  ; time of tpa time step
! Surface Temperature   ; surface temperature of the waste
!                         package outer layer prior to
!                         corrosion
! Critical Potential    ; critical potential for localized
!                         corrosion initiation
! Corrosion Potential   ; corrosion potential
! Chloride Flag         ; flag indicating that critical
!                         chloride concentration has been
!                         exceeded
! Layer Thickness       ; remaining thickness of waste
!                         package outer layer
! Mode                  ; mode of corrosion
!                         dry oxd: dry air oxidation
!                         hmd oxd: humid air oxidation
!                         local:   aqueous localized corrosion
!                         general: aqueous general corrosion

 Step        Time       Surface       Critical      Corrosion  Chloride        Layer      Mode
                    Temperature     Potential      Potential      Flag    Thickness
           (year)   (degrees C)   (volts SHE)    (volts SHE)                    (m)
    2  2.31016E+00  5.71807E+01   0.00000E+00    0.00000E+00         0  2.00000E-02   dry oxd
    3  4.67440E+00  6.13628E+01   0.00000E+00    0.00000E+00         0  2.00000E-02   dry oxd
    4  7.09399E+00  6.31162E+01   0.00000E+00    0.00000E+00         0  2.00000E-02   dry oxd
    5  9.57023E+00  6.40163E+01   0.00000E+00    0.00000E+00         0  2.00000E-02   dry oxd
.
.
.
  129  1.80962E+03  1.10607E+02   9.68401E-01    3.59270E-01         1  1.98565E-02   general
  130  1.85430E+03  1.09161E+02   9.81965E-01    3.59372E-01         1  1.98526E-02   general
  131  1.90002E+03  1.07728E+02   9.95394E-01    3.59541E-01         1  1.98488E-02   general
failt: Outer overpack LC initiated at 1946.810000000000  years
failt: Outer overpack LC initiated at 1935.112500000000  years
failt: Outer overpack LC initiated at 1917.566250000000  years
failt: Outer overpack LC initiated at 1914.641875000000  years
failt: Outer overpack LC initiated at 1916.104062500000  years
failt: Outer overpack LC initiated at 1915.372968750000  years
  132  1.94681E+03  1.06308E+02  -1.09187E+00    3.07832E-01         1  1.17446E-02   local
failt: Inner overpack LC initiated at 1946.810000000000  years
```

Extract of *failt.out* from version 5.1a

```
! SECTION 4 ; WASTE PACKAGE CORROSION FAILURE DATA
!
! This section contains LC corrosion failure data versus time
! for the waste package outer layer only. LC corrosion credit
! is restricted to the waste package outer layer.
!
! Step                  ; tpa time step
! Time                  ; time of tpa time step
! Surface Temperature   ; surface temperature of the waste
!                         package outer layer prior to
!                         corrosion
! Critical Potential    ; critical potential for localized
!                         corrosion initiation
! Corrosion Potential   ; corrosion potential
! Chloride Flag         ; flag indicating that critical
!                         chloride concentration has been
!                         exceeded
! Layer Thickness       ; remaining thickness of waste
!                         package outer layer
! Mode                  ; mode of corrosion
!                         dry oxd: dry air oxidation
!                         hmd oxd: humid air oxidation
!                         local:   aqueous localized corrosion
!                         general: aqueous general corrosion

 Step         Time      Surface      Critical     Corrosion  Chloride        Layer      Mode
                    Temperature     Potential     Potential      Flag    Thickness
                (year) (degrees C)  (volts SHE)  (volts SHE)                   (m)
    2  2.31016E+00  5.71807E+01  0.00000E+00  0.00000E+00          0  2.00000E-02  dry oxd
    3  4.67440E+00  6.13628E+01  0.00000E+00  0.00000E+00          0  2.00000E-02  dry oxd
    4  7.09399E+00  6.31162E+01  0.00000E+00  0.00000E+00          0  2.00000E-02  dry oxd
    5  9.57023E+00  6.40163E+01  0.00000E+00  0.00000E+00          0  2.00000E-02  dry oxd
.
.
.
  129  1.80962E+03  1.10607E+02  9.68401E-01  3.59270E-01          1  1.98565E-02  general
  130  1.85430E+03  1.09161E+02  9.81965E-01  3.59372E-01          1  1.98526E-02  general
  131  1.90002E+03  1.07728E+02  9.95394E-01  3.59541E-01          1  1.98488E-02  general

  132  1.94681E+03  1.06308E+02 -1.09187E+00  3.07832E-01          1  1.17446E-02  local
```

Therefore, the file *failt.out* does not include extra print statements.

Test 1.2:

Perform the runs with TPA 5.1 and 5.1a, one realization, subarea 3 only to verify that (I) the time of localized corrosion of the WP body is ignored in TPA 5.1, and (ii) the problem is fixed in TPA 5.1a. The time of localized corrosion is reported in the files *failt.out* (WP body) and *weldfail.out* (WP welds). The failure time is passed to the file *ebstrh.dat* as input to EBSREL computations. The file *ebstrh.dat* for TPA 5.1 incorrectly ignores the time of localized corrosion of the waste package body.

Run b01
Changes to force localized corrosion (WP body and welds):
AA_1_1[C/m2/yr]=1.60e3
EnvironmentII_Wastepackage_DeltaECrit[VSHE]=-2.0
No initially defective WPs: DefectiveFractionOfWPs/cell=0.0
Subarea 3 only, Realization 1

Run b02
Same as b01 with
WeldCritChlorideConc[mol/L]=100.0 (no localized corrosion of WP welds)

Run b03
Same as b01 with
CritChlorideConcForFirstLayer[mol/L]=100.0 (no localized corrosion of the WP body)

Results:

Run b01_51, TPA 5.1

File *ebstrh.dat*
```
    5.165000E+00     1.659000E+00          | WP length[m], WP diameter[m]
    4.852900E-02                           | Weld surface fraction
     1             1.9769145420E+03        | Weld Failure Flag (1 = failure), Weld Failure Time[yr]
     0             1.0000000000E+04        | WP Breach by General Corrosion Flag (1 = general
corrosion failure, 0 otherwise), Time of WP Breach by General Corrosion[yr]
     0             1.0000000000E+04        | Localized Corrosion Breach of WP Body Flag (1 =
failure), Time of Localized Corrosion Breach of WP Body[yr]
```

The flag indicates that localized corrosion on the WP body is ignored (flag=0). Localized corrosion is reported to occur in the file *failt.out* at around 1946.81 years. That time is ignored in *ebstrh.dat*.

Run b01, TPA 5.1a
File ebstrh.dat
```
    5.165000E+00     1.659000E+00          | WP length[m], WP diameter[m]
    4.852900E-02                           | Weld surface fraction
     1             1.9769145420E+03        | Weld Failure Flag (1 = failure), Weld Failure Time[yr]
     0             1.0000000000E+04        | WP Breach by General Corrosion Flag (1 = general
corrosion failure, 0 otherwise), Time of WP Breach by General Corrosion[yr]
     1             1.9468100000E+03        | Localized Corrosion Breach of WP Body Flag (1 =
failure), Time of Localized Corrosion Breach of WP Body[yr]
```

In this case, both flags equal 1, indicating that both failure times (weld and body) are well read by the TPA code version 5.1a.

Run b02_51, TPA 5.1
File ebstrh.dat
```
    5.165000E+00     1.659000E+00          | WP length[m], WP diameter[m]
    4.852900E-02                           | Weld surface fraction
     0             1.0000000000E+04        | Weld Failure Flag (1 = weld failure, 0 otherwise), Weld
```

```
Failure Time[yr]
     0            1.0000000000E+04      | WP Breach by General Corrosion Flag (1 = general
corrosion failure, 0 otherwise), Time of WP Breach by General Corrosion[yr]
     0            1.0000000000E+04      | Localized Corrosion Breach of WP Body Flag (1 =
failure), Time of Localized Corrosion Breach of WP Body[yr]
```

In this case, the TPA code 5.1 ignores the presence of localized corrosion on the WP body (flag=0). Localized corrosion is reported to occur in the file failt.out at around 1946.81 years. That time is ignored in *ebstrh.dat*.

Run b02, TPA 5.1a
File *ebstrh.dat*

```
    5.165000E+00     1.659000E+00           | WP length[m], WP diameter[m]
    4.852900E-02                            | Weld surface fraction
     0            1.0000000000E+04      | Weld Failure Flag (1 = weld failure, 0 otherwise), Weld
Failure Time[yr]
     0            1.0000000000E+04      | WP Breach by General Corrosion Flag (1 = general
corrosion failure, 0 otherwise), Time of WP Breach by General Corrosion[yr]
     1            1.9468100000E+03      | Localized Corrosion Breach of WP Body Flag (1 =
failure), Time of Localized Corrosion Breach of WP Body[yr]
```

The TPA code version 5.1a properly recognizes the presence of LC on the WP body (flag=1)

Test 1.3

The seepage factor for the waste package is reported in the file *ebsflo.dat*, column labeled fwc. If properly computed, the WP seepage factor for run b01 must equal the sum of run b02 and b03.

Value of fwc seepage factor (file *ebsflo.dat*) in run b01: 8.6792E-02
Value of fwc seepage factor (file *ebsflo.dat*) in run b02: 3.8263E-02
Value of fwc seepage factor (file *ebsflo.dat*) in run b03: 4.8529E-02

Indeed 8.6792E-02 = 3.8263E-02 + 4.8529E-02

Therefore, the seepage factor fwc is correctly computed for the cases when LC occurs only on the WP body or the welds or both areas in version 5.1a.

I conclude that the changes to the TPA code were properly implemented and that requirement 1 is fulfilled.

Requirement 2. The SZFT module calculates R values for actinides using a grain density value, but should be using the bulk density. See Attachment A for details.

Objective: verify that Kd values for tuff are corrected by a factor 1/(1-porosity). Kd values are reported in the file *sz_kdrd.out*

Approach:
Run TPA 5.1 and correct the values of Kd by the factor 1/(1-porosity). Compare the corrected values to values of Kd reported in the file *sz_kdrd.out* for TPA Version 5.1a.

I run the TPA codes Version 5.1 and 5.1a with the following changes to the *tpa.inp*:

DefectiveFractionOfWPs/cell=loguniform(0.999, 0.9999)
Subarea 3 only.

Output files were saved in the directory *kd_test.*

I used Excel to compare the kd and rd values for tuff computed with Version 5.1 and correct by the factor 1/(1-porosity). The corrected values compared well to values in the output file *sz_kdrd.out* from Version 5.1a. I noted a divergence of the order of 0.03% or less. I discussed the small divergence with J. Winterle as he explained that the small difference was due to a negligible correction on the Kd to account for colloidal transport.

The comparison of the values is summarized in the excel file *kd_test.xls.*

I conclude that the change for requirement 2 was properly implemented.

Requirement 3. *tpa.inp* values for PGA in seismic curve are mean values versus median . Mean values are specified, but code is based on median. Attachment B contains the new seismic hazard curve values.

I verified that values for the parameter hazardcurve were updated in *tpa.inp*:

```
hazardcurve
Seismic_MAPE_PGV_PGAm_PGAsd_CFmin_CFmax[1/yr,m/s,m/s2,_,_,_]
5
1.0e-4  0.47  0.38  0.64  0.10  0.20
1.0e-5  1.05  1.85  0.64  0.20  0.40
1.0e-6  2.44  4.13  0.53  0.30  0.60
1.0e-7  5.35 11.04  0.53  0.40  0.60
1.0e-8  5.35 11.04  0.53  0.40  0.60
```

Requirement 4. EBSREL calculates Fmult using a natural log function but the input parameters, BfmultCoefficient and X0fmultCoefficient are based on Log-10.

I verified that the parameters BfmultCoefficient and X0fmultCoefficient were updated in *tpa.inp* by a factor LN(10)=2.3

```
constant
BFmultCoefficient
0.5
**
triangular
X0FmultCoefficient
2.3, 3.4, 4.6
```

REGRESSION TEST FOR VALIDATION

RT#: 1	Project#: 06002.01.354
Software Name: TPA	Version: 5.1a
Test ID: **P-9**	Test Series Name: Waste Package Corrosion

Test Method

□ Code Inspection	■ Spreadsheet
■ Output Inspection	■ Graphical
■ Hand Calculation	□ Comparison with External Code Results

Test Objective: This is a regression test to maintain assurance in the original validation tests (see Attachment A).

Test Environment Setup

Hardware (platform, peripherals): Desktop PC with Intel Pentium 4 processor.

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

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

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

Test Procedure:
See Attachment A

Test Results

Location: See attached CD labeled "TPA Version 5.1a Regression Tests for Validation Task P-9

Test Criterion and Analysis of Results: See Attachment A

Test Evaluation (Pass/Fail): Pass

Notes:

Tester: R. Janetzke *R. Janetzke*	Date: Sep. 22, 2007

Attachment A

TPA Version 5.1a Regression Tests for Validation Task P-9
Objectives, Assumptions, Test Descriptions

OBJECTIVES

This is one of the tests of the TPA V5.1a that constitutes the regression testing for the validation of the TPA code after the implementation of SCR695. A subset of the previously performed P-9 validation test is performed to satisfy the regression testing requirement for modification of validated code. The objective of Software Validation Report (SVR) P-9 is to verify process level calculations performed by the TPA module EBSFAIL (waste package failure). The specific issues to be retested by this SVR are #4, #5, and #6:

1. The ebsfail.f module provides correct input to the failt.f code.

2. Time varying corrosion potentials and passive current densities are correctly calculated.

3. Modification to the critical potential to account for the action of inhibiting anions is correctly calculated.

4. Times of failures by general corrosion and localized corrosion on welds and the waste package body are correctly reported by *failt.f*.

5. Changes to specified failure depth thresholds (i.e., fraction of total thickness at which waste package is assumed to have failed) result in proportional changes to calculated corrosion failure times.

6. Localized corrosion does not occur until the drift wall temperature falls below a threshold value for onset of seepage.

ASSUMPTIONS

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

- The input parameters and their distributions supplied by *tpa.inp* are consistent with the abstractions of the modeled processes.

- Previous validation testing of this module and testing of subsequent SCRs affecting this module have been properly performed, and may be cited as evidence of module performance.

TESTS

The following tests sequentially address the objectives of this SVR.

4a. First, the time of waste package failure due to general corrosion was tested. The *tpameans.out* file generated by reference case for TPA Version 5.1a was renamed *tpameansRefCase.out* and used as the *tpa.inp* file. The input values of the following six parameters were changed in accordance with the table below:

Parameter	**Value**
CriticalRelativeHumidityHumidAirCorrosion	0.2
CriticalRelativeHumidityAqueousCorrosion	0.2
OuterActivationEnergyPassiveCurrDens[J/mol]	0
AA_1_1[C/m2/yr]	3.2E5
OuterOverpackErpIntercept	100000
ErpInterceptWeld	100000

By assigning the same values of CriticalRelativeHumidityHumidAirCorrosion and CriticalRelativeHumidityAqueousCorrosion, the humid air corrosion is deactivated. Similarly, by assigning large values for OuterOverpackErpIntercept and ErpInterceptWeld, it is ensured that localized corrosion will not activate. In the test, the temperature independent general corrosion rate is implemented by assigning OuterActivationEnergyPassiveCurrDens[J/mol] to zero. In addition, the general corrosion rate is increased by four orders of magnitude to ensure that waste package outer container thickness reduces to zero before 10,000 years. The waste package thickness should change linearly with time due to temperature-independent general corrosion rate. The TPA code was executed for one reference case realization for subarea 3. The general corrosion rate at each time step and time of failure for mill-annealed and welded Alloy 22 is stored in file *failt.out* and *weldfail.out*, respectively. The time of failures were hand-calculated (H-C) for both materials and compared to the values provided by the TPA code.

Pass/Fail criteria
The relative difference between two computed values of times of failures should be less than 5 percent.

Results:
The TPA code was simulated using the procedure outlined above. The results are summarized in the following Table.

Summary of Results for Test Case 4a

	Hand-Calculation		TPA Code	
	WP Body	Welds	WP Body	Welds
Initiation Time for general corrosion (years)	**750.2829**	**760.2724**	**750.2829**	**760.2724**
Time of Failure (yrs)	2768.1627	2778.1522	2768.1289	2778.1067
Net General Corrosion Time (yrs)	2017.8798	2017.8798	**2017.8460**	**2017.8343**
	Ave. 2017.8798		Ave. 2017.8402	
	Ratio (H-C/TPA) = 1.000020E+00			

The times of failures for the waste package body (WP Body) and the welds (Welds) provided by TPA code are consistent with the values obtained by hand-calculation.

The computed results demonstrate that the failure times due to general corrosion for the WP Body and the Welds are correctly reported by EBSFAIL. The relative difference between the hand-calculated values and TPA code values for failure time is much less than 5 percent for both mill-annealed and welded materials. These results are presented as evidence that test objective has been successfully met.

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

4b. The time of waste package failure due to localized corrosion was tested. The *tpameans.out* file generated by reference case for TPA Version 5.1a was renamed *tpameansRefCase.out* and used as the *tpa.inp* file. The input values of following two parameters were changed in accordance with the table below:

Parameter	Value
OuterOverpackErpIntercept	-100000
ErpInterceptWeld	-100000

The large negative values of OuterOverpackErpIntercept and ErpInterceptWeld ensures that the corrosion potential is much larger than the repassivation potential for mill-annealed and welded Alloy 22. The TPA code was executed for one reference case realization for subarea 3. The time of failure due to localized corrosion for mill-annealed and welded Alloy 22 is stored in file *failt.out* and *weldfail.out*. The time of failure was hand-calculated and compared to the values provided by the TPA code.

Pass/Fail criteria
The relative difference between two computed values of time of failure should be less than 5 percent.

Results
The TPA code was simulated using the procedure outlined above. The results are summarized in the following Table.

Summary of Results for Test Case 4b

	Hand-Calculation		TPA Code	
	WP Body	Welds	WP Body	Welds
Start Time (Initiation Time) (yrs)	**750.3874**	**760.2190**	**750.3874**	**760.2190**
Finish Time (Time of Failure) (yrs)	830.3702	840.2030	830.3701	840.2032
Net Localized Corrosion Time (yrs)	**79.9828**	**79.9840**	**79.9827**	**79.9842**
	Ave. 79.9834		Ave. 79.9834	
	Ratio (H-C/TPA) = 9.999995E-01			

The times of failures for the waste package body (WP Body) and the welds (Welds) provided by TPA code are consistent with the values obtained by hand-calculation.

These results demonstrate that the waste package failure times due to localized corrosion for the WP Body and the Welds are correctly reported by EBSFAIL. The relative difference between the hand-calculated values and TPA code values for failure time is much less than 5 percent for both mill-annealed and welded materials.

These results are presented as evidence that test objective has been successfully met.

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

5a. The test procedure outlined in 4a was repeated with additional change in values of the two parameters according to the following table

Parameter	Value
WPFractionThicknessPenetratedForFailureByCorrosion[]	0.75
WPWeldFractionThicknessPenetratedForFailureByCorrosion[]	0.75

The time of waste package failure should reduce by 25 percent by changing values of the two parameters from 1 to 0.75. The output values of time of waste package failure by TPA code were compared to the hand-calculated values. The relative difference between two computed values was less than 5 percent.

Pass/Fail criteria
The relative difference between two computed values of time of failure should be less than 5 percent.

Results:
The TPA code was simulated using the procedure outlined for test case 5a. The results are summarized in the following Table.

Summary of Results for Test 5a

	Hand-Calculation		TPA Code	
	WP Body	Welds	WP Body	Welds
Start Time (Initiation Time) (yrs)	**750.2829**	**760.2724**	**750.2829**	**760.2724**
Finish Time (Time of Failure) (yrs)	2263.6927	2273.6823	2263.6674	2273.6150
Net General Corrosion Time (yrs)	1513.4099	1513.4099	**1513.3845**	**1513.3426**
	Ave. 1513.4099		Ave. 1513.3635	
	Ratio (H-C/TPA) = 1.000031			

The times of failures for the waste package body (WP Body) and the welds (Welds) provided by TPA code are consistent with the values obtained by hand-calculation.

The computed results demonstrate that the EBSFAIL failure times for the WP Body and the Welds by general corrosion are correctly reported by EBSFAIL. The relative difference between the hand-calculated values and TPA code values for failure time is much less than the 5 percent for both mill-annealed and welded materials.

The following table summarizes the net times at two different values of fraction (i.e., 1 and 0.75) in the case of general corrosion. As shown in this table, the net times are reduced approximately 25 percent by reducing values of failure criteria from 1 to 0.75.

Changes of Net Times at Different Specified Failure Depth Threshold in the Case of General Corrosion Mode.

Specified Failure Depth Thresholds (fraction)	Ave. Net Time by Hand-Calculation (yrs)	Ave. Net Time by TPA Code (yrs)
1 0.75	2017.8798 1513.4099	2017.8402 1513.3635
Fraction of Changes of Net Time		
-0.25	-0.2435	-0.2500
	Ave. -0.2468	

These results are presented as evidence that test objective has been successfully met.

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

5b. The test procedure outlined in 4b was repeated with additional changes in values of the two parameters according to the following table

Parameter	Value
WPFractionThicknessPenetratedForFailureByCorrosion[]	0.75
WPWeldFractionThicknessPenetratedForFailureByCorrosion[]	0.75

The time of failure should reduce by 25 percent because of the change in values of the above two parameters. The output values of time of failure by TPA code were compared to the hand-calculated values.

Pass/Fail criteria
The relative difference between two computed values of time of failure should be less than 5 percent.

Results:
The TPA code was simulated using the procedure outlined for test case 5b. The results are summarized in the following Table.

Summary of Results for Test Case 5b

	Hand-Calculation		TPA Code	
	WP Body	Welds	WP Body	Welds
Start Time (Initiation Time) (yrs)	**750.3702**	**760.2040**	**750.3702**	**760.2040**
Finish Time (Time of Failure) (yrs)	810.3702	820.2040	810.3700	820.1920
Localized Corrosion Failure Time (yrs)	60.0000	60.0000	**59.9998**	**59.9880**
	Ave. 60.0000		Ave. 59.9939	
	Ratio (H-C/TPA) = 1.000102			

The times of failures for the waste package body (WP Body) and the welds (Welds) provided by TPA code are consistent with the values obtained by hand-calculation.

The computed results demonstrate that the failure times by localized corrosion for the WP Body and the Welds are correctly reported by EBSFAIL. This is also supported by the very low value of ratio (-0.010), which is much less than 5 percent as a criterion.

The following Table summarizes the net times at two different values of fraction (i.e., 1 and 0.75) in the case of localized corrosion. As shown in this table, the net times are reduced approximately 25 percent by reducing values of fractions from 1 to 0.75.

Changes of Net Time at Different Specified Failure Depth Threshold in the Case of Localized Corrosion Mode.		
Specified Failure Depth Thresholds (fraction)	Ave. Net Time by Hand-Calculation (yrs)	Ave. Net Time by TPA Code (yrs)

1 0.75	80.0000 60.0000	79.9834 59.9939
Fraction of Changes of Net Time		
-0.25	-0.2500	-0.2499
	Ave. -0.2500	

These results are presented as evidence that this objective has been successfully tested.
Test Results (PASS/FAIL): **PASS**

6. This procedure tested the onset of localized corrosion when drift wall temperature falls below a threshold value. The *tpameans.out* file generated by reference case for TPA Version 5.1a was renamed *tpameansRefCase.out* and used as the *tpa.inp* file. The corrosion potential model for Alloy 22 in the TPA code predicts higher values in low pH environment than in high pH. The repassivation potential model predicts a low value in high chloride and low nitrate concentration solutions. Using these two facts, the following parameters values in *tpa.inp* were changed according to the following table.

Parameter	Value
SeismicDisruptiveScenarioFlag(yes=1,no=0)	0
DriftDegradationScenarioFlag(yes=1,no=0)	0
DSFractionThicknessPenetratedForFailureByCorrosion[]	0
EnvironmentII_Cl_Subarea_3[mol/L]	50.0 mol/L
EnvironmentII_pH_Subarea_3[]	3
EnvironmentII_NO3_Subarea_3[mol/L]	0.01 mol/L
SeepageThresholdT[C]	90 °C

These parameter values ensure that the repassivation potential for localized corrosion initiation is much lower than the corrosion potential at each time step in Environment II. The TPA code was executed for one reference case realization for subarea 3. The time for localized corrosion initiation for mill-annealed and welded material is recorded in files *failt.out* and *weldfail.out*. The drift wall temperature as a function of simulation time is recorded in *nfenv.rlt* for each time step. The simulation time was obtained from the file when drift wall temperature reaches the value of SeepageThresholdT[C] as specified in *tpa.inp*. The corresponding localized corrosion initiation time was obtained from output files *failt.out* and *weldfail.out*. The localized initiation time and the time when drift wall temperature reaches the value of SeepageThresholdT[C] were found to be same.

Pass/Fail criteria

The localized corrosion initiation temperature is at or below the value specified by input parameter SeepageThresholdT[C].

Results:

The tpa code was executed as mentioned above. The drift wall temperature reached to 89.82 °C at time 1723.31 years. The localized corrosion of mill-annealed Alloy 22 started at time 1723.31 years. Similarly, localized corrosion welded material also started 1723.3 years. The results of this test are presented in Figure 5 as shown below. The blue diamond symbols represent the drift wall temperature versus simulation time, the pink and green symbols represent the waste package (mill-annealed Alloy 22) and welded material thickness.

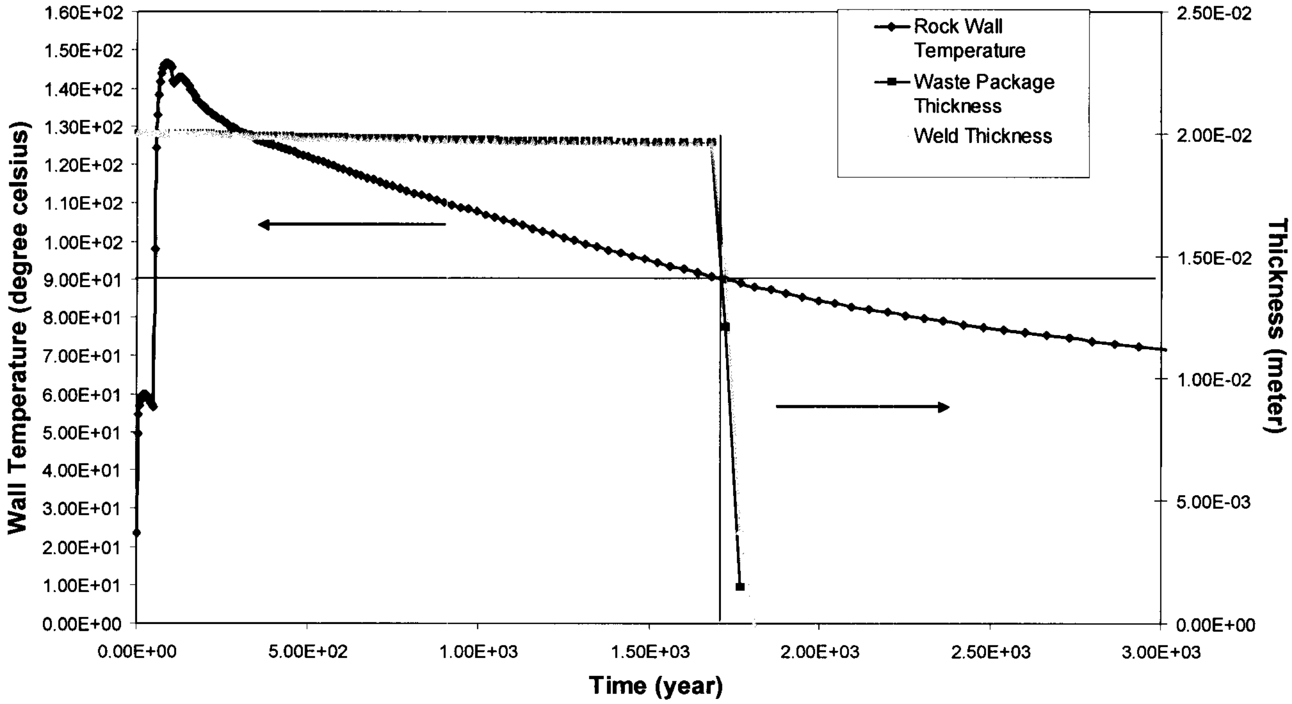

Figure 5: Simulation results for test case 6.

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

REGRESSION TEST FOR VALIDATION

RT#: 2	Project#: 06002.01.354
Software Name: **Total-system Performance Assessment (TPA)**	Version(s): **5.1a**
Test ID: **P-13**	Test Series Name: **Saturated Zone Flow and Transport**

Test Method

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

Test Objective: This is a regression test to maintain assurance in the original validation tests (see Attachment A).

Test Environment Setup

Hardware (platform, peripherals): Desktop PC

Software (OS, compiler, libraries, auxiliary codes or scripts): Windows XP; no auxiliary codes or scripts were used other than a spreadsheet for calculations for comparison to code results;

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

Assumptions, constraints, and/or scope of test:
Scope is limited to evaluating functionality of SZFT module and its outputs.

Test Procedure: See Attachment A.

Test Results

Location: See CD labeled "TPA Version 5.1a Regression Tests for Validation Task P-13."

Test Criterion and Analysis of Results: See Attachment A

Test Evaluation (Pass/Fail): PASS

Notes:

Tester: J. M. Menchaca *J.M. M[signature]*	Date: Sep. 21, 2007

Attachment A

Test Cases for TPA Version 5.1a Regression Tests for Process-Level Validation Task P-13
Objectives, Assumptions, Test Procedures

OBJECTIVES

This is one of the tests of TPA V5.1a that constitutes the regression testing for the validation of the TPA code after the implementation of SCR695. A subset of the previously performed P-13 validation test is performed to satisfy the regression testing requirement for modification of validated code. As described in the Software Validation Plan for TPA Version 5.1, Process-Level Task 13 (P-13), the objectives of the test activities described in this attachment are to verify that

1. Releases to the saturated zone for each repository subarea are assigned to the appropriate stream tube in *strmtube.dat* for use in transport calculations.
2. Repository Partition and retardation coefficients are correctly adjusted to account for reversible colloid transport and correctly reported in *sz_revers.out.*
3. Calculated partition and retardation coefficients for actinides are correctly reported in *sz_kdrd.out.*

The specific issue to be retested by this SVR is #3:

ASSUMPTIONS

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

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

TEST CASES:

The following test addresses the objectives of this SVR.

Test 3: Calculation of Kd and Rd Values

Test 3 Criteria

- Output values of pH and pCO_2 are consistent with input distributions and correlations.
- K_A values (calculated from output K_D values) for the five actinide species Am, Np, Pu, Th, and U, are consistent with the underlying surface complexation model over the input range of pH and pCO_2 values.
- Output for saturated tuff (STFF) effective surface area is correct.
- Conversion of K_D to R_D values for actinide species are correctly computed.
- Calculated K_D values for Cm and Am are the same (i.e., an intentional simplification in the abstraction is that the calculated coefficient for Am is used also for Cm in transport calculations).

Test 3 Description and Results

TPA Version 5.1a was used to run a 500-realization simulation for Subarea 1 only. TPA outputs file *sz_kdrd.out* and *sz_revers.out.* files were examined and used in spreadsheet calculations to ensure correct calculation of retardation coefficients and to conduct graphical comparisons of output to surface complexation model-predicted curves representing specific area normalized distribution coefficient (KA) values for each of the five actinides over a range of pH and at several CO2 values. The following analysis of results is presented in the order of the above-specified criteria.

Check pH and Log-CO_2 Distribution and Correlation

Output values of pH and Log-CO_2 are reported in the *sz_kdrd.out* file. The *tpa.inp* input files specifies that these outputs should be correlated with a correlation coefficient value of −0.95. The plot in figure 1 shows a regression of pH and Log-CO_2. The calculated correlation coefficient for these values is −0.947770, which is very close to the specified value. Additionally, the output values are within the ranges of user-specified values in the *tpa_include.inp* file.

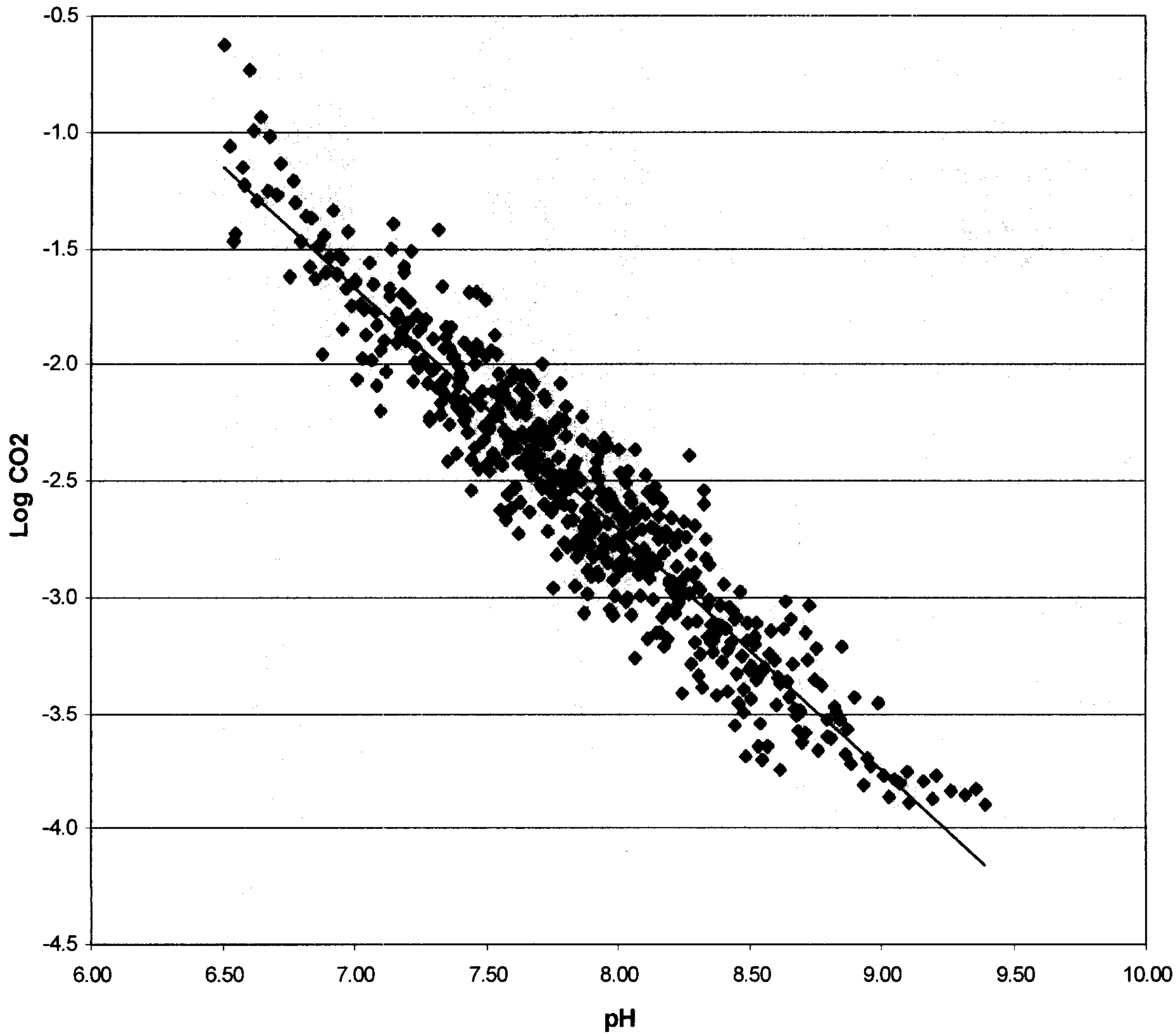

Figure 1. Correlation of pH and Log-pCO_2

<u>Check Calculated K_A Values</u>

The next step was to evaluate whether K_A values for the five actinide species Am, Np, Pu, Th, and U, are consistent with the underlying surface complexation model. This was done by first converting the output K_D values (in m^3/kg) for Am, Np, Pu, Th, and U to K_A values (in ml/m2) by dividing by specific surface area (ssarea) and a factor of 10^{-6}. These K_A values were then compared to the surface complexation model K_A curves for each of the five actinides over a range of pH and pCO_2. The surface complexation model curves are produced by the same data used to generate the information contained within the *coefkdeq.dat* auxiliary file. Generated K_A values for each of the five actinides should plot within the sorption envelope produced by the surface complexation model predicted K_A curves. Note that all K_A values should plot between below the envelope for Log pCO_2 = −4.0 and above the envelope for Log pCO_2 = −0.5. Figures 2–6 below show that the K_A values fit the desired profile and, hence, the K_D properly represent the underlying model. The spreadsheet file named *sz_kdrd_TPA51a.xls* contains the calculations for conversion of output data to K_A values and generation of Figures 1–6.

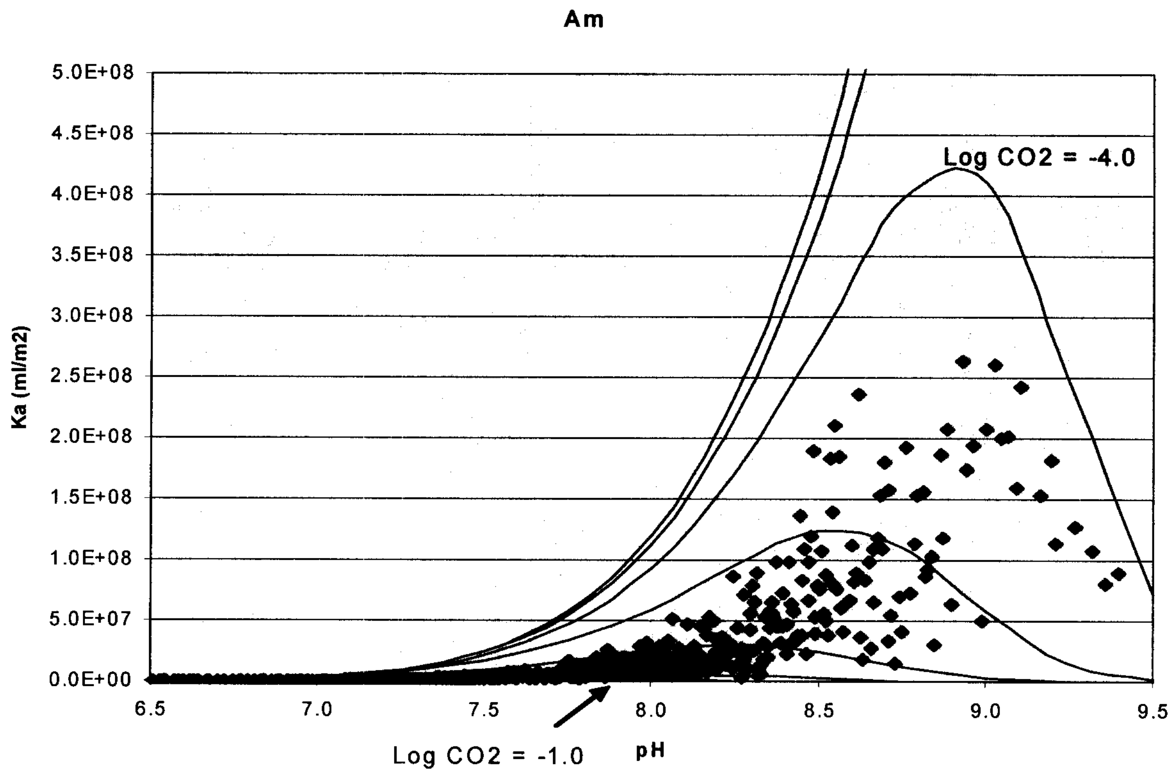

Figure 2. Plot of K_A values for Am, compared to complexation model envelopes.

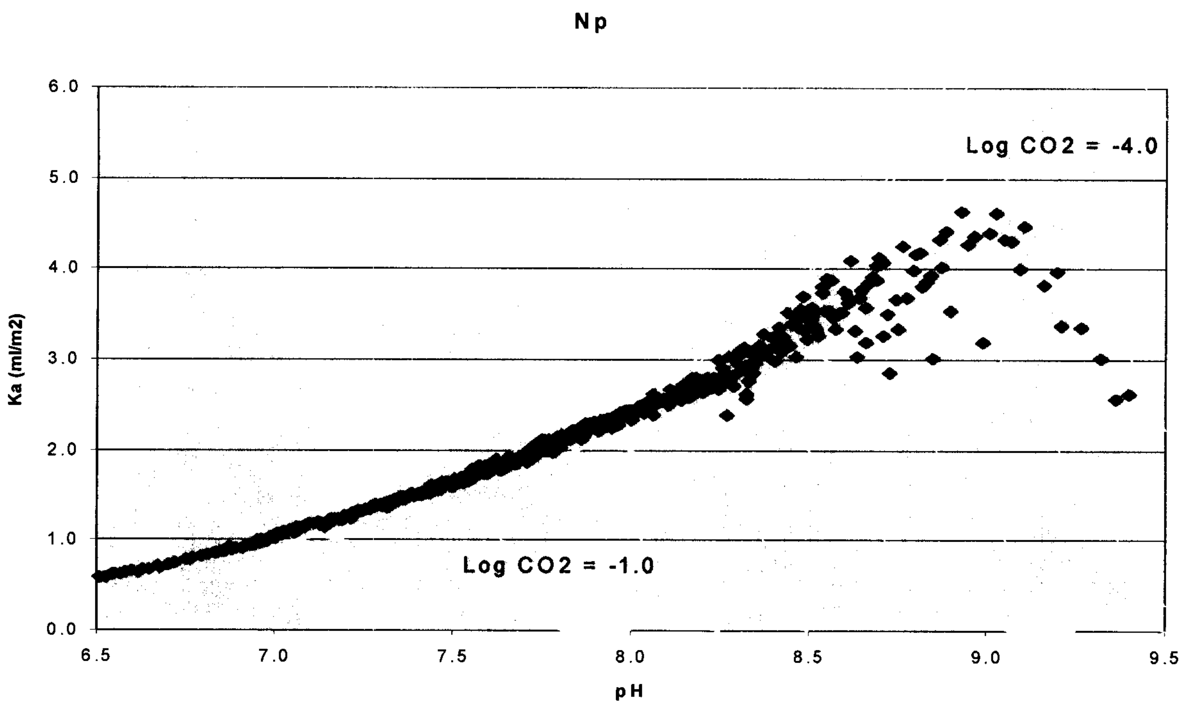

Figure 3. Plot of K_A values for Np, compared to complexation model envelopes.

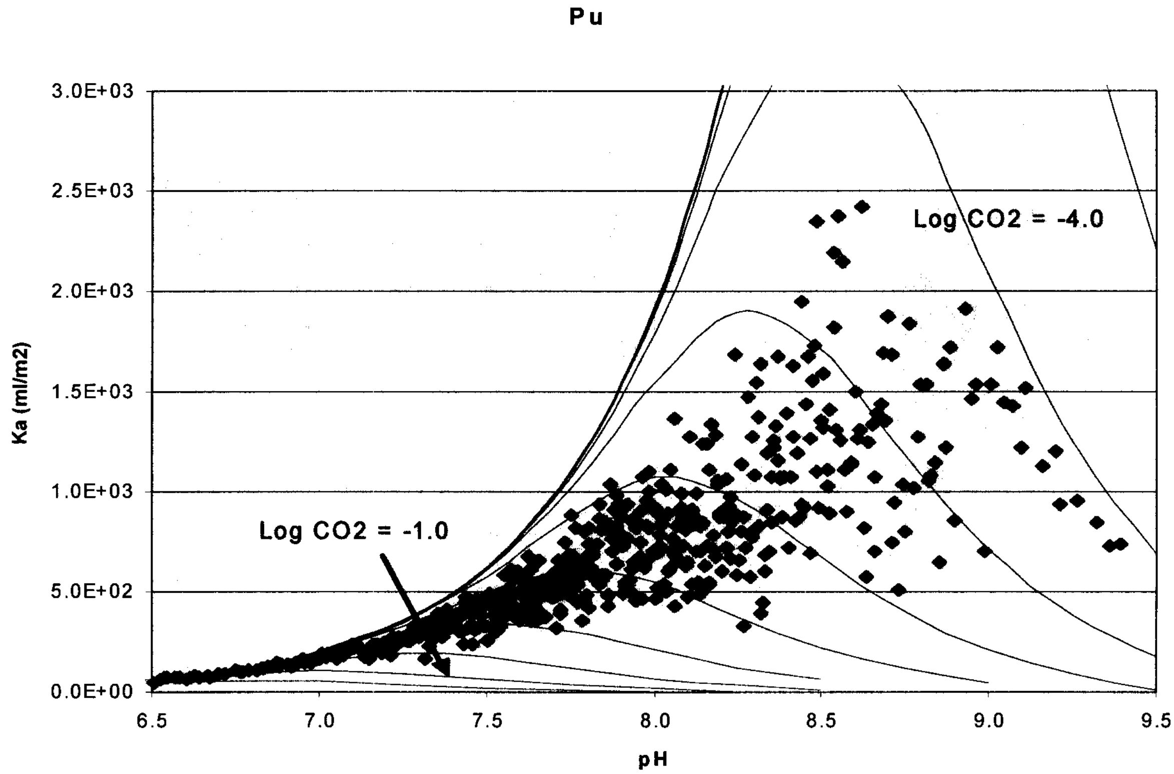

Figure 4. Plot of K_A values for Pu, compared to complexation model envelopes.

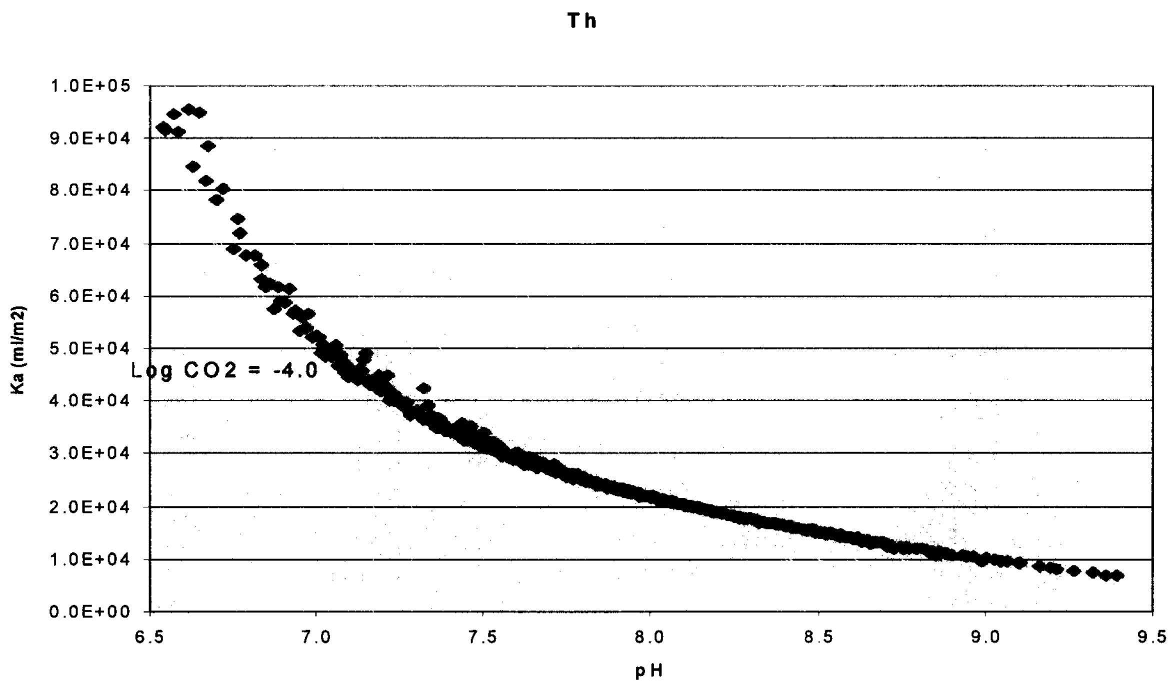

Figure 5. Plot of K_A values for Th, compared to complexation model envelopes.

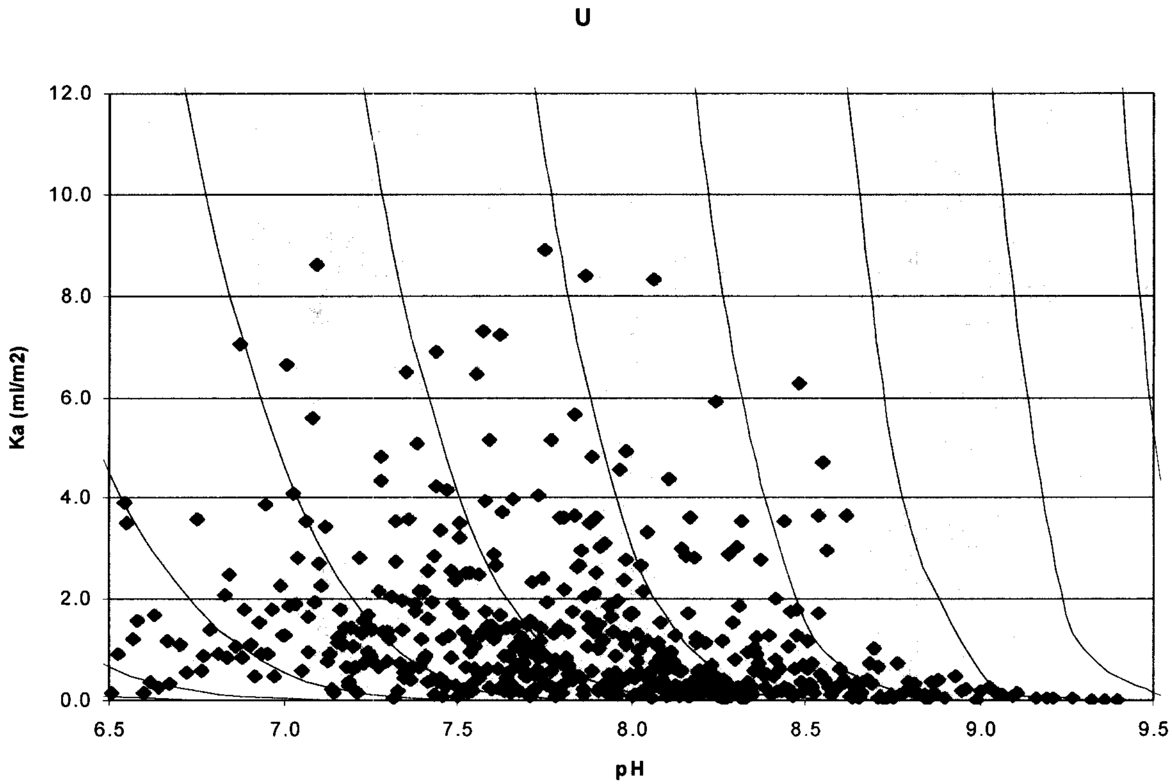

Figure 6. Plot of K_A values for U, compared to complexation model envelopes.

Check Saturated Tuff Effective Surface Area

Calculations to verify that output for saturated tuff (STFF) effective surface area is correct were performed using the equation:

$$ESA = \frac{3\theta}{\rho(1-\theta)r}$$

where

ESA = effective surface area (m^2/kg)

θ = porosity (ImmobilePorosity_STFF)

ρ = grain density (kg/m^3) (ImmobileGrainDensity_STFF)

r = pore radius (m) (ImmobilePoreRadius_STFF)

ImmobilePorosity_STFF, ImmobileGrainDensity_STFF, and ImmobilePoreRadius_STFF are assigned constant values of 0.2, 2470 kg/m^3, and 5.0E-8 m, respectively, in the *tpa.inp* file. Based on the above equation, these values yield ESA = 6,073 m^2/kg, which is identical to the output value reported for the tuff transport leg in *sz_kdrd.out* (this parameter is identified as 'ssarea' in the TPA files).

Check Conversion of K_D to R_D Values for Actinide Species

Calculations to verify TPA correct conversion from K_D to R_D for the actinide species were performed using the equation:

$$R_D = 1 + \frac{\rho(1-\theta)}{\theta} K_D$$

where

R_D = retardation factor

K_D = distribution coefficient

ρ = grain density

θ = porosity

Using the K_D, porosity, and density values reported in the *sz_kdrd.out* file R_D was calculated by hand using the above equation and compared the reported R_D value in *sz_kdrd.out*. These hand calculations were performed only for the first two lines of *sz_kdrd.out* file, which represent tuff matrix and alluvium for the first realization of the simulation; since all realizations perform the same calculation, there was no need to repeat for other realizations. The hand calculations produced R_D values identical to those reported in *sz_kdrd.out*.

Check that K_D values for Cm and Am are the Same

The K_D and R_D values for Cm are not reported in the *sz_kdrd.out* file, but the R_D values for tuff and alluvium are written to the NEFMKS input file *nefii.inp* for use in transport calculations. Below is an excerpt from the *nefii.inp* file, which represents the NEFMKS input for the 500th realization of the simulation. In this excerpt, Element Index 1 represents Cm and Index 3 represents Am; Leg 2 is tuff and Leg 3 is alluvium. It can be seen that the highlighted R_D values below for Cm and Am are identical. These R_D values also reflect the correction to account for the effects of reversible sorption to colloids, which are reported in the output file *sz_revers.out* (See for Test 2 for discussion of the correction for colloid effects).

ELEM. INDEX	SOLUBILITY (KG/KG)	LEG #	MOBIL RD	IMMOBILE RD	MASS XFER MOD FACTOR
1	0.000E+00	1	0.248E+02	0.100E+01	0.139E-02
		2	0.248E+02	0.993E+07	0.139E-02
		3	0.241E+07	0.100E+01	0.000E+00
2	0.000E+00	1	0.108E+01	0.100E+01	0.992E+00
		2	0.108E+01	0.167E+02	0.992E+00
		3	0.180E+02	0.100E+01	0.000E+00
3	0.000E+00	1	0.248E+02	0.100E+01	0.139E-02
		2	0.248E+02	0.993E+07	0.139E-02
		3	0.241E+07	0.100E+01	0.000E+00

Test 3 Evaluation (Pass/Fail): PASS