Scientific Notebook No. 170E: Total Performance Assessment (TPA) 3.2 Development (April 3, 1996 through September 16, 2003)

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by

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INITIAL ENTRIES

Scientific Notebook: #170

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Account Number: 20-5708-762

Title: TPA

Participants: George Adams

April 1, 2002, GADAMS:
The objectives of this task are in accordance with SCR Number: PA-SCR-346 and section 2.1 of the Software Requirements Description for the Total-System Performance Assessment Version 5.0 code. The objectives are: "C3 Add shallow infiltration variance factor in UZFLOW."

The approach to achieving the objectives will be in accordance with the Software Development Plan for the Total-System Performance Assessment Version 5.0 Code. C3-Add shallow infiltration variance factor in UZFLOW is referenced in section 3.1.3.

Qualifications: Proficiency in developing, implementing and testing FORTRAN 77 code.

For this coding effort, TPA code was checked-out in accordance with configuration procedures identified in the Software Development Plan for the Total-System Performance Assessment Version 5.0 Code. During software development, the TPA code was placed on the following machine: GRADAMS2.datasys.swri.edu. This is a Microsoft Windows 2000 laptop. The source code directory is: c:\CNWRA\tpa.

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The software development directory is: c:\CNWRA\Project_20-1402-762\PA-SCR-346. Software will be developed on this machine using the Lahey-Fujitsu FORTRAN 95 v5.6 development environment.

In-Process Entries

April 2, 2002, GADAMS:
Performed the following code moudule modifications in addition to those specified in PA-SCR-346:
Module itym - Removed calls to get_data_file. This routine was removed from itymutils.f. It generated a compiler warning: istatus is used but never set.

Module estimator - (within print_summary) Removed references to vMAT and vMAP. These two variables generated the following compiler warning: vMAT/vMAP is used but never set. (Within calc_MAI_table) The variable nDEM was referenced in a "do" loop. The reference generated the following compiler warning: nDEM is used but never set. The variable nDEM was replaced with mnDEM. (Within calc_MAI_DEM) Added a print statement to display the results for each realization. This allows the operator to see that the program is progressing towards a reslult.

Module itymutils - Removed module get_data_file. The calling module itym.f had the calls commented out, and get_data_file generated the compiler warning message istatus is used but never set. (Within tailDTBL) Removed ztype and zfile. These two arguments created the following compiler errors: Variable ztype/zfile with asterisk length specification must be a dummy argument.

Module uncertain - (within get_par_maps) Modified sixth argument in call to set_1par_map. The following run-time error occurred: The subscript or substring iTab is out of the specified range (reference value: 1,6, specification value: 1:1, 1:5). (Within set_1par_map) Changed the value of the sixth parameter from the caller to prevent an array index out of bounds run-time error. (Within map_cover_bedrock _pairs) Changed call check_i_le to check_ii_le and changed the order of parameters.

The following run-time errors were obtained: The reference and definition numberr of arguments is different (actual number: 5, dummy number: 4). ***>>> Error in map_cover_bedrock_pairs <<<*** nCurCBTab .le. MnCBTrow nCurCBTab = 1 mnCBTrow = 1600

Module zportpc - (within ZPORTFDATEFUN) Removed assignment of DateString(1:1) = TimeZoneString(1:1). This assignment generated the following run-time error: The variable (TimeZoneString(1:1)) has an undefined value.

April 9, 2002, GADAMS:
Modified module SEISMO to remove references to sh. References to sh generated linker errors.

Modified module ZPORTPC. Changed function GETENV to a subroutine.

April 11, 2002, GADAMS:
Module estimator - (within print_summary) Added input parameters vMAT and vMAP. This change was recommended by SS per e-mail 4-5-02. (Within calc_MAI_table) The following line was added: nDEM = nint(BaseDEMStat(mDEMnxy). This change was recommended by SS per e-=mail 4-5-02. (Within do_all_cover_bed_pairs) Modified the argument list to include the array indices '(1)'. Otherwise, the following run-time error was generated: An attribute of argument 2 is inconsistent (actual argument pixK: array name, dummy argument pixK: scalar variab). Change made in call to calc_soil_params.

Module itym - Modified the calls to retrieve the current time. The functions zporttime and zportctime were used instead of the call to zportfdate. Time was not printed out in output files. Uncommented the calls to get_data_file per SS recommendation on e-mail 4-5-02. Within these calls, added an additional call using zMASWtbl and substituted zBUnitDEM, zSUnitDEM, and zSUnitDEM for current parameters. Concurrence from SS by e-mail 4-10-02.

Module itymutils - Resotored module get_data_file. Uncommented calls within this module to zportsh per recommendation from SS by e-mail 4-5-02.

Module uncertain.f - (Within get_par_maps) Modified the calls to set_1par_map to include the additional parameters: mnClTcol, ... This change was recommended by SS per e-mail 4-5-02. (Within set_1par_map) Modified the parameter list to include the additional parameter nTcol). This change was recommended by SS by e-mail 4-5-02.

Module uzflow - (calc_mai) - Replaced calc_mai with a new routine received from SS by e-mail 4-11-02. The following was documented within this routine, "replaced interpolation of log10(E[MAI]) with sampled values based on E[log10(MAI)] and std[log10(MAI)] and converted interpolation to use inline function."

4-23-02 GADAMS:
Code modules in addition to UZFLOW will be edited and documented in this scientific notebook. Previous entries applied to the UZFLOW and ITYM code. In future entries, the code module will be referenced along with the date.

4-23-02 weldfailt, GADAMS:
WP2 - Weld Corrosion

The objectives of this task are in accordance with SCR number PA-SCR-365 and Section 3.1.7 of the Software Development Plan for the Total-System Performance Assessment Version 5.0 Code and Section 2.4 of the Software Requirements Description for the Total-System Performance Assessment Version 5.0 Code.

For this development effort, new code modules were developed. These modules are described as follows: weldfailt.f, SelectCorrRate.f, CorrFunctions.f, corrPot.f, and library modules int.f, linearInterp.f, and searchPosition.f.

Qualifications for performing this work are proficiency in developing, implementing, and testing FORTRAN 77 code.

The code modules were modified to read the number of time steps in file "ebstrhc.inp" and initialize the arrays with tihis number of time steps.

A new input file was added, "deltaEcOL.inp". This file provides an offset or additive value to the critical potential for each time step.

During software development, the code was placed on the following machine: GRADAMS2.datasys.srwri.edu. This is a Microsoft Windows 2000 laptop. The software development directory is: c:\CNWRA\Project_20-1402-762\PA-SCR-365. Software will be developed on this machine using the Lahey-Fujitsu FORTRAN 95 v5.6 development environment.

4-25-02 weldfailt PA-SCR-365 GADAMS:
Testing was performed on the following process level tests: PL-1, PL-2, and PL-3. Testing was performed in accordance twith the Test Plan for TPA SCR#365. The following compurter was used for the tests: Host Machine: PITOR (domain CNWRA), Windows NT 4.00.1381. The testing was performed by GADAMS with verification of corrosion potential and critical corrosion potential performed by Osvaldo Pensado for test PL-3. This verification was performed using Mathematica. The code modules successfully passed all three process level tests.

5-3-02 dsfail/dsfailt PA-SCR-348 GADAMS:
The objectives of this task are in accordance with SCR Number: PA-SCR-348 and section 2.3 of the Software Requirements Description for the Total-System Performance Assessment Version 5.0 Code.

For this development effort, one new standalone module was developed, "dsfailt." In addition, a new module was integrated into the TPA code. The integrated module is "dsfail." Software development was performed on the following machine: GRADAMS2.datasys.swri.edu. The software development directory was c:\tpabuild_348(DS1).

Qualifications for performing this work are proficiency in developing, implementing, and testing FORTRAN 77 code.

Module dsfail is called by the executive (module exec). Module dsfail then creates the input files, "fluoride.dat" and dsfailt.inp for use by the standalone module dsfailt.

Fluoride concentration values were obtained from multiflo.dat. An additional fluoride column was added to this file. After creating the input files, module dsfail invokes module dsfailt. After dsfailt executes, module dsfail retrieves the drip shield thickness versus time from the dsfailt output file dsfailt.out. These values for drip shield thickness versus time are then returned to the executive.

Both process level and system level (integration testing) was successfully completed in accordance with test plan, "Test Plan for TPA SCR#348." Testing was performed on the following machine: PITOR (domain CNWRA). The Host OS is: Windows NT 4.001381. Test results were archived in directory: c:\PROJ-1402-762\PA-SCR-348 on this machine.

5-13-02 dsfail/dsfailt PA-SCR-348 GADAMS:

The previous testing with this module did not include poundary level testing. Therefore the test plan was modified to include one additional process level test, PL-4, and one additional system level test SL-2. The process level test, PL-4, verified that the module would work correctly if drip shield thickness is set to 0 or negative. It also verified the module would operate correctly at invalid input parameters such as fluoride minimum greater than fluoride maximum. Both process level and system level testing was successfully completed in accordance with test plan, "Test Plan for TPA SCR#348." This test plan was updated from the previous test to include test PL-4 and test SL-2. Testing was performed on the following machine: PITOR(domain CNWRA). The Host OS is: Windows NT 4.001381. Test results were archived in directory: c:\PROJ-1402-762\PA-SCR-348(DS1) on this machine. Previous test results were moved to a subdirectory of this one labeled, "Testing050302."

5-14-02 weldfail/failt PA-SCR-365 GADAMS:

Module weldfailt was renamed weldfail to make it less than or equal to 8 characters. Module weldfail was rewritten to be a subroutine instead of a standalone module. Weldfail was integrated into module failt. For this integration, the weldfail module and associated TPA code was placed in directory, "c:\tpabuild_365(WP2)." Software development for this module is being performed in this directory on machine, "GRADAMS2.datasys.swri.edu."

5-28-02 weldfail/failt PA-SCR-365 GADAMS:
The output file for failt, ebstrh.dat, was setup to pass drip shield failure and weld/waste package failure information to releaset. Module releaset retrieves this failure information for use in its qin calculation. Two subroutines were added to releaset. The first one, getDSFactor, retrieves the drip shield factor used in modifying the calculation for qin. The second one, getWeldWPFactor, retrieves the weld/waste package factor used in modifying the calculation for qin.

5-29-02 itym/uzflow PA-SCR-346 GADAMS:
The software development and code directory was changed to c:\tpabuild_346(C3) on machine GRADAMS2.datasys.swri.edu. An error was discovered in the itym preprocessor code when the code was run at 1000 realizations and 16 tables. The following error occurred: ***>>> Error in sample_unctab_props <<<***. A modification was made to subroutine sample_unctab_props within the uncertain.f code module to set the constant mntry to a value of 100. With this change, convergence occurred at 1000 realizations.

5-29-02 releaset PA-SCR-394 GADAMS:
The objectives of this task are the following: To extract additional information from the RELEASET module and store this information in the ebsrel.rlt file. The following additional information is needed: 1) waste package fill-up time 2) the period over which the solubility limit is activated for each nuclide, and 3) the spent fuel dissolution time.

During software development, the code was placed on the following machine: GRADAMS2.datasys.swri.edu. The software development and source code directory is: c:\tpabuild_394. Software will be developed on this machine using the Lahey-Fujitsu FORTRAN 95 v5.6 development environment.

6-5-02 dsfail/dsfailt PA-SCR-395 GADAMS:
The objectives of this task are the following: 1) Initialize the fraction of failed drip shields versus time array, 2) modify dsfail tpa.inp parameters to spell-out names and units, and 3) include a group of files (dcagw.ech, dcf.cum, ebsfail.rlt, ebsrel.rlt, nfenv.rlt, szft.rlt, uzflow.rlt, and uzft.rlt) for post processing. This group will be

included as an append option in tpa.inp.

During software development, the code was placed on the following machine: GRADAMS2.datasys.swri.edu. The software development and source code directory is: c:\tpabuild_395. Software will be developed on this machine using the Lahey-Fujitsu FORTRAN 95 v5.6 development environment. The baseline software release is 4.2 retrieved as the current software version using UNIX script gettpa on 6-4-2.

6-5-02 releaset PA-SCR-394 GADAMS:
Code changes were integrated into baseline software release 4.2 retrieved as the current software version using the UNIX script gettpa on 6-4-02. The code was modified such that relcum.out was expanded to include waste package fill time, and dissolution time for a subarea and this information was retrieved by the EXEC module to place in ebsrel.rlt. In addition, waste package fill time and dissolution time were placed in relfrac.ut for retrieval by ebsrel. Solubility limit affected information was placed in trelease.out, ebsnef.dat and ebsnef2.dat. The code modules exec, ebsrel, ebsfilt, and releaset were modified to incorporate the changes.

The code modules were tested in accordance with process level test PL-1 and system level test SL-1 included in Test Plan for TPA SCR*394. The code modules passed both tests. For process level test pl-1, releaset produced the required additional information of dissolution time, waste package fill time, and solubility limit affected. It placed this information correctly in file relfrac.out, relcum.out, ebsnef.dat, and trelease.out. For process level test pl-1, the information was correctly stored. For system level test sl-1, the additional information produced by releaset was correctly processed and stored in ebsrel.rlt. This includes subarea averages for solubility limit affected and number of cycles. It includes correct waste package fill time data and dissolution time retrieved from subareas and summarized at the end of ebsrel.rlt.

6-10-02 dsfail/dsfailt PA-SCR-395 GADAMS:
Successfully completed the testing of this module in accordance with Test Plan for TPA SCR#395. This test plan includes 4 process level tests designed to verify that dsfailt can correctly return drip shield thickness and failure information. In addition, three system level tests were performed to verify that module dsfailt was correctly

integrated into the code along with its companion module dsfail. Additionally, one of the system level tests sl-3 verifies that files required by the graphical post-processor could be generated. Additionally, bug fixes were added to the code and are identified as follows: 10 Set the failure time in dsfailt when the drip shield thickness is zero. Previously, the code would ablort if the failure time was not initialized for this case. 2) Send output from module dsfailt to dsfailt.dat instead of dsfailt.out. Otherwise, screen output messages from dsfailt would appear on the screen when screen captures were performed on UNIX boses. 3) The initialization flag passed to dsfail was incorrect. EXEC needed to check istartreal for the realization number instead of checking the starting realization against 1. 4) On pcs, the 'cat' command could not be successfully executed. Changed the command to 'type' in zportpc.

Testing of the changes was performed on spock, SUN Ultra-4 server unsder Solaris 5.8. Output files were compared to previously generated output files generated under PA-SCR-348. This comparison was done to verify that changes did not affect previous output results.

6-11-02 releaset PA-SCR-394 GADAMS:
Moved the code that was previously integrated into version 4.2d to c:\tpabuild_394\backup and integrated the code changes into release 4.1k of the software. For this new integration, the development directory remained the same at c:\tpabuild_394 on machine GRADAMS2.datasys.swri.edu.

Moved the test results for the previous integration of the code into version 4.2d to $HOME/PA-SCR-394/integration4.2d. Tested the new integration into 4.1k on machine spock in accordance with Test Plan for TPA SCR#394. This is the same test plan that was previously executed for the integration into 4.2d. The new integration into 4.1k successfully passed the process level test pl-1 and the system level test sl-1. The module releaset successfully generated the solubility limit affected, dissolution time and waste package fill time. For system level test sl-1, the ebsrel.rlt file showed the correct averages for waste package fill time and solubility limit affected. It also showed the correct minimum and maximum for waste package fill time. In addition, this result file showd the accumulated dissolution times across all realizations and subareas.

The new release of the code with these changes integrated will be identified as version 4.1.1.

6-14-02 PA-SCR-394 GADAMS:
Modified version 4.1.1 of the tpa code, module releaset to generate values for sareat, total internal surface area in the wetted porton of spent fuel. A single realization test was performed and included in directory c:\tpatest_394\test6-13-02 and a mean value test was performed and included in directory c:\tpatest_394\test6-14-02. Both directories are on GRADAMS2.datasys.swri.edu.

6-20-02 PA-SCR-365 weldfail/failt GADAMS:
Modified code modules under this SCR were integrated into release 4.2d of the tpa code and tested. Testing was performed in accordance with Test Plan for TPA SCR#365. Testing was performed on machine spock. This machine is a SUN Ultra-4 Server with Solaris 5.8.

The testing of the code changes was successfully completed. The testing involved four process level tests and two system level tests. The process level tests were designed to verify that the welfail and failt modules could produce the correct results. The system level tests were designed to verify that output from these modules could be retrieved for use in releaset. Test results were archived in directory $HOME/PA-SCR-365/pltest/pl1,2,3,4 and $HOME/PA-SCR-365/pltest/sl-1,2. These test results are on machine spock.

6-25-02 PA-SCR-394 GADAMS:
The test results and code for this SCR were moved to directory $HOME/PA-SCR-394/integration4.1.1 on machine spock. This directory contains the baseline integrated code and test results for the initial integration into version 4.1k of the tpa code.

6-27-02 PA-SCR-394 GADAMS:
Made additional modifications to the code and placed the changes on machine spock in directory $HOME/VERS, correction, in directory $HOME/PA-SCR-394/VERSION4.1.1CHG1. The following additional changes swere incorporated: 10 The total internal surface area in the wetted portion of the spent fuel was added to

ebsrel.rlt. 2) The dissolution times for all 8 failure types was added to ebsrel.rlt. 3) The code was cleaned up with large time dependent arrays removed from releaset. This change allows the code to operate at time steps greater than 401.

The code changes were tested in accordance with Test Plan for TPA SCR#394 as was done for the baseline version. The code change successfully passed the process level and system level test and results were archived on machine spock in directory $HOME/PA-SCR-394/VERSION4.1.1CHG1.

7-2-02 PA-SCR-394 GADAMS:
Made additional modifications to the code and placed the changes on machine spock in directory $HOME/PA-SCR-394/VERSION4.1.1CHG2. The following additional changes were incorporated: 1) Changed the waste package fill time to the difference between the time the release rate goes positive and the time of initial failure. Formerly, the fill time used the total release which was affected by the initialization parameters. 2) Modified the solubility limit affected flag to only be set when flowrate out of the waste package (qout) is greater than 0. This avoids the flag being set where the initialization parameters are affecting the results.

The code changes were tested in accordance with Test Plan for TPA SCR#394 and the test results were archived on machine spock in directory $HOME/PA-SCR-394/VERSION4.1.1CHG2. The code successfully passed the process level test, pl-1, and the system level test, sl-1.

Additionally, three separate teste were performed on the code. The first test, TEST1, used 5 realizations of equal time steps over 10 thousand years. The second test, TEST2, used 100 realizations of equal time steps over 100 thousand years. And, the third test, TEST3, used the mean data over 10 thousand years. Results were archived in directory $HOME/PA-SCR-394/run/TEST7-1-02 on machine spock. These tests produced output results which showed the changes to solubility limit affected and waste package fill time.

7-3-02 PA-SCR-394 GADAMS:
The change to the releaset module in which solubility limit affected is set if qout is

greater than zero has a significant effect on the output results over a 10,000 year analysis period. Therefore, an additional test was performed similar to the test on 7-2-02 TEST2. In this test, however, the simulation period was limited to 10,000 years instead of 100,000 years. The number of realizations was kept at 100. This test was identified as TEST1 and the results have been archived in directory $HOME/PA-SCR-394/run/TEST7-2-02. The code for which this test has been run was archived in directory $HOME/PA-SCR-394/VERSION4.1.1CHG2. The code and test results are located on machine spock. The test revealed that the following radionuclides are solubility limited: U-238, U-234, Pu-239, Pu-240, Nb-94, Am-241, Am-243, Np-237, Th-230, Cm-246, Cm-245, and Ra-226. The following radionuclides are not solubility limited: Pb-210, Cs-135, I-129, Tc-99, Ni-59, Se-79, and Cl-36.

7-8-02 PA-SCR-365 GADAMS:

The following parameters were added as part of this SCR:

Parameter	Value	Reference
DripShieldTimeMark[yr]	10000	Configuration parameter no reference
WPWeldThickness[m]	3.50e-2	Lid thickness (25 mm outer lid + 10 mm inner lid, CRWM M&O, 2000, p. 21)
StandardExchangeCurrOxygen Reduction[C/(m^2 yr)]	1.232E-25	Assumed value derived from information information in Bockis and Reddy (1970), Calvo (1997), and Calvo and Schriffrin (1988)
EquilibriumPotentialOxygenReduction[VSHE]	1.229	Bard and Faulkner, 1980, p. 701
ErpInterceptWeld[mVSHE]	1541.2	Brossia et al., 2001, p. 3-34
TempCoefOfErpInterceptWeld [mVSHE/C]	-13.1	Brossia et al., 2001, p. 3-34
ErpSlopeWeld[mVSHE]	-362.7	Brossia et al., 2001, p. 3-34
TempCoefOfErpSlopeWeld[mVSHE/C]	2.3	Brossia et al., 2001, p. 3-34

FractionWeldSurface[]	0.004	Fraction derived from data in CRWM M&O, 2000. Calculation follows: waste package surface area[m^2] = 2 * pi{3.1416} * radius of waste package[m]{0.782, CRWM M&O, 2000, p. 36 and Table 1} * length of waste package[m]{4.775, CRWM M&O, 2000, p. 36 and Table 1} + 2 * pi * radius of waste package ^ 2 weld surface area[m^2] = 2 * pi * radius of waste package * Weld thickness by direct measurement of official DOE weld[m]{0.02} fraction weld surface = weld surface area / waste package surface area

References:
Civilian Radioactive Waste Management System, Management and Operating Contractor.
WAPDEG Analysis of Waste Package and Drip Shield Degradation, Rev 00 ICN 01. 11/9/2000
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7-9-02 PA-SCR-365 GADAMS:

Integrated drip shield thickness from the version 4.2d release into the code modules for this SCR. The code modules that changed were exec.f and seismo.f. Previously, seismo computed a drip shield thickness but this was only temporary until the drip shield thickness from dsfail was integrated into the code. Now, module seismo receives the drip shield thickness versus time produced from dsfail/dsfailt.

7-15-02 PA-SCR-365 GADAMS:
Three TPA input parameters were changed to spell out their names. This change affected module EBSFAIL and the tpa.inp file. The parameters that changed are the following: 1) StandardExchangeCurrOxygenReduction[C/(m^2 yr)] was changed to StandardExchangeCurrentDensityforOxygenReduction[C/(m^2 yr)]. 2) TempCoefOfErpInterceptWeld[mVSHE/C] was changed to TemperatureCoefficientOfErpInterceptWeld[mVSHE/C]. 3) TempCoefOfErpSlopeWeld[mVSHE/C] was changed to TemperatureCoefficientOfErpSlopeWeld[mVSHE/C].

7-16-02 PA-SCR-394 GADAMS:
Incorporated additional changes into the code. The following additional changes were made: 1) Configured the code modules to use a maximum number of time steps defined in maxntime.i. The value set for the maximum number of tiem steps was 2001. 2) Performed additional code cleanup on module releaset. Eliminated variables that were no longer being used. Also eliminated redundant variable arrays. Performed regression testing on the software and added one additional system level test (SL2) to the test plan (Test Plan for PA-SCR-394). The additional system level test is designed to verify that the results obtained in ebsrel.rlt are comparable to those obtained at 251 time steps. The updated code successfully passed the process level test pl1 and the system level tests sl1 and sl2. This code update and test results are archived on machine spock in directory $HOME/PA-SCR-394/VERSION4.1.1CHG3.

7-23-02 PA-SCR-374 GADAMS:
Performed formal testing of the software in accordance with Test Plan for TPA SCR #374. Testing was performed on machine spock under Sun Solaris 5.8. The baseline version of the code for the SCR change was 4.1j. The tested version was 4.2d. The code module that changed for this SCR was uzft.f. The testing involved one function level test FLT1 and four system level tests, SLT1, 2, 3, and 4. The software successfully passed the function level test and all system level tests. The TPA code was built on machine spock in directory $HOME/PA-SCR-374. Testing was performed in directory $HOME/PA-SCR-374/test. Test results were archived on a CD labeled, "Test Plan and Test results for TPA SCR #374, 7-23-02."

7-25-02 PA-SCR-394 GADAMS:

The test results for the entry identified as 7-3-02 PA-SCR-394 GADAMS conducted under this SCR are summarized in the following table. This test was conducted using the bathtub model.

Averages over all realizations and subareas(Ordered by average length of time release is solubility-limited)

Nuclide	Average Number of Time Steps with Solubility Controlling	Average length of time release is solubility-limited[yr]	Time span (out of 10,000 years) over which the nuclide is solubility Limit-controlled	Ranking by the average length of time release is solubility-limited	Average Number of Cycles Release Switches from Solubility-Limited to Dissolution-Limited	Ranking by the average number of cycles release switches from solubility limited to dissolution-limited
U238	2.4480E+01	1224.000	12.2%	1	1.0000E-03	9
U234	2.4480E+01	1224.000	12.2%	1	1.0000E-03	9
Pu239	2.4474E+01	1223.700	12.2%	3	1.0000E-03	9
Pu240	2.4474E+01	1223.700	12.2%	3	1.0000E-03	9
Nb94	2.3884E+01	1194.200	11.9%	5	1.8000E-02	8
Am241	2.1310E+01	1065.500	10.7%	6	7.3000E-02	6
Am243	2.1310E+01	1065.500	10.7%	6	7.3000E-02	6
Np237	1.5297E+01	764.850	7.6%	8	1.4900E-01	1
Th230	1.0261E+01	513.050	5.1%	9	1.4200E-01	4
Cm246	5.7150E+00	285.750	2.9%	10	1.4300E-01	2
Cm245	5.7150E+00	285.750	2.9%	10	1.4300E-01	2
Ra226	4.7270E+00	236.350	2.4%	12	8.0000E-02	5
Pb210	0.0000E+00	0.000	0.0%	13	0.0000E+00	13
Cs135	0.0000E+00	0.000	0.0%	13	0.0000E+00	13
I129	0.0000E+00	0.000	0.0%	13	0.0000E+00	13
Tc99	0.0000E+00	0.000	0.0%	13	0.0000E+00	13
Ni59	0.0000E+00	0.000	0.0%	13	0.0000E+00	13
Se79	0.0000E+00	0.000	0.0%	13	0.0000E+00	13
Cl36	0.0000E+00	0.000	0.0%	13	0.0000E+00	13

7-25-02 PA-SCR-394 GADAMS:

Performed two tests using the flowthru model instead of the bathtub model. The first test, test1, used the mean data set with uniform time steps of 50 years over a period of 10,000 years. The second test, test2, used 100 realizations with uniform time steps of 50 years over a period of 10,000 years. VERSION4.1.1CHG2 of the TPA code was used for these tests. The tests were performed on machine spock in the following directories: $HOME/PA-SCR-394/run/TEST7-25-02/TEST1 and $HOME/PA-SCR-394/run/TEST7-25-02/TEST2. The results for test2 are summarized in the following table.

Averages over all realizations and subareas(Ordered by average length of time release is solubility-limited)

Nuclide	Average Number of Time Steps with Solubility Controlling	Average length of time release is solubility-limited[yr]	Time span (out of 10,000 years) over which the nuclide is solubility Limit-controlled	Ranking by the average length of time release is solubility-limited	Average Number of Cycles Release Switches from Solubility-Limited to Dissolution-Limited	Ranking by the average number of cycles release switches from solubility limited to dissolution-limited
U238	4.1493E+01	2074.650	20.7%	1	1.0000E-03	14
U234	4.1493E+01	2074.650	20.7%	1	1.0000E-03	14
Pu239	4.1487E+01	2074.350	20.7%	3	1.0000E-03	14
Pu240	4.1487E+01	2074.350	20.7%	3	1.0000E-03	14
Nb94	4.0897E+01	2044.850	20.4%	5	1.8000E-02	12
Am241	3.8348E+01	1917.400	19.2%	6	7.2000E-02	8
Am243	3.8348E+01	1917.400	19.2%	6	7.2000E-02	8
Np237	3.1810E+01	1590.500	15.9%	8	1.9300E-01	6
Th230	2.4876E+01	1243.800	12.4%	9	2.7200E-01	5
Cm246	1.8423E+01	921.150	9.2%	10	3.8000E-01	1
Cm245	1.8423E+01	921.150	9.2%	10	3.8000E-01	1
Ra226	1.6791E+01	839.550	8.4%	12	2.9500E-01	3
Ni59	6.0430E+00	302.150	3.0%	13	2.8800E-01	4
Pb210	5.7730E+00	288.650	2.9%	14	2.9000E-02	11
Tc99	4.5400E-01	22.700	0.2%	15	8.6000E-02	7
Cs135	1.1700E-01	5.850	0.1%	16	3.5000E-02	10
I129	1.4000E-02	0.700	0.0%	17	7.0000E-03	13
C14	0.0000E+00	0.000	0.0%	18	0.0000E+00	18
Se79	0.0000E+00	0.000	0.0%	18	0.0000E+00	18
Cl36	0.0000E+00	0.000	0.0%	18	0.0000E+00	18

7-25-02 PA-SCR-394 GADAMS:

Performed a series of tests using VERSION 4.1.1CHG3 of the code. Change 3 of the code was designed to allow the TPA code to execute with a large number of time steps. Test1 was performed using the mean data se~~over 150 real~~ GADAMS 7-25-02 over 10,000 years. Test2 was performed using 150 realizations over 10,000 years. In both tests, the time steps were set to 201, 501, 1001, and 2001time steps. The peak mean dose and year for test1 is tabulated below.

Number of Years in Time Step	Number of Time Steps	Peak Mean Dose (rem/yr)	Year
50	201	3.0410E-05	10000
20	501	7.1487E-06	9600
10	1001	7.1011E-06	9590

5	2001	7.0676E-06	9595

The peak mean dose and year for test2 is tabulated below.

Number of Years in Time Step	Number of Time Steps	Peak Mean Dose (rem/yr)	Year
50	201	2.0816E-05	7850
20	501	1.0296E-05	9540
10	1001	1.0137E-05	9550
5	2001	1.0038E-05	9550

The tests were performed on machine spock in the following directories: $HOME/PA-SCR-394/run/TEST7-17-02/test1 and $HOME/PA-SCR-394/run/TEST7-17-02/test2.

7-25-02 PA-SCR-394 GADAMS:

Performed a test in which the WastePackageFlowMultiplicationFactor is decreased to observe the effects on number of time steps that solubility is limited. This test was performed using VERSION4.1.1CHG2 of the TPA code. The test was performed using the bathtub model with the mean data set over 10,000 years with uniform time steps of 50 years. The test was performed for a single subarea (subarea 1). The test was run on machine spock in the following directory: $HOME/PA-SCR-394/run/TEST7-25-02/TEST3.

The following table summarizes the results of running this test.

WastePackageFlowMultiplicationFactor	Number of Time Steps with Solubility Limited
5.751086854	36 out of 201
3.00	23 out of 201
1.00	0 out of 201
0.50	0 out of 201

7-26-02 PA-SCR-394 GADAMS:

Performed a test using the flowthru model in which the WastePackageFlowMultiplicationFactor is increased from the GADAMS 7-26-02 mean data set value. The purpose of the test was to observe the effect on Number of Time Steps with Solubility Limited for U238. The test was performed using version4.1.1CHG2 of the TPA code. The time period was 10,000 years with uniform

time steps of 50 years. The test was performed for a single subarea (subarea 1). The DripShieldFailureTime was set to 0.0 years. The following table summarizes the results of running this test. Testing was performed on machine spock in the following directory: $HOME/PA-SCR-394/run/TEST7-25-02/TEST4.

WastePackageFlowMultiplicationFactor	Number of Time Steps with Solubility Limited (U238)
5.7510868538042(mean data value)	187
1000	187
10000	187
20000	187
25000	176

7-30-02 PA-SCR-394 GADAMS:

Performed a code modification to VERSION4.1.1CHG2~~A~~ GADAMS 7-30-02 of the TPA code. The new code version is VERSION4.1.1CHG2A. The change involved displaying the average number of cycles in which the flowrate out of the waste package is positive. This new value is added to the ebsrel.rlt file for each realization and for the average over all realizations. The functionality of the code was not changed, only an additional parameter, the number of time steps in which flowrate out of the waste package is positive, is tracked. Regression testing was performed with VERSION4.1.1CHG2 of the TPA code. The ebsrel.rlt files associated with entry 7-3-02 PA-SCR-394 GADAMS were compared to verify that information that was already present did not change. In addition, verification was performed against the system level test ebsrel.rlt file.

7-30-02 PA-SCR-394 GADAMS:

A series of tests was conducted on 7-26-02 and 7-29-02 to 7-30-02. These tests were performed using VERSION4.1.1CHG2A of the TPA code. Test1 was designed to repeat the test performed on 7-3-02 under entry 7-3-02 PA-SCR-394 GADAMS. The test was performed over 10,000 years with 100 realizations and uniform time steps of 50 years. As in previous tests, the tpa.inp file for version 4.1j was used with modifications to include checkpointrestart and generate restartfiles. This test produced the same results as those displayed under entry 7-25-02 PA-SCR-394 GADAMS as expected with one additional output, average cycles with positive flowrate out of the waste package. The average over all realizations for positive

flowrate out of the waste package was 24.523 time steps of 50 years per time step. Test 1 generated the following values for the percentage of the actual flow period over which the release is solubility limit controlled: (U-238 99.8%, U-234 99.8%, Pu-239 99.8%, Pu-240 θ GADAMS 7-30-02 99.8%, Nb-94 97.4%, Am-241 86.9%, Am-243 86.9%, Np-237 62.4%, Th-230 41.8%, Cm-246 23.3%, Cm-245 23.3%, Ra-226 19.3%, Pb-210 0%, Cs-135 0%, I-129 0%, Tc-99 0%, Ni-59 0%, Se-79 0%, and Cl-36 0%.

Test 2 was a series of tests that were performed as verification of results. The first of these tests was a study on flowrates where flowrates were set to constant low, mean, and high values. **Hi**gh and low flowrates from the mean case were selected in these tests. The~~resuls~~ GADAMS 7-30-02 results indicated that against the mean data case, flowrate changes did not affect the rankings for solubility limit affected radionuclides. The second of these tests involved changing the radionuclide inventory. A low inventory of 3.83E-6 was selected for all radionuclides and a high inventory of 2.883E4 was selected. The results indicate that with high inventories, radionuclides such as PB-210, Cs-135, I-129, and Ni-59 will shift from not solubility limited to 100% solubility limited. The third of these tests involved changing the halflife of **ra**dionuclides. A low value of 2.23E1, a high value of 4.468E9 were used. Also, the halflife of Pb-210 was set to 1E4 in a separate test. The results indicated that changing the halflife of Pb-210 to 1E4 years did not affect its ranking when compared to the mean data case. The last test involved considering the radionuclides outside of chains. The ebspac.nuc file was modified such that 20 radionuclides were analyzed instead of 13 chains. The result of this test indicated that pulling the radionuclides outside of chains and setting a high inventory(2.883E4) made Cs-135, I-129, Ni-59, and Se-79 solubility limited. Pulling the radionuclides outside of~~chan~~ GADAMS 7-30-02 chains and setting a long halflife caused some radionuclides such as U-238 and Np-237 to no longer be solubility limited. And last, pulling the radionuclides ~~outsic~~ GADAMS 7-30-02 outside of chains and setting a long halflife(1E4) and large inventory(2.883E4) moved Pb-210 and Ni-59 from not solubility limited to 100% solubility limited.

All tests were performed on machine spock in directory $HOME/PA-SCR-394/run/TEST7-26-02.

8-2-02 PA-SCR-394 GADAMS:
Performed an edit to VERSION4.1.1CHG2A. The edit affected the releaset module and incorporated a way to calculate the waste package fill time using the difference in time between the points where the flowrate out of the waste package becomes positive and the flowrate into the waste package becomes positive. The new code version is VERSION4.1.1CHG2B. The code was placed on machine spock in directory $HOME/PA-SCR-394/VERSION4.1.1CHG2B. Testing on this code version was conducted to compare the output generated in file ebsrel.rlt to system level test sl-1 for VERSION4.1.1, regression testing to VERSION4.1k, and a comparison of output results to VERSION4.1.1CHG2A for mean and 100 of 100 realizations. The output corresponded to the previous results and the new code version successfully passed these tests.

The following table summarizes the results obtained for waste package fill time.

Minimum(years)	Average(years)	Maximum(years)	Simulation
0	840.1	5800	100 realizations
800	1130	1550	mean case 10,000 years
800	1080	1600	mean case 100,000 years

The above test results and fill times were obtained on machine spock in directory $HOME/PA-SCR-394/run/TEST8-1-02.

8-6-02 PA-SCR-365 GADAMS:
Successfully completed the testing for this SCR in accordance with the Test Plan for SCR #365. Testing was conducted on machine spock. The test plan consisted of four process level tests and two system level tests. The process level tests were designed to verify that the WELDFAIL module could correctly calculate failure of the welds and that the WELDFAIL module was integrated into FAILT without affecting the corrosion failure calculations of the waste package. The two system level tests

verified that the information produced by WELDFAIL could be retrieved by module RELEASET for use in its calculations for water infiltration into the waste package.

The software successfully passed all process level and system level tests in accordance with the Test Plan for TPA SCR #365. The test plan and test results were included with the SCR and placed on a CD labeled, "Test Plan and Test Results for TPA SCR #365, 8-6-02." Testing that was performed during development on this SCR was also placed on this CD. This included the testing that was performed on 4-25-02 and 6-20-02.

8-7-02 PA-SCR-394 GADAMS:

Performed a series of verification studies for the flowthru model similar to the ones identified under entry 7-30-02 PA-SCR-394 GADAMS for the bathtub model. For the flowthru model, VERSION4.1.1CHG2B of the code was used over a period of 10000 years mean case for subarea 1. The solubility limited results were compared for two radionuclides (Pb-210, and U-238). The range of tests included low, mid, and high values for reference flowrate, inventory, and halflife. In addition, tests were performed for parent-only ~~radionuclidd~~ GADAMS 8-7-02 radionuclide activity involving high inventory and halflife. The results of these verification studies with a comparison to those obtained using the bathtub model is included in the following tables:

Total Steps	**200**								
	Reference Flowrate[m^3/yr] (Bathtub Model)								
	Low: 6.53E-2			**Mid: 7.5E-2**			**High: 8.46E-2**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	103	100	**52**	116	100	**58**	125	100	**63**
Pb-210	0	0	0	0	0	0	0	0	0
qout > 0	103			116			125		
	Reference Flowrate[m^3/yr] (Flowthru Model)								
	Low: 6.53E-2			**Mid: 7.5E-2**			**High: 8.46E-2**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	198	100	**99**	198	100	**99**	198	100	**99**
Pb-210	0	0	**0**	0	0	**0**	0	0	**0**

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qout > 0	198			198			198		
	Inventory[ci] (Bathtub Model)								
	Low: 3.83E-6			**Mid: 1.44E4**			**High: 2.88E4**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	0	0	**0**	36	100	**18**	36	100	**18**
Pb-210	0	0	**0**	36	100	**18**	36	100	**18**
qout > 0	36			36			36		
	Inventory[ci] (Flowthru Model)								
	Low: 3.83E-6			**Mid: 1.44E4**			**High: 2.88E4**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	0	0	**0**	52	100	**26**	52	100	**26**
Pb-210	0	0	**0**	52	100	**26**	52	100	**26**
qout > 0	52			52			52		
	Halflife[yr] (Bathtub Model)								
	Low: 2.23E1			**Mid: 2.23E9**			**High: 4.47E9**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	0	0	**0**	0	0	**0**	0	0	**0**
Pb-210	0	0	0	0	0	0	0	0	0
qout > 0	36			36			36		
	Halflife[yr] (Flowthru Model)								
	Low: 2.23E1			**Mid: 2.23E9**			**High: 4.47E9**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	0	0	**0**	0	0	**0**	0	0	**0**
Pb-210	0	0	**0**	0	0	**0**	0	0	**0**
qout > 0	52			52			52		
	Parent-only radionuclide activity (Bathtub Model)								
	Inventory High: 2.88E4			**Halflife High: 1E4**			**Inventory High: 2.88E4, Halflife High: 1E4**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	36	100	**18**	0	0	**0**	36	100	**18**
Pb-210	0	0	0	0	0	0	36	100	18

qout > 0	36			36			36		
	Parent-only radionuclide activity (Flowthru Model)								
	Inventory High: 2.88E4			**Halflife High: 1E4**			**Inventory High: 2.88E4, Halflife High: 1E4**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	52	100	**26**	1	2	**1**	52	100	**26**
Pb-210	0	0	**0**	0	0	**0**	52	100	**26**
qout > 0	52			52			52		

Conducted another test using the flowthru model to repeat the one conducted under entry 7-25-02 PA-SCR-394 GADAMS. The test was conducted on machine spock using version ~~4.4~~ GADAMS 8-7-02 4.1.1CHG2B of the TPA code. The test was performed using 100 realizations over 10000 years with uniform time steps of 50 years. An additional value, "average cycles with positive flowrate out of the waste package" was generated. For this test case, there were 41.536 cycles with positive flowrate out of the waste package. The results for this test are summarized in the following table.

Averages over all realizations and subareas(Ordered by average length of time release is solubility-limited)

Nuclide	Average Number of Time Steps with Solubility Controlling	Average length of time release is solubility-limited[yr]	Time span (out of 10,000 years) over which the nuclide is solubility limit-controlled	Time span (with qout > 0) over which the nuclide is solubility limit-controlled	Ranking by the average length of time release is solubility-limited	Average Number of Cycles Release Switches from Solubility-Limited to Dissolution-Limited	Ranking by the average number of cycles release switches from solubility limited to dissolution-limited
U238	4.1493E+01	2074.650	20.7%	99.9%	1	1.0000E-03	14
U234	4.1493E+01	2074.650	20.7%	99.9%	1	1.0000E-03	14
Pu239	4.1487E+01	2074.350	20.7%	99.9%	3	1.0000E-03	14
Pu240	4.1487E+01	2074.350	20.7%	99.9%	3	1.0000E-03	14
Nb94	4.0897E+01	2044.850	20.4%	98.5%	5	1.8000E-02	12
Am241	3.8348E+01	1917.400	19.2%	92.3%	6	7.2000E-02	8
Am243	3.8348E+01	1917.400	19.2%	92.3%	6	7.2000E-02	8
Np237	3.1810E+01	1590.500	15.9%	76.6%	8	1.9300E-01	6
Th230	2.4876E+01	1243.800	12.4%	59.9%	9	2.7200E-01	5
Cm246	1.8423E+01	921.150	9.2%	44.4%	10	3.8000E-01	1
Cm245	1.8423E+01	921.150	9.2%	44.4%	10	3.8000E-01	1
Ra226	1.6791E+01	839.550	8.4%	40.4%	12	2.9500E-01	3
Ni59	6.0430E+00	302.150	3.0%	14.5%	13	2.8800E-01	4

Pb210	5.7730E+00	288.650	2.9%	13.9%	14	2.9000E-02	11
Tc99	4.5400E-01	22.700	0.2%	1.1%	15	8.6000E-02	7
Cs135	1.1700E-01	5.850	0.1%	0.3%	16	3.5000E-02	10
I129	1.4000E-02	0.700	0.0%	0.0%	17	7.0000E-03	13
C14	0.0000E+00	0.000	0.0%	0.0%	18	0.0000E+00	18
Se79	0.0000E+00	0.000	0.0%	0.0%	18	0.0000E+00	18
Cl36	0.0000E+00	0.000	0.0%	0.0%	18	0.0000E+00	18

These tests were conducted on machine spock in directory $HOME/PA-SCR-394/run/Test8-3-02.

8-7-02 PA-SCR-394 GADAMS:

Repeated the flowrate verification study for the bathtub model. In the previous results the flowfactr value in ebsflo.dat was set to 1.0. In order to use the value from the mean data set and to have the same ~~inpt~~ GADAMS 8-7-02 input that was used for this case in the flowthru analysis, this value was set to 0.5751086854E+01. The test results are summarized in the table below.

Total Steps	**200**								
	Reference Flowrate[m^3/yr] (Bathtub Model)								
	Low: 6.53E-2			**Mid: 7.5E-2**			**High: 8.46E-2**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	182	100	**91**	184	100	**92**	186	100	**93**
Pb-210	0	0	0	0	0	0	0	0	0
qout > 0	182			184			186		

The testing was performed on machine spock in directory $HOME/PA-SCR-394/run/TEST8-7-02.

8-8-02 PA-SCR-394 GADAMS:

When halflives are the same for parent and daughter radionuclides, subroutine decay in code module releaset will produce a divide by zero error. It sets the value for p2 to zero, and this local variable is used in the denominator. For this reason, the verification studies previously conducted on halflife and summarized under entry 8-7-

02 PA-SCR-394 GADAMS were repeated. The halflives of parent and daughter radionuclides was modified in ebspac.nuc so that the difference between the two would not be exactly zero and lead to the code error. The results of this analysis are included in the following table.

Total Steps	**200**								
	Halflife[yr] (Bathtub Model)								
	Low: 2.23E1			**Mid: 2.23E9**			**High: 4.47E9**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	0	0	**0**	36	100	**18**	36	100	**18**
Pb-210	0	0	**0**	0	0	**0**	36	100	**18**
qout > 0	36			36			36		
	Halflife[yr] (Flowthru Model)								
	Low: 2.23E1			**Mid: 2.23E9**			**High: 4.47E9**		
	steps	% flow	%time	steps	%flow	%time	steps	%flow	%time
U-238	0	0	**0**	52	100	**26**	52	100	**26**
Pb-210	0	0	**0**	0	0	**0**	52	100	**26**
qout > 0	52			52			52		

The testing was performed on machine spock in directory $HOME/PA-SCR-394/run/TEST8-8-02.

8-9-02 PA-SCR-394 GADAMS:

The radionuclide C-14 was not identified in the solubility limit analysis discussed under entry 7-30-02 PA-SCR-394 GADAMS. Under the bathtub model in test1 under entry 7-30-02 PA-SCR-394 GADAMS, C-14 showed no solubility limited release over the analysis period. This result was obtained from the ebsrel.rlt file associated with the test for this entry and run on machine spock in directory $HOME/PA-SCR-394/run/TEST7-26-02.

8-12-02 PA-SCR-397 GADAMS:

The objective of this task is to correct an error observed in TPA code version 4.2i. The error is as follows:

DSFAIL crashes during the checkpoint/restart ~~featue~~ GADAMS 8-12-02 feature.
The following scenario would produce the error in version 4.2i of the TPA code:
1) Run for 3 realizations with the restart flag on.
2) Interrupt the run with control-C during the second realization.
3) Re-run (restart) TPA without removing any files from the run directory.
The module DSFAIL crashes on the first DSFAIL call after restart.

This objective is in accordance with SCR PA-SCR-397. It was accomplished through the modification of two code modules: DSFAIL and EXEC. The reason DSFAIL crashed is its initialization flag was not set after a restart. In order to correct this error, EXEC no longer passes an initialization flag to DSFAIL. Instead DSFAIL manages this flag on its own. The first time DSFAIL is called, this flag is true, and DSFAIL changes it to false. The state of this flag is maintained statically by DSFAIL. This modification ensures that the flag will be true on the first call to DSFAIL (whenever this call occurs) and will be false afterwards.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All software development and testing was performed on machine spock in directory $HOME/PA-SCR-397. This machine is a Sun Ultra-4 server with Solaris 5.8.

Version 4.2i of the TPA code was used as a baseline software version. Code modules DSFAIL and EXEC were updated such that DSFAIL manages the initialization flag. The software was tested in accordance with the Test Plan for TPA SCR #397. This test plan contained a single system level test designed to verify that the error in the code was corrected. The software successfully passed the system level test and the code executes correctly on restart. The test plan and test results as well as the build archive from spock are included on a CD labeled, "Test Plan and Test Results for TPA SCR #397, 8-12-02."

9-9-02 PA-SCR-398 GADAMS:
The purpose of this task is to include the dryout region for analysis of five values: chloride, fluoride, pH, carbonate, and delta potential critical. This objective is

accomplished through the modification of two code modules: exec.f and nfenv.f. Formerly, nfenv.f used file multiflo.dat. With the update, nfenv.f uses multifbe.dat for the period before dryout and multifaf.dat for the period after dryout. The dryout region is calculated directly.

~~WG~~GADAMS 9-9-02 Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All software development is performed on machine spock in directory $HOME/PA-SCR-398. This machine is a Sun Ultra-4 server with Solaris 5.8.

Version 4.2k of the TPA code was used as a baseline software version. Code module exec.f was updated to send and receive carbonate to and from nfenv.f. Module nfenv.f was updated to retrieve values for the five parameters before, during, and after the dryout period.

9-10-02 PA-SCR-394 GADAMS:
A series of tests was conducted on machine spock using VERSION 4.1.1 CHG2B of the TPA code. There were 8 tests conducted and they are summarized in the table below.

Test Identifier	Test Description
Test 1	Bathtub Model, 350 Realizations, Uniform time steps,400 years per time step, Analysis performed over 100,000 years
Test 2	Flowthrough Model, 350 Realizations, Uniform time steps,400 years per time step, Analysis performed over 100,000 years
Test 3	Bathtub Model, 350 Realizations, Uniform time steps, 50 years per time step, Analysis performed over 10,000 years
Test 4	Flowthrough Model, 350 Realizations, Uniform time steps, 50 years per time step, Analysis performed over 10,000 years
Test 5	Bathtub Model, 350 Realizations, Uniform time steps, 50 years per time step, Leaching Model 1, Analysis performed over 10,000 years
Test 6	Bathtub Model, 350 Realizations, Uniform time steps, 50 years per time step, Leaching Model 3, Analysis performed over 10,000 years
Test 7	Bathtub Model, 350 Realizations, Uniform time steps, 50 years per time step, Leaching Model 4, Analysis performed over 10,000 years
Test 8	Bathtub Model, 350 Realizations, Uniform time steps, 50 years per time step, Grain Size Model, Analysis performed over 10,000 years

The results for these tests is summarized in the following table.

	Time span (with qout > 0) over which the nuclide is solubility limit-controlled							
					Modifications to Test 3			
Nuclide	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6	Test 7	Test 8
Cm246	1.30%	2.89%	23.18%	46.24%	59.73%	0.00%	0.00%	59.87%
U238	95.97%	96.09%	99.66%	99.80%	99.90%	97.37%	0.00%	99.91%
Cm245	1.30%	2.89%	23.18%	46.24%	59.73%	0.00%	0.00%	59.87%
Am241	21.03%	23.23%	86.62%	92.21%	97.98%	35.06%	0.00%	97.94%
Np237	24.90%	27.13%	63.91%	78.12%	91.51%	3.71%	0.00%	91.25%
Am243	21.03%	23.23%	86.62%	92.21%	97.98%	35.06%	0.00%	97.94%
Pu239	84.97%	85.45%	99.41%	99.66%	99.85%	95.81%	0.00%	99.86%
Pu240	84.97%	85.45%	99.41%	99.66%	99.85%	95.81%	0.00%	99.86%
U234	95.97%	96.09%	99.66%	99.80%	99.90%	97.37%	0.00%	99.91%
Th230	27.77%	30.00%	43.55%	63.99%	82.86%	0.00%	0.00%	82.46%
Ra226	18.48%	21.75%	18.62%	41.62%	53.06%	0.00%	0.00%	53.55%
Pb210	0.00%	12.24%	0.00%	11.73%	0.00%	0.00%	0.00%	0.00%
Cs135	0.00%	0.00%	0.00%	0.19%	0.00%	0.00%	0.00%	0.00%
I129	0.00%	0.00%	0.00%	0.01%	0.00%	0.00%	0.00%	0.00%
Tc99	0.00%	0.02%	0.00%	0.81%	0.00%	0.00%	0.00%	0.00%
Ni59	0.00%	0.51%	0.00%	13.67%	0.00%	0.00%	0.00%	0.01%
C14	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Se79	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Nb94	58.21%	59.56%	96.53%	97.97%	99.58%	74.23%	0.00%	99.58%
Cl36	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

The testing was performed on machine spock in the following directory: $HOME/PA-SCR-394/run/TEST8-15-02.

9-19-02 PA-SCR-346 GADAMS:

Software development was moved to machine spock in the following directory: $HOME/PA-SCR-346/code42u. The code modules for this SCR were integrated into version 4.2u of the TPA code. The following changes were made to the code. The itym code was modified to create output Digital Elevation Model (DEM) Tables (DTBL) for Mean Annual Infiltration (MAI), log10(MAI), and the standard deviation stdev(log10(MAI)). In addition, parameter sampling was corrected. Module UZFLOW was modified to receive two DTBL files. The file maydtbl.dat contains the

log10(MAI) values generated by itym. The file smaydtbl.dat contains the stdev(log10(MAI)) values generated by itym. In addition, a new sampled parameter was added, UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)]. This parameter is normally distributed with zero mean and unit variance.

10-17-02 PA-SCR-410 GADAMS:
The purpose of this task is to correct the screen output for ITYM and place repository averages in file infilper.res. This objective is accomplished through the modification of two code modules: exec.f and estimator.f. In addition, a modification was made to reader.f to correct a compiler error. The following warning was generated: endofcolloidalnuclides is used but never set.

The following changes were made to the code modules: 1) In estimator.f, the values for EsI are printed in double precision scientific notation. 2) In exec.f, the variable percinfil(isa,jj,1) is summed and then divided by repository area instead of summing a subarea averaged percinfil(isa,jj,1) and then dividing by the number of subareas. 3) In reader.f, endofcolloidalnuclides was included as part of an output string instead of being used as a variable name.

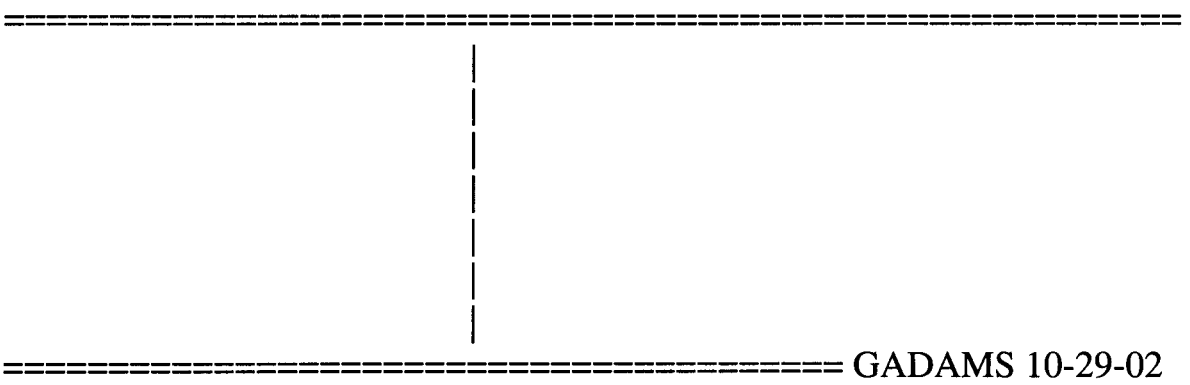
Qualifications for performing this work are proficiency in developing, implementing, and ~~maini~~GADAMS 10-17-02 maintaining FORTRAN 77 code.

All software development is performed on machine spock in directory $HOME/PA-SCR-410. This machine is a Sun Ultra-4 server with Solaris 5.8.

Version 5.0 beta of the TPA code was used as a baseline software version.

10-29-02 PA-SCR-394 GADAMS:
The following table summarizes a series of test results not included in entry 9-10-02 PA-SCR-394 GADAMS. The testing was performed on machine SPOCK in directory: $HOME/PA-SCR-394/run/TEST8-15-02. It was performed using VERSION 4.1.1CHG2B of the TPA code. The table shows the percentage of the 10,000 year simulation period over which the release is solubility limit controlled in addition to the percentage of the actual flow period over which the release is solubility

limit controlled.



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	Bathtub Model		Flow-through Model	
Radionuclide	**Percentage of the 10,000 year Simulation Period over which the Release is Solubility Limit Controlled**	**Percentage of the Actual Flow Period over which the Release is Solubility Limit Controlled**	**Percentage of the 10,000 year Simulation Period over which the Release is Solubility Limit Controlled**	**Percentage of the Actual Flow Period over which the Release is Solubility Limit Controlled**
U-238	11.4%	99.7%	19.6%	99.8%
U-234	11.4%	99.7%	19.6%	99.8%
Pu-239	11.4%	99.4%	19.5%	99.7%
Pu-240	11.4%	99.4%	19.5%	99.7%
Nb-94	11.0%	96.5%	19.2%	98.0%
Am-241	9.9%	86.6%	18.1%	92.2%
Am-243	9.9%	86.6%	18.1%	92.2%
Np-237	7.3%	63.9%	15.3%	78.1%
Th-230	5.0%	43.6%	12.5%	64.0%
Cm-246	2.7%	23.2%	9.1%	46.2%
Cm-245	2.7%	23.2%	9.1%	46.2%
Ra-226	2.1%	18.6%	8.2%	41.6%
Ni-59	0%	0%	2.7%	13.7%
Pb-210	0%	0%	2.3%	11.7%
Tc-99	0%	0%	0.2%	0.8%
Cs-135	0%	0%	0%	0.2%
I-129	0%	0%	0%	0%
Se-79	0%	0%	0%	0%
Cl-36	0%	0%	0%	0%
C-14	0%	0%	0%	0%
Test Parameters: 350 realizations, 50 years per time step, Leaching Model 2, Particle Model, 10,000 years				

11-4-02 PA-SCR-411 GADAMS:

The purpose of this task is to correct errors in code modules releaset.f and ebsrel.f implemented under PA-SCR-367, PA-SCR-369, and PA-SCR-370. The following errors were observed: 1) File ebsrel.inp contains a zero (0) drip shield failure time when it should contain the first time of drip shield failure contained in ebstrh.dat. 2) In subroutine derivs of releaset.f, the variable amass0 is used instead of y(3). The coefficients for the ODE integration should be calculated using the input parameter y(3) instead of the initial parameter amass0. 3) When tfirstflow is obtained from the information retrieved in ebsflo.dat, it is more precise than the TPA time step value retrieved from ebstrh.dat. For example, in one test case, the value 811.31698403 was retrieved from ebsflo.dat; whereas, 811.317 was retrieved from ebstrh.dat. This difference in precision will result in integration performed in liqrel to start one time step early.

The code was modified and the following files were affected: releaset.f, ebsrel.f, and ebsrel.def/ebsrel.inp. Version 5.0Beta of the TPA code was used as a baseline software version.

The following changes were made to the code modules: 1) Since the reference flowrate in ebsflo.dat will only be positive when the time is greater than or equal to the drip shield failure time, the retrieval of drip shield failure time from ebsrel.inp into dsfailtime is not necessary. Therefore, dsfailtime was eliminated from releaset.f and ebsrel.def/ebsrel.inp. 2) Replaced references to amass0 in subroutine derivs of releaset.f with y(3). 3) Rounded variable tfirstflow (releaset.f) using the following statement: tfirstflow = DBLE(DNINT(tfirstflow * 10000.0D0)) / 10000.0D0.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All software development is performed on machine spock in directory $HOME/PA-SCR-411. This machine is a Sun Ultra-4 ~~Seer~~ GADAMS 11-4-02 Server with Solaris 5.8.

11-8-02 PA-SCR-411 GADAMS:
The software successfully passed the Test Plan for TPA SCR#411. This test plan consisted of four process level tests designed to verify the following: 1) Release rates are comparable to TPA version 4.1j release rates when diffusion is not included, no protection is provided by the cladding, and the glass source term model is not included. 2) Glass Model release rates are comparable to hand calculations. 3) Diffusion release rates are comparable to hand calculations. 4) Release rates with cladding protection are comparable to hand calculated release rates.

Test ~~resusl~~ GADAMS 11-8-02 results and archives were placed on a CD labeled, "Test Plan and Test results for TPA SCR #411." The software was tested on machine spock in directory $HOME/PA-SCR-411.

11-12-02 PA-SCR-415 GADAMS
The purpose of this task is to ~~correct adjustable arrays~~ GADAMS 11-12-02 change automatic arrays to adjustable arrays. FORTRAN 95 and FORTRAN 90 accept automatic arrays; however, earlier versions of FORTRAN 77 do not.

Version 5.0Beta of the TPA code will be used as the baseline for these changes.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All software development will be performed on machine spock in directory $HOME/PA-SCR-415.

11-13-02 PA-SCR-415 GADAMS:
In order to eliminate automatic arrays from the FORTRAN code, the ~~fi~~ GADAMS 11-13-02 following files were changed: 1) nfenv.f, 2) seismo2.f, 3) exec.f, 4) mechfail.f, 5) failt.f, 6) weldfail.f, 7) dsfailt.f, and 8) integrt.f. The following files were added: 1) nfenvadj.i, 2) seisadj.i, 3) failtadj.i. These files were originally modified using the automatic array declaration of f77 version 5.0. Automatic arrays are not supported in the f77 version 4.2 compiler.

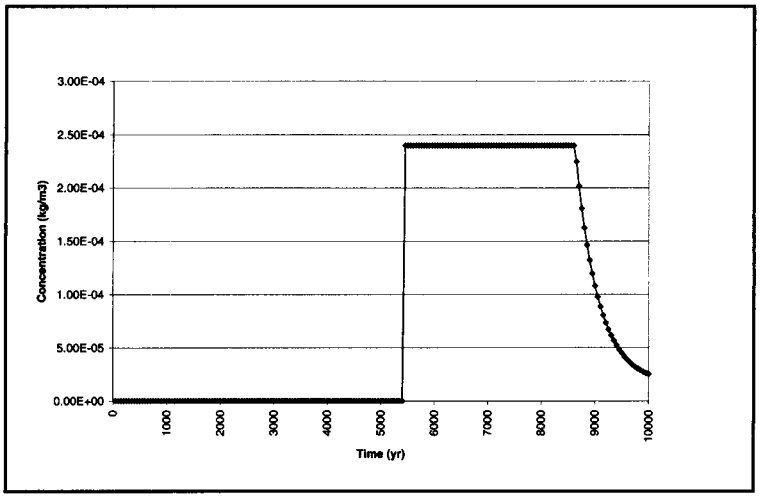
The following changes were made to the files:
NFENV.F: Added include file nfenvadj.i. This include file is used in subroutine assignConcentrations.
SEISMO2.F: Subroutine buildMechfailInputFile. Modified local variable arrays to use maxnsubarea defined in maxnsuba.i.
EXEC.F: Moved variable maxseismicevents to include file seisadj.i.
MECHFAIL.F: Added references to maxnsuba.i, maxntime.i, and added new include files mechadj.i and seisadj.i. Mechfail uses these files to dimension its local arrays and check its input number of subareas, number of time steps, number of block size points and number os seismic events against the maximums identified in these files.
FAILT.F: Removed automatic arrays from subroutine calculateWeldFailure. Moved nintv to include file, failtadj.i. This include file is used to dimension arrays in FAILT.F and WELDFAIL.F.
WELDFAIL.F: Eliminated automatic arrays by redimensioning local variable arrays from include file failtadj.i.
DSFAILT.F: Removed automatic arrays from subroutine getDSThickness and subroutine dsfailtime.
INTEGRT.F: Subroutine getIntegral was modified to accept a maximum dimension for alignment purposes.

11-14-02 PA-SCR-415 GADAMS:
The software successfully passed the Test Plan for TPA SCR#415. This test plan consisted of one system level test, sl-1, designed to ~~verfi~~ GADAMS 11-14-02 verify that the TPA code generates the same output data when automatic arrays are removed from the code. The ~~s~~ GADAMS 11-14-02 test was a comparison between the code 5.0 Beta output and the new TPA code built from the modified files. The test was performed on machine spock in directory $HOME/PA-SCR-415. The test plan and test results were placed on a CD labeled, TPA SCR#415, 11-14-02.

11-15-02 PA-SCR-415 GADAMS:
The CD referenced in entry 11-14-02 PA-SCR-415 GADAMS was labeled TPA SCR#415. This label was not consistent with the Test Plan or the SCR. A new cd was made and the test plan and test results were placed on this new CD labeled, Test Plan and Test Results for TPA SCR#415, 11-15-02.

11-22-02 PA-SCR-394 GADAMS:

A test was conducted using VERSION 4.1.1CHG2B of the TPA code in which the code was run for one realization (realization 12) of 350 realizations. The purpose of the test was to extract values for the radionuclide concentration of Cm-246. The values were extracted from trelease.out and plotted below:



This test was conducted on machine spock in directory $HOME/PA-SCR-394/run/TEST11-18-02.

~~**11-22-02 PA-SCR-394 GADAMS:**~~ **GADAMS 11-22-02**

11-22-02 PA-SCR-413 GADAMS:

The purpose of this task is to make modifications to the UZFLOW TPA code module and its associated preprocessor ITYM as a result of recommended changes from a code review conducted on 11-4-02. The following changes were identified: 1) For module UZFLOW.F, The previous uzflow_init subroutine was renamed old_uzflow_init. Instead of keeping the renamed subroutine in the code, rename it uzflow_init and comment it out. This alternative is preferable to leaving subroutines in the code that are no longer being used. 2) For module UZFLOW.F, subroutine calc_ainit uses the number of pixels in a subarea and teh repository to determine the fractional contribution of each subarea to infiltration. This causes teh infiltration generated in file infilper.res to not correspond to the ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] since the rest of the TPA code calculates the area using a quadrilateral to determine the fractional contribution of

each subarea. 3) Create a base case itym.dat file. Include the default values for all options. Those options that are not needed for the base case will be commented out. This change was recommended because the ITYM code module will execute whether or not an option is present in the file. a user who is not familiar with the code would not know what options are available. 4)For file TPA.INP, it is difficult for a user unfamiliar with the UZFLOW code to understand the relationship between the following parameters: UZFLOWSampleMode, UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)], ArealAverageMeanAnnualInfiltrationAtStart[mm/yr], MeanAnnualPrecipitationMultiplierAtGlacialMaximum, and MeanAnnualTemperatureIncreaseAtGlacialMaximum. Therefore, the recommendation was to group all of these parameters and include specific instructions for their use as comments in file tpa.inp. 5) In the section of the file (tpa.inp) marked, "Number and Location Of SubAreas[m] Based On EDA-II Design," the identifier for subarea 6 is edaii 6-c. It should be edaii 6-cw. For subareas 9 and 10, the fifth coordinate should match the first coordinate to generate a closed polygon for the subarea. 6) For the test plan, add a system level test to the test plan that eliminates variation over time from the UZFLOW code. This test would include, for example, a) Setting the UZFLOWSampleMode to 1 to eliminate the effects of standard deviation on mean annual infiltration. b) Setting the ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] to a constant value, c) Setting the MeanAnnualPrecipitationMultiplierAtGlacialMaximum to 1.0 to eliminate the variation in precipitation over time, and d) Setting the MeanAnnualTemperatureIncreaseAtGlacialMaximum to 0.0 to eliminate the variation in temperature over time. 7) For ITYM/UZFLOW, There is a minor difference between the temperature of the current climate used in the UZFLOW modules versus the temperature used in the ITYM preprocessor. The UZFLOW module uses a value of 17.38 degrees Celcius, the ITYM code uses the value 17.28 degrees Celcius. The code needs to be modified to use the same value.

Version 5.0BetaB of the TPA code will be used as the baseline for this work.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All software development will be performed on machine spock in directory: $HOME/PA-SCR-413.

11-26=02 PA-SCR-414 GADAMS:
The purpose of this task is to modify the TPA code to address major and minor defects identified during the DSFAIL (DS1) code review conducted on 11-11-02 and the SEISMO (SA1) code review conducted on 11-18-02. In addition, this SCR addresses changes to the SEISMO module following its initial implementation. The changes identified include the following: 1) Place drip shield failure result information in a .res file similar to the wpsfail.res file. 2) Return drip shield failure time to the executive. 3) Invoke drip shield failure on a subarea basis. 4) Modify the coefficients in some of the equations to account for a change in units from kg to tonnes. 5) Update parameters in the tpa.inp file to include the seismic hazard curve, drip shield buckling load, and fractional rock types.

Version 5.0BetaB of the TPA code will be used as the baseline for this work.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All software development will be performed on machine spock in directory: $HOME/PA-SCR-414.

12-12-02 PA-SCR-414 GADAMS:
Implemented the code changes for this task. The following modules were affected: dsfail.f, dsfailt.f, seismo2.f, exec.f, mechfail.f, seisbs1.dis, seisbs2.dis, mechfail.def, multifaf.dat, multifbe.dat, and tpa.inp. The major change to the code involved invoking dsfail and seismo for each subarea rather than each realization. The code changes were integrated into version 5.0BetaD instead of version 5.0BetaB. This was because the current version of the TPA code was version 5.0BetaD.

The software changes were tested in accordance with the Test Plan for TPA SCR #414. This test plan consisted of one process level test designed to compare the MECHFAIL standalone code module results to hand calculated (Excel Spreadsheet)

values. The test plan also contained three system level tests designed to verify the integration of the SEISMO/DSFAIL/MECHFAIL code into the current TPA code. The software successfully passed the process level and system level tests.

Code modules were built and tested on machine spock in directory $HOME/PA-SCR-414.

12-20-02 PA-SCR-413 GADAMS:
Implemented the code changes for this task. The following modules were affected: uzflow.f, estimator.f, init_itym.f, itym.i, itym.dat, and tpa.inp. Originally, the code changes were integrated into version 5.0BetaB of the TPA code. However, because of updates to the TPA code, the changes were instead placed in version 5.0BetaE. The software was tested in accordance with the Test Plan ~~foor~~ GADAMS 12-20-02 for TPA SCR #413. This test plan consisted of one process level test designed to verify the ITYM Preprocessor output has changed as expected for a change in the current climate from 17.28 C to 17.38 C. In addition, the test plan consisted of one system level test designed to verify that the average infiltration can be constant and equal to the ArealAverageMeanAnnualInfiltrationAtStart[mm/yr]. The software successfully passed the process level test and the system level test.

Code modules were built and tested on machine spock in directory $HOME/PA-SCR-413.

1-3-03 PA-SCR-417 GADAMS:
Performed testing of the importance analysis feature of the TPA code in accordance with the Test Plan for TPA SCR #417. This test plan consisted of two system level tests designed to verify the operation of the importance analysis feature. System level test 1 verifies the TPA code will execute to completion when importance analysis is invoked. System level test 2 verifies the TPA code will abort execution and generate the appropriate error message when a negative leaching rate is calculated.

The software successfully passed the system level tests in accordance with the Test Plan for TPA SCR #417. Testing was performed on machine spock in directory $HOME/PA-SCR-417.

1-3-03 PA-SCR-390 GADAMS:
Testing was conducted on the integrated 5.0Beta version of the software on 11-1-2002 by C. Scherer. Test results were summarized for both a process level test and a system level test in accordance with Test Results for TPA SCR #390. The tests were designed to verify that infiltration increases in areas of the repository where runon occurs. The software passed both the system level test, sl-1, and the process level test, pl-1.

1-24-03 PA-SCR-394 GADAMS:
The following includes a set of test results not included in entry 9-10-02 PA-SCR-394 GADAMS. The testing was performed on machine SPOCK in directory: $HOME/PA-SCR-394/run/TEST8-15-02.

The average flowing period for the bathtub model was 1144 years.
The average flowing period for the flow-through model was 1959 years.

2-7-03 PA-SCR-346(continued) GADAMS:
This SCR is a continuation of changes previously included in SCR 346. The following modifications were continued: 1) File UZFLOW.F was modified to only include two UZFLOW sample modes instead of 3. In sample mode 1, the ArealAverageInfiltrationAtStart is sampled and the UZFLOWHydraulicPropertyUncertaintyDeviation is not used. In sample mode 2, the ArealAverageInfiltrationAtStart is not used and the UZFLOWHydraulicPropertyUncertaintyDeviation is sampled. 2) Since the number of sample modes was changed, the comments in the UZFLOW section of the TPA.INP file were modified to reflect the two sample modes instead of the three sample modes. 3) In addition, since the compiler has been upgraded on SPOCK, in order to build the ITYM code with the 4.2 compiler, a new make file, makefile4.2, was generated.

Code modifications were made to version 5.0betai of the TPA code. The code modifications were tested and they passed the three system level tests identified on Test Plan and Test Results for TPA SCR#346(continued). In addition, the process level tests from the Test Plan for TPA SCR#346 were summarized on the same

document. These process level tests were conducted previously by C. Scherer. The code passed these three process level tests as well.

All code modifications and testing were performed on machine spock in directory: $HOME/PA-SCR-346.

2-11-03 PA-SCR-420 GADAMS:
Performed testing of the EBSFILT code module. In addition, made one change to this module which was to bypass calculations for invert thickness less than or equal to 0. This change was made to version 5.0BetaO of the TPA code.

The test plan for TPA SCR #420 consists of one process level test designed to verify that oscillations in the release of radionuclides through the invert has been corrected and that the release through the invert of at least one other radionuclide is reasonable.

The software successfully passed the process level test in accordance with the Test Plan for TPA SCR#420.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All code modifications and testing were performed on machine spock in directory: $HOME/PA-SCR-420.

2-13-03 PA-SCR-423 GADAMS:
Performed testing of the code changes. The test plan for TPA SCR #423 consisted of one process level test designed to verify that the "choose source of temperature data" section and the "other temperature parameters" section of ebsfail.def/ebsfail.inp could be removed without affecting the output. In addition, the test plan contained one system level test designed to verify that the correct chemistry is obtained from NFENV using the waste package temperature instead of the repository temperature. The software successfully passed the process level test and the system level test in accordance with the Test Plan for TPA SCR #423.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All testing was performed on machine spock in directory: $HOME/PA-SCR-423.

2-17-03 PA-SCR-425 GADAMS:
The purpose of this SCR was to correct an error observed in UZFLOW. When the AnnualInfiltrationLossMode was set to 0, the code would abort. The problem was in UZFLOW where the subarea area was used before it was set. Additional changes were made in accordance with the following: 1) UZFLOW: Modified the parameter list to pass the isfirstsubarea flag to UZFLOW. Formerly, subarea 1 was used for initialization and screen output messages; however, the flag, isfirstsubarea is passed because subarea 1 may not necessarily be the first subarea. 2) DCAGS: Modified to copy env.e, envin.e, and associated data files to the run directory. The DCAGS module would not copy the files over if the DirectReleaseOnlyFlag was set. 3) EXEC: Modified EXEC to not generate EBSREL subarea summary information when the DirectReleaseOnlyFlag is set. Also, moved the AAP and AAT calculations used as input to DCAGS and DCAGW to within the isfirstsubarea IF-THEN statement preceding the call to UZFLOW. 4) TPA.INP: Modified tpa.inp to include the clarifying comment, "ClimatePerturbationSet should be greater than zero."

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All code modifications were performed on machine spock in directory: $HOME/PA-SCR-425.

2-18-03 PA-SCR-368 GADAMS:
Performed testing of the code changes. The test plan for TPA SCR #368 consists of two system level tests designed to verify the implementation of colloidal radionuclides. The first system level test verifies that when colloids are turned off, the release rates obtained are equivalent to those obtained from a previous code version in which colloids were not yet implemented. The second system level test verifies the additional (colloidal) NEFTRAN input for the saturated zone is correctly retrieved

from the TPA.INP file. The software successfully passed the two system level tests in accordance with the Test Plan for TPA SCR #368. The test plan and test results are included on a CD labeled, "Test Plan and Test Results for TPA SCR #368" submitted with this SCR.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All testing was performed on machine spock in directory: $HOME/PA-SCR-368.

2-21-03 PA-SCR-421 GADAMS:
Performed testing of the code changes. The test plan for TPA SCR #421 consisted of one system level test designed to verify the movement of Ja243 in chain number 2 from its position as parent to Pu239 to parent of Jp239. Print statements were generated to the screen to display the moles per MTU for the individual radionuclides after the call to subroutine allchains within INVENT.F. In the new code version, (5.0BetaV), the amount of Pu239 decreased and the amount of Jp239 increased as expected. This comparison was performed against a baseline version, 5.0BetaL. The software successfully passed the system level test in accordance with the Test Plan for TPA SCR #421. The test plan and test results are included on a CD labeled, "Test Plan and Test Results for TPA SCR #421."

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All testing was performed on machine spock in directory: $HOME/PA-SCR-421.

2-26-03 PA-SCR-441 GADAMS:
Performed testing of the code changes. The Test Plan for TPA SCR #441 consisted of one system level test designed to verify that the SZFT module will no longer generate a parameter not found error message when Importance Analysis is selected. Previously, a parameter not found error message (name = FractureRD_STFF_Jc) was generated. The software successfully passed the system level test in accordance with the Test Plan for TPA SCR #441. The original code version was 5.0BetaZ, the tested

code version was 5.0BetaZa.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

All testing was performed on machine spock in directory: $HOME/PA-SCR-441.

3-4-03 PA-SCR-426 GADAMS:
The purpose of this SCR was to include an initial ventilation period and an operation period in the code. During the active ventilation period, the chemistry values are set to their dryout values and the relative humidity is set to zero. The code changes were placed in the 5.0BetaV version of the tpa code; however, they were not included in the 5.0 release due to time constraints. The files/modules which were modified are as follows: exec.f, uzft.f, szft.f, dcagw.f, reader.f, nfenv.f, and tpa.inp.

Qualifications for performing this work are proficiency in developing, implementing and maintaining FORTRAN 77 code.

The modified code modules were integrated, and the updated code was built and run on machine spock in directory: $HOME/PA-SCR-426.

3-25-03 EXEC CODE VALIDATION GADAMS:
Created validation code modules for the following subroutines: checknr, checknsa, cleanupwd, cumfail, findpkmndose, writehead, and writehead2.

Checknr.t was created with two test cases designed to check the handling of a low number of realizations and a high number of realizations.

Checknsa.t was created with two test cases designed to check the handling of a low number of subareas and a high number of subareas.

Cleanupwd.t was created with a single test case to verify that files which should not be present in the write directory at the beginning of a TPA run are not present.

Cumfail.t was created with two test cases. Each test case contains a set of predefined failure data and each test case verifies that the correct cumulative fraction of waste package failures is obtained.

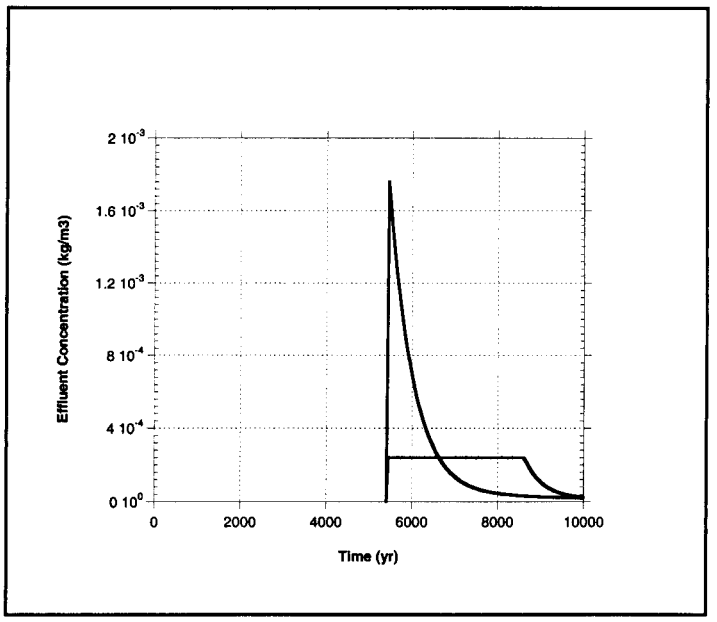
Findpkmndose.t was created with three test cases. The first test case places the peak mean dose at the first time step. The second test case places the peak mean dose at the last time step. And, the third test case places the peak mean dose at an intermediate time step. Each test case verifies that the code places the peak dose at the correct time step.

Writehead.t and Writehead2.t were created with as many test cases as there are files requiring ~~head4crs~~ GADAMS 3-25-03 headers written. These test cases verify that the correct header information is written to the files.

Qualifications for performing this work are proficiency in developing, implementing and maintaining FORTRAN 77 code.

The code modules were integrated into TPA Version 5.0 on machine spock in directory: $HOME/exec_validation/tpabuild_50_test.

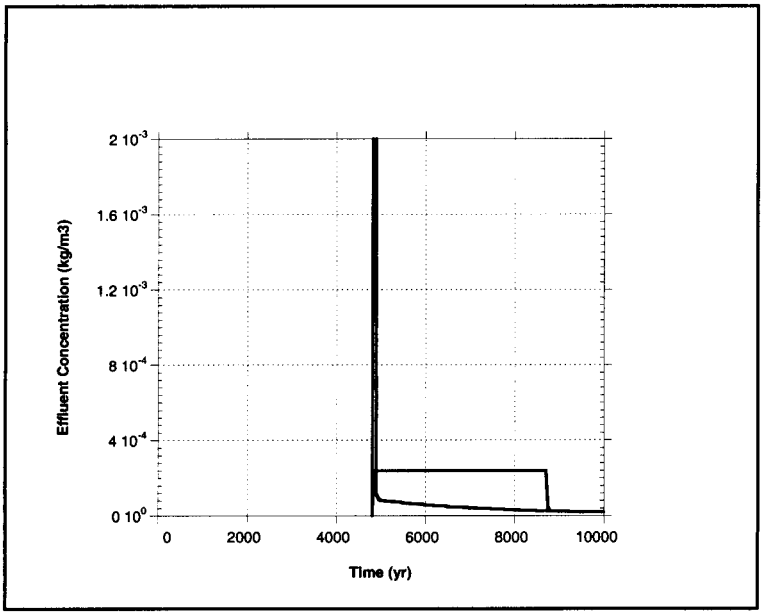
3-26-03 PA-SCR-394 GADAMS:
A test was conducted using VERSION4.1.1CHG2B of the TPA code in which the code was run for one realization (realization 12) of 350 realizations. This test was similar to the test conducted under entry 11-22-02 PA-SCR-394 GADAMS except the solubility limit for Cm was changed from 2.4e-4 to 2.0e2. The solubility limit was set artificially high to observe the effect of Cm concentration in the effluent. The values were extracted from trelease.out and plotted below(with the previous values from the test conducted for entry 11-22-02 PA-SCR-394 GADAMS):



This test was conducted on machine spock in directory: $HOME/PA-SCR-394/run/TEST3-26-03.

3-26-03 PA-SCR-394 GADAMS:

The test conducted in the previous entry was repeated using the flowthrough model instead of the bathtub model. As in the previous test, the solubility limit for Cm was changed from 2.4e-4 to 2.0e2. The values from trelease.out at both solubility limits is plotted in the following graph:

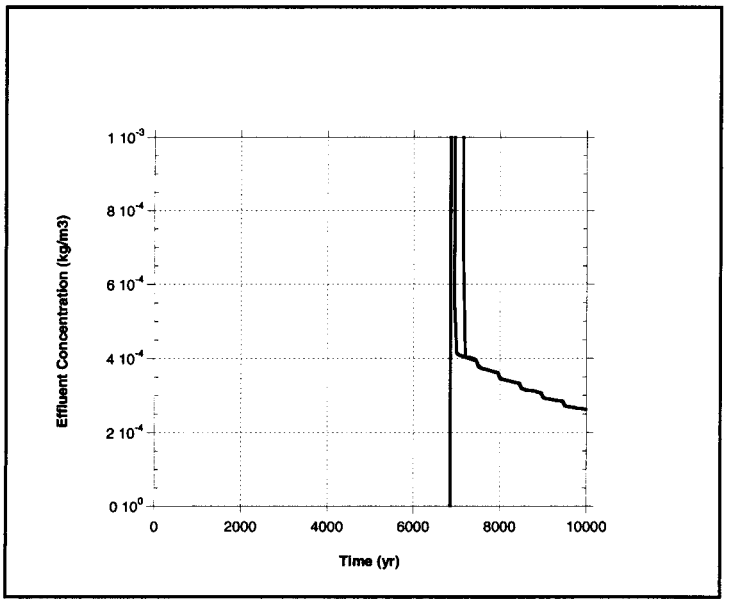


This test was conducted on machine spock in directory: $HOME/PA-SCR-394/run/TEST3-26-03/FLOWTHRU.

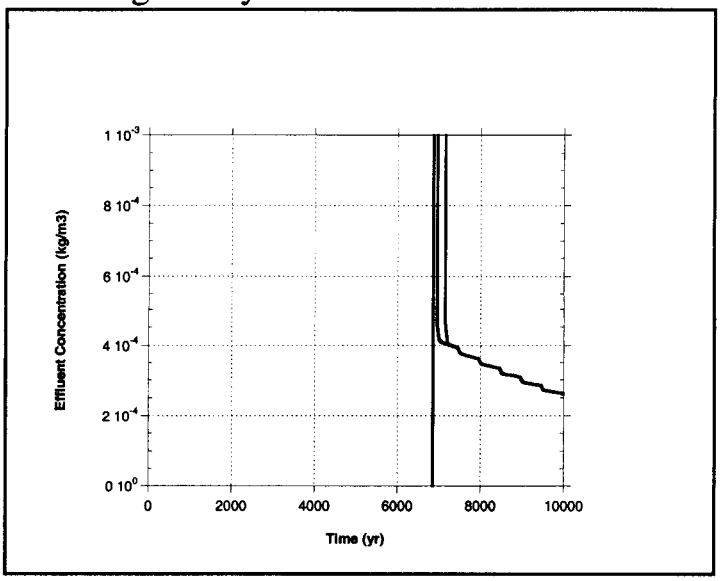
3-28-03 PA-SCR-394 GADAMS:

A test was conducted using ~~using~~ GADAMS 3-28-03 VERSION 4.1.1CHG2B of the TPA code in which the code was run for one realization (realization 12) of 350 realizations. This test was similar to the test conducted under entry 11-22-02 PA-SCR-394 GADAMS and the two tests identified under entries 3-26-03 PA-SCR-394 GADAMS. The difference in this test is Np was analyzed instead of Cm. Four individual test cases were run: 1) Basecase bathtub model with Np solubility a constant at the center value of its logtriangular distribution (3.4e-2). 2) Bathtub model with Np solubility set to a constant high value of 1e4. 3) Basecase flowthrough model with Np solubility set to a constant value of 3.4e-2. 4) Flowthrough model with Np solubility set to a constant high value of 1e4.

Plots for the bathtub analysis are included in the following diagram:



Plots for the flowthrough analysis are included on the following diagram:



This test was conducted on machine spock in directory: $HOME/PA-SCR-394/run/TEST3-28-03.

4-4-03 PA-SCR-394 GADAMS:

A test was conducted to analyze the differences between Test Case 3 conducted within TEST8-15-02 documented under entry 9-10-02 PA-SCR-394 GADAMS in which the radioelements had the standard solubility limits and a test case in which the solubility limits were set artificially high to 1e4. At all solubility limits set to 1e4, the peak mean dose is 3.06e-5 rem/yr at 10000 yr. The previous TEST8-15-02 test case 3 showed that the peak mean dose with normal solubility limits was 1.78e-5 rem/yr at 9450 yr. Both the test conducted under this entry and under the TEST8-15-02 test case were performed with TPA Version 4.1.1CHG2B.

An additional test was performed against tpa version 4.1k to verify the output dose information. The peak mean dose compared well to the 4.1.1CHG2B version; however, there was a difference. The peak mean dose from version 4.1k was 3.05741e-5 rem/yr compared to 3.06067e-5 rem/yr in 4.1.1CHG2B. The difference was at realization 64, subarea 2 where a stepsize underflow occurred in the Cash-Karp Runge-Kutta method of Version 4.1.1 CHG2B.

All testing was performed on machine spock in directory: $HOME/PA-SCR-394/run/TEST3-28-03350REAL.

4-7-03 PA-SCR-446 GADAMS:
Modified the failt module to generate the correct mode to the screen and corrode.out output file. In addition, for corrosion other than aqueous, the corrosion potential (ecor) and the critical potential (ecrit) are both set to zero.

Qualifications for performing this work are proficiency in developing, implementing and maintaining FORTRAN 77 code.

All code modifications were placed on machine spock in directory: ~~$HOME/PA-SCR-39~~ GADAMS 4-7-03 $HOME/PA-SCR-446. TPA code version 5.0c was used for this development work.

4-15-03 EXEC CODE VALIDATION GADAMS:
Created validation code modules for the following subroutines: ccdfindexed, epaccdf, epaccdf_c, putfailwp, setfiles, writedata, writeepaccdf. Some code modules were no

longer used and were commented out. The following modules were commented out: getspnam, putfault, putseism, and putvolcan.

Ccdfindexed.t was created with two test cases each with a set of predefined parameters designed to verify that the subroutine correctly indexes the parameters sent to it.

Epaccdf.t was created with two test cases containing different parameter sets. The test cases are designed to save the current relgwgs.res file, build an input file to replace it, and verify that the correct information is written to the module generated output files (gwccdf.res, gsccdf.res, relccdf.res).

Epaccdf_c.t was created with two test cases containing different parameter sets. The test cases are designed to save the current rlgwgs_c.res file, build an input file to replace it, and verify that the correct information is written to the module generated output files (gwccdf_c.res, gsccdf_c.res, rlccdf_c.res).

Getspnam is no longer invoked and was therefore commented out.

Putfailwp.t was created to run any number of test cases. The executive invokes this routine for each subarea. The test cases are designed to retrieve information from the module variable database and verify that the values passed into the subroutine are the values placed in the database.

Putfault is no longer invoked and was therefore commented out.

Putseism is no longer invoked and was therefore commented out.

Putvolcan is no longer invoked and was therefore commented out.

Setfiles.t was created with a single test case. The setfiles subroutine operates under 4 different modes depending on the value for iflagsetfiles. The 4 modes are tested under test case 1 to verify that the file manipulations for each test mode are carried out.

Writedata.t was created with three test cases. Each of the test cases varies the input parameter set to writedata and ~~vari~~ GADAMS 4-15-03 verifies that the input data set was correctly placed in the subroutine's output file.

Writeepaccdf.t was created with two test cases. The first test case takes a set of nonzero numerical values over 6 time periods and 3 radionuclides and verifies that the writeepaccdf subroutine correctly places the results in the module variable database. The second test case takes a set of zero numerical values over 6 time periods and 3 radionuclides and verifies that the write epaccdf subroutine correctly places the results in the module variable database.

Cumfail.t was modified to run the test cases without changing the normal tpa code output.

The code modules were integrated into TPA Version 5.0 on machine spock in directory: $HOME/exec_validation/tpabuild_50_test1.

4-18-03 PA-SCR-394 GADAMS:
A series of 8 tests was conducted on machine spock using VERSION 4.1.1CHG2B of the TPA code. These tests were the same tests conducted under entry 9-10-02 PA-SCR-394 GADAMS except the solubility limits for some radioelements were modified from constants to distributions. Those radioelements affected are described below:

Solubility_U[kg/m3] was changed from {constant 7.6e-3} to {logtriangular 2.4e-6, 7.6e-3, 2.4e0}

SolubilityCm[kg/m3] was changed from {constant 2.4e-4} to {uniform 2.4e-8, 2.4e-4}

SolubilityTh[kg/m3] was changed from {constant 2.3e-4} to {loguniform 2.3e-7, 2.3e-1}

SolubilityRa[kg/m3] was changed from {constant 2.3e-5} to {logtriangular 2.3e-7,

2.3e-5, 2.3e-3}

SolubilityPb[kg/m3] was changed from {constant 6.6e-5} to {logtriangular 2.1e-6, 6.6e-5, 2.1e-3}

SolubilityNi[kg/m3] was changed from {constant 1.1e-1} to {logtriangular 5.9e-5, 1.1e-1, 5.9e0}

SolubilityNb[kg/m3] was changed from {constant 9.3e-7} to {loguniform 9.3e-8, 9.3e-6}

A table summarizing the results for the eight tests is shown below:

	Time span (with qout > 0) over which the nuclide is solubility limit-controlled							
					Modifications to Test 3			
Nuclide	Test 1	Test 2	Test 3	Test 4	Test 5	Test 6	Test 7	Test 8
Cm246	3.57%	5.55%	35.22%	58.78%	74.81%	0.29%	0.00%	74.72%
U238	92.77%	92.99%	99.05%	99.45%	99.82%	92.71%	15.77%	99.81%
Cm245	3.57%	5.55%	35.22%	58.78%	74.81%	0.29%	0.00%	74.72%
Am241	20.69%	22.99%	88.83%	93.60%	97.88%	31.41%	0.00%	97.79%
Np237	25.29%	27.42%	62.96%	77.72%	90.10%	3.74%	0.00%	89.89%
Am243	20.69%	22.99%	88.83%	93.60%	97.88%	31.41%	0.00%	97.79%
Pu239	85.06%	85.54%	99.64%	99.79%	99.88%	95.97%	0.00%	99.88%
Pu240	85.06%	85.54%	99.64%	99.79%	99.88%	95.97%	0.00%	99.88%
U234	92.77%	92.99%	99.05%	99.45%	99.82%	92.71%	15.77%	99.81%
Th230	38.74%	39.88%	49.08%	58.86%	61.52%	20.55%	0.00%	61.85%
Ra226	20.37%	22.15%	20.29%	40.97%	45.70%	0.03%	0.00%	45.77%
Pb210	0.83%	9.06%	0.00%	12.70%	0.00%	0.00%	0.00%	0.00%
Cs135	0.00%	0.01%	0.00%	0.42%	0.00%	0.00%	0.00%	0.00%
I129	0.00%	0.00%	0.00%	0.04%	0.00%	0.00%	0.00%	0.00%
Tc99	0.00%	0.03%	0.00%	1.39%	0.00%	0.00%	0.00%	0.00%
Ni59	3.71%	5.02%	11.45%	28.71%	28.88%	0.11%	0.00%	29.03%
C14	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Se79	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Nb94	55.90%	57.23%	94.88%	97.04%	99.15%	69.77%	0.00%	98.94%
Cl36	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%

These tests were conducted on machine spock in directory: $HOME/PA-SCR-394/run/TEST4-7-03.

4-24-03 EXEC CODE VALIDATION GADAMS:

The following code modules were edited in order to generate standard validation testing messages to the screen: 1) ccdfindexed.t, 2) setfiles.t, 3) checknr.t, 4) checknsa.t, 5) cleanupwd.t, 6) cumfail.t, 7) epaccdf.t, 8) epaccdf_c.t, 9) findpkmndose.t, 10) putfailwp.t, 11) writeepaccdf.t, 12) writedata.t, 13) writehead.t, 14) writehead2.t.

The code modules were integrated into TPA Version 5.0 on machine spock in directory: $HOME/exec_validation/tpabuild_50_test2.

4-25-03 PA-SCR-394 GADAMS:

A test was conducted to evaluate the effect of flow on the solubility limited release of radionuclides. A mean value case was studied using as a baseline the test4 tpa.inp file from the TEST8-15-02 test included under entry 9-10-02 PA-SCR-394 GADAMS. A mean value tpa.inp file was built and modifications were made to the file as follows: 1) For all test cases, the number of realizations was set to 1 and the test was run for subarea 1 only. 2) For test case 1, the tpa code was run with the ArealAverageMeanAnnualInfiltrationAtStart left at the default value of 8.5. 3) For test case 2, the ArealAverageMeanAnnualInfiltrationAtStart was set to the minimum value of 4.0. 4) For test case 3, the ArealAverageMeanAnnualInfiltrationAtStart was set to the maximum value of 13.0. This testing was conducted on machine spock using VERSION4.1.1 CHG2B of the tpa code. The following table summarizes the test results:

Radionuclide	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 8.5	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 4.0	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 13.0
U238	100%	100%	100%
U234	100%	100%	100%
Pu239	100%	100%	100%
Pu240	100%	100%	100%
Nb94	100%	100%	100%
Am241	100%	100%	100%

Radionuclide	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 8.5	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 4.0	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 13.0
Am243	100%	100%	100%
Np237	100%	100%	100%
Th230	100%	100%	100%
Cm246	42.31%	100%	25%
Cm245	42.31%	100%	25%
Ra226	30.77%	100%	15.38%
Ni59	1.92%	7.69%	1.92%
Pb210	0.0%	0.0%	0.0%
Tc99	0.0%	0.0%	0.0%
Cs135	0.0%	0.0%	0.0%
I129	0.0%	0.0%	0.0%
Se79	0.0%	0.0%	0.0%
Cl36	0.0%	0.0%	0.0%
C14	0.0%	0.0%	0.0%

The testing was conducted in directory: $HOME/PA-SCR-394/run/TEST4-18-03.

5-1-03 PA-SCR-394 GADAMS:

A second test was conducted to evaluate the effect of flow on the solubility limited release of radionuclides. For this test, a baseline tpa.inp file from test4 of TEST8-15-02 identified under entry 9-10-02 PA-SCR-394 GADAMS was used. The tpa.inp file was modified for this test as follows: 1) For test case 1, the ArealAverageMeanAnnualInfiltrationAtStart was set to a constant of 8.5. 2) For test case 2, the ArealAverageMeanAnnualInfiltrationAtStart was set to the minimum value of 4.0. 3) For test case 3, the ArealAverageMeanAnnualInfiltrationAtStart was set to the maximum value of 13.0. The testing was conducted on machine spock using VERSION4.1.1 CHG2B of the tpa code. The following table summarizes the test results:

Radionuclide	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 8.5	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 4.0	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 13.0
U238	99.76%	99.85%	99.68%
U234	99.76%	99.85%	99.68%
Pu239	99.55%	99.66%	99.49%
Pu240	99.55%	99.66%	99.49%
Nb94	97.84%	98.68%	96.83%
Am241	92.25%	95.56%	89.79%
Am243	92.25%	95.56%	89.79%
Np237	77.24%	83.29%	71.89%
Th230	63.49%	73.33%	56.56%
Cm246	46.75%	58.52%	39.97%
Cm245	46.75%	58.52%	39.97%
Ra226	42.53%	54.52%	35.85%
Ni59	13.39%	23.01%	9.43%
Pb210	11.82%	18.19%	7.90%
Tc99	1.54%	1.71%	0.97%
Cs135	0.55%	0.54%	0.34%
I129	0.06%	0.05%	0.03%
Se79	0.0%	0.0%	0.0%
Cl36	0.0%	0.0%	0.0%
C14	0.0%	0.0%	0.0%

The testing was conducted in directory: $HOME/PA-SCR-394/run/TEST4-25-03.

5-16-03 PA-SCR-394 GADAMS:

A test was conducted to evaluate the effect of flow on the solubility limited release of radionuclides in which the solubility limits were changed to distributions for 7 radionuclides. The baseline tpa.inp file used in these tests was taken from test 4 of TEST8-15-02 identified under entry 9-10-02 PA-SCR-394 GADAMS. The tpa.inp

file was modified such that the solubility limits were changed to distributions for several radionuclides as was done under TEST4-7-03 entry 4-18-03 PA-SCR-394 GADAMS.
The following solubility limit information was changed:
1) Solubility_U[kg/m3] was changed from {constant 7.6e-3} to {logtriangular 2.4e-6, 7.6e-3, 2.4e0}.
2) ~~Solubility_~~ GADAMS 5-16-03 SolubilityCm[kg/m3] was changed from {constant 2.4e-4} to {uniform 2.4e-8, 2.4e-4}.
3) SolubilityTh[kg/m3] was changed from {constant 2.3e-4} to {loguniform 2.3e-7, 2.3e-1}.
4) SolubilityRa[kg/m3] was changed from {constant 2.3e-5} to {logtriangular 2.3e-7, 2.3e-5, 2.3e-3}.
5) SolubilityPb[kg/m3] was changed from {constant 6.6e-5} to {logtriangular 2.1e-6, 6.6e-5, 2.1e-3}.
6) SolubilityNi[kg/m3] was changed from {constant 1.1e-1} to {logtriangular 5.9e-5, 1.1e-1, 5.9e0}.
7) SolubilityNb[kg/m3] was changed from {constant 9.3e-7} to {loguniform 9.3e-8, 9.3e-6}.

Secondly, the effect of flow on the solubility limited release of radionuclides was evaluated as was done under TEST4-25-03 entry 5-1-03 PA-SCR-394 GADAMS. The following values were set for ArealAverageMeanAnnualInfiltrationAtStart:
1) For test case 1, it was set to a constant of 8.5.
2) For test case 2, it was set to a constant of 4.0.
3) For test case 3, it was set to a constant of 13.0.

The testing was conducted on machine spock using VERSION4.1.1CHG2B of the tpa code. The following table summarizes the test results:

Radionuclide	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 8.5	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 4.0	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 13.0
U238	99.35%	99.60%	99.01%
U234	99.35%	99.60%	99.01%

Radionuclide	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 8.5	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 4.0	Time span with qout > 0 over which the nuclide is solubility limit controlled. InfiltrationAtStart = 13.0
Pu239	99.54%	99.76%	99.31%
Pu240	99.54%	99.76%	99.31%
Nb94	96.15%	97.83%	95.01%
Am241	93.47%	95.65%	91.28%
Am243	93.47%	95.65%	91.28%
Np237	78.57%	84.39%	74.10%
Th230	56.61%	63.63%	53.80%
Cm246	58.81%	69.99%	52.13%
Cm245	58.81%	69.99%	52.13%
Ra226	39.30%	50.42%	33.87%
Ni59	30.20%	39.40%	27.53%
Pb210	10.86%	18.06%	8.42%
Tc99	0.58%	1.92%	0.77%
Cs135	0.16%	0.66%	0.35%
I129	0.03%	0.08%	0.08%
Se79	0.00%	0.00%	0.00%
Cl36	0.00%	0.00%	0.00%
C14	0.00%	0.00%	0.00%

The testing was conducted in directory: $HOME/PA-SCR-394/run/TEST5-9-03.

5-23-03 PA-SCR-394 GADAMS:

The following information was generated as part of TEST4-7-03 identified under entry 4-18-03 PA-SCR-394 GADAMS:

The radionuclides Pu-239 and Pu-240 showed the longest solubility limited control over the 10,000 year analysis period for the bathtub model. They were solubility limited for 11.6% of the 10,000 year analysis period. In addition, in the flowthrough

model, Pu-239 and Pu-240 were solubility limited for 20.1% of the analysis period and U-238 and U-234 were solubility limited for 20.0% of the analysis period.

The average flowing periods during the 10,000 year simulation periods for the bathtub model and the flowthrough model were 1165.15 years and 2015.8 years, respectively.

5-28-03 PA-SCR-394 GADAMS:
A test was conducted to show the radioelement solubility sampling used for Test 3 of TEST4-7-03 identified under entry 4-18-03 PA-SCR-394 GADAMS. The number of realizations was set to 1000 and the run was interrupted after the first realization. Only the solubility limit sampled values were needed.

A separate code module was used to extract the information for the sampled distributions. This code is titled readsp.f. The module was modified to not retrieve dose information from gwpkdos.res.

The following sampled parameters were analyzed:
SolubilityAm[kg/m3]
SolubilityNp[kg/m3]
Solubility_U[kg/m3]
SolubilityCm[kg/m3]
SolubilityPu[kg/m3]
SolubilityTh[kg/m3]
SolubilityRa[kg/m3]
SolubilityPb[kg/m3]
SolubilityNi[kg/m3]
SolubilityNb[kg/m3].

The testing was conducted on machine spock in directory: $HOME/PA-SCR-394/run/TEST5-23-03.

6-12-03 SVTP Testing GADAMS:
The objective of this task is to perform testing in accordance with the Software Validation Test Plan for the Total-System Performance Assessment Version 5.0 Code.

Test C7-3 was conducted for the Software Validation Test Plan for the Total-System Performance Assessment Version 5.0 Code. The testing was conducted to verify that radionuclide concentrations do not exceed the solubility limits and to evaluate the release rates for low solubility radionuclides. In order to conduct the test, a mean value case was run for one realization and one subarea. In addition, diffusive release was eliminated from the calculations as well as cladding protection. In addition, in order to make the calculations simpler, uniform time steps were used.

For this test, version 5.0f of the TPA code was used. All testing was performed on machine spock. The code was built using f77 version4.2.

Qualifications for performing this work are proficiency in developing, implementing and maintaining FORTRAN 77 code.

For this test, three radionuclides were analyzed: Tc-99, Nb-94, and Ni-59. The expected release rates calculated for these three radionuclides compared well with the values retrieved from file ebsrel.rlt. In addition to the release rates, the concentrations for these three radionuclides were analyzed. Of the three radionuclides, only Nb-94 was solubility limited. However, for all three test cases with both solubility limited and non-solubility limited radionuclides, the radionuclide concentration does not exceed the solubility limit. Therefore, test C7-3 successfully passed.

Test results and build files are located in directory: SPOCKHOMEsvtp_c7-3.

6-12-03 SVTP Testing GADAMS:

Test C1-3 was conducted to verify that the uzflow module could correctly calculate the expected infiltration for each subarea at the current climate. For this test, an external code module, svtp_uzflow_may, was used to generate maydtbl.dat and smaydtbl.dat files for 30, 60, and 120-meter pixels containing nine tables with table 5 at the current climate. Within each table, each subarea contained a different value for the infiltration.

Test C1-3 successfully passed. Infiltration values for the current climate matched the expected values for each of the subareas to within 0.1%. In addition, plots of the

repository with the infiltration values extracted from maydtbl_30m.dat, maydtbl_60m.dat, and maydtbl_120m.dat for the current climate overlaying the subareas confirmed the spatial orientation of infiltration values retrieved by uzflow and averaged for each subarea.

For this test, version 5.0 of the TPA code was used. The code was built using f77 version4.2. All testing was performed on machine spock in directory: SPOCKHOMEsvtp_c1-3.

6-16-03 SVTP Testing GADAMS:
Test E13-1 was conducted to verify that the checkpoint restart feature allows the code to be interrupted and subsequently resumed, and to identify limitations checkpoint restart places on the code in terms of execution speed and storage requirements.

A series of eight tests were conducted to evaluate the checkpoint restart feature. Most of the tests were conducted over ten realizations and the results of these tests were that checkpoint restart took approximately one additional minute of system time. In addition, checkpoint restart took approximately 68 MB of additional storage. This additional storage was used for the checkpoint restart file, check.pnt (67,938,784 bytes). qq GADAMS 6-16-03

A problem was discovered when the output for tests 6 and 7 were compared. The screen output for test 6 showed a peak mean dose of 2.17747e-5; whereas, the screen output for test 7 showed a peak mean dose of 2.18017e-5.

For this test, version 5.0f of the TPA code was used. All testing was performed on machine spock in directory: SPOCKHOMEsvtp_e13-1.

6-26-03 PA-SCR-447 GADAMS:
The objective of this task was to perform testing of the software changes for SCR PA-SCR-447.

Testing was conducted in accordance with the Test Plan for TPA SCR #447 which consisted of one system level test designed to verify that colloid release data is

generated on a subarea basis by the SZFT module. The system level test verified that select append file options could be set to generate the required nefiisz.cum file and that this file contained radionuclide discharge rates to include those for colloidal radionuclides.

The software successfully passed the system level test in accordance with the Test Plan for TPA SCR #447. For this testing, version 5.0h of the tpa code was used. All testing was performed on machine spock in directory: $HOME/PA-SCR-447.

Qualifications for performing this work are proficiency in developing, implementing and maintaining FORTRAN 77 code.

7-1-03 PA-SCR-426 GADAMS:

A series of code changes were made to version tpa 5.0g to correct errors in the code modules. The following changes were made:

1) tpa.inp: Pre and post temperature peak chemistry values as well as delta ecrit values were corrected. Previously, the chemistry values were constants, they were changed to distributions. The delta ecrit values were modified to zero values. Within the SEISMO section of tpa.inp, the references to GridElement were changed to Subarea. Parameter FractionWeldSurface[] was changed to WeldAdvectiveFraction[] to account for the fraction of the surface area from failed welds and is used in the calculation of advective release from the waste package. Three parameters were added to the NFENV section of tpa.inp: IndriftEvaporationTemperature[C], RelativeHumidityTransitionTimeAfterClosure[yr], and RelativeHumidityForVentilatedAir[]. These three parameters are used to modify the calculation for relative humidity at the waste package to reflect conditions in the drift during the operational period and the period immediately following.

2) Module FILEUTIL.F was created. This new module takes file utility routines from SEISMO2 and NFENV, one of which was duplicated between SEISMO2 and NFENV. The following routines were taken from SEISMO2: getRealArray, setRealArray, setStringValue, setRealValue, setIntegerArray, and setIntegerValue. The following routine was taken from NFENV: getIntegerValue.

3) Module MECHFAIL was modified to use the time that backfill is emplaced as the end of the operational period and skip mechanical failure calculations until the

operational period has ended. With this change, drift degradation does not start until after the operational period and any effects due to seismicity are ignored until after the operational period. The major change in the code was to skip any calls to subroutine processElements until after the operational period.

4) Module SEISMO2 was modified such that references to sampled parameters containing the phrase 'GridElement' were replaced with 'Subarea.' The mechfail analysis assigns two grid elements per subarea and each of the parameters is sampled on a subarea basis and not a grid element basis.

5) Module EXEC was modified to sample the hazard curve once per realization instead of once per subarea. Also modified exec.f to reformat the seismo.ech file. This file includes information applicable to all subareas and realizations (the analysis times), applicable to all subareas for a realization (the seismic event history), and applicable to each subarea (the drip shield thickness versus time analysis). In addition, the subroutine writeepaccdf was modified to eliminate the ikey parameter, change the return parameter for the module variable query on 'ArealMassLoading[MTU/acre] to iaml, this query was moved to within the one-time block.

6) Module NFENV was modified to remove the hard-coded z-direction of 2.5 and replaced with the calculated value of (drift diameter / 2). Modified the calculation for relative humidity at the waste package to include the relative humidity at the drift wall. The relative humidity at the drift wall varies from a value retrieved from tpa.inp (RelativeHumidityForVentilatedAir[]) to 1.0 beginning with the first tpa time step after closure.

7) Modified EBSFAIL/EBSFAIL.DEF to use tpa.inp parameter WeldAdvectiveFraction[] instead of FractionWeldSurface[].

8) Modified module RELEASET to pass parameter ftilt (the fraction of the waste packages tilted in the correct orientation for diffusion) to subroutine getWeldWPFactor. If ftilt is positive, the resulting factor is set to FractionWeldSurface[]; otherwise, the resulting factor is set to zero. Also, corrected the code to use the minimum corrosive failure time of either the waste package or the weld.

All code modifications were performed on machine spock in directory: $HOME/PA-SCR-426.

7-3-03 SVTP Testing GADAMS:
Successfully completed three software validation tests using version tpa 5.0i. SVTP C1-1 was an automated test conducted for module UZFLOW. SVTP S6 was conducted for SEISMO2/MECHFAIL. SVTP C7-3 was conducted for EBSREL.

All testing was performed on machine spock in the following directories:
C1-1: $HOME/svtp_c1-1
S6: $HOME/svtp_s6_7-1-03
C7-3: $HOME/svtp_c7-3_7-1-03

7-3-03 SVTP Testing GADAMS:
Successfully completed a software validation test using version tpa 5.0i. SVTP E13-1 was conducted on the checkpoint restart feature of EXEC.

All testing was performed on machine spock in the following directory:
$HOME/svtp_e13-1_7-1-03

7-7-03 SVTP Testing GADAMS:
Successfully completed a software validation test using version tpa5.0i. SVTP C1-3 was conducted on module UZFLOW. This test was used to verify the infiltration values calculated by the UZFLOW module on a subarea basis.

All testing was performed on machine spock in the following directory:
$HOME/svtp_c1-3_7-1-03

7-10-03 SVTP Testing GADAMS:
Successfully completed a software validation test on tpa version 5.0j. SVTP C7-4 was conducted on module EBSREL. This test was used to examine the qualitative correctness of release rate trends with respect to: i) solubility limit, ii) half life, iii) inventory, and iv) radionuclide position in the decay chain. The software validation test passed.

All testing was performed on machine spock in the following directory:
$HOME/svtp_c7-4_7-3-03.

7-14-03 PA-SCR-459 GADAMS:
The objective of this task was to perform testing of the software changes for SCR PA-SCR-459.

Testing was conducted in accordance with the Test Plan for TPA SCR #459 which consisted of one process level test designed to verify that the EBSFILT module correctly bounds variable thigh and that variable dti is no longer negative.

The software successfully passed the process level test in accordance with the Test Plan for TPA SCR #459. For this testing, version 5.0j of the tpa code was used. All testing was performed on machine spock in directory: $HOME/PA-SCR-459.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

7-15-03 PA-SCR-464 GADAMS:
The purpose of this task was to perform error corrections to two tpa files: mechfail.f and itym.dat. Within itym.dat, a typographical error was corrected (line 24, modified Atothoff96 to Stothoff96) in addition, comments were added at lines 306 and 762. Within mechfail.f, the addition to drift height due to seismic activity was limited so that drift height did not exceed the maximum drift failure height. In addition, a debug constant, ID_DEBUG_ROCK was added to allow the user to select the type of rock for debug analysis.

Code modifications were made to tpa version 5.0k. The modified code was executed on machine spock in directory: $HOME/PA-SCR-464.-

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

7-21-03 PA-SCR-464 GADAMS:
Made additional changes to the ITYM preprocessor under this SCR. The following additional changes were made: i) Within itym.dat, the MAP_scheme, MAT_scheme, and MAV_scheme options were removed. ii) Within file estimator.f, the subroutine

calc_DEM_props was removed.

Code modifications were made to tpa version 5.0k. The modified code was executed on machine spock in directory: $HOME/PA-SCR-464_continued.

7-21-03 PA-SCR-451 GADAMS:
The objective of this task was to perform testing of the software changes implemented under scr, PA-SCR-451.

Testing was conducted in accordance with the Test Plan for TPA SCR #451. The testing consisted of two process level tests and two system level tests. The process level tests were designed to verify that i) the dcagw.f code file and the data files (tpa.inp, repdes.dat, and drythick.dat) modified under this scr contained the correct information and ii) the releaset code no longer generates release values when the flow values in ebsflo.dat are all zero. The system level tests were designed to verify that i) subroutine buildCharacterString performs error checking and ii) subroutine cleanupwd removes the required files.

The software successfully passed the process level tests and system level tests in accordance with the Test Plan for TPA SCR #451. For this testing, version 5.0f and 5.0m of the TPA code was used. All testing was performed on machine spock in directory: $HOME/PA-SCR-451.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

7-22-03 SVTP Testing GADAMS:
Successfully completed a software validation test using version tpa 5.0m. SVTP E5-1 was conducted on the SUBAREA module. This validation test was designed to verify that the information generated by module SUBAREA agreed with the information supplied by READER.

All testing was performed on machine spock in the following directory: $HOME/svtp_e5-1

7-25-03 SVTP Testing GADAMS:
Successfully completed a software validation test using version tpa 5.0m. SVTP E5-3 was conducted on the SUBAREA module. This validation test was an automated test designed to verify that calculations of elements (points, circles and lines) within a specified subarea are performed correctly. In this case, the subarea was an assumed area made for the test cases. Validation was performed by verifying that the code correctly detected points, circles, and lines within the subarea and outside the subarea.

All testing was performed on machine spock in the following directory: ~~$HOME/svtp_35-3~~ GADAMS 7-25-03 $HOME/svtp_e5-3.

7-25-03 SVTP Testing GADAMS:
Successfully completed a software validation test using version tpa 5.0m. SVTP E5-2 was conducted on the SUBAREA module. This validation test was designed to verify that the information generated by module SUBAREA is valid when subarea size is changed by dividing one larger subarea into four smaller subareas. In this test, subarea one was split using the midpoints of subarea one's boundaries. The subarea areas were compared before and after the subarea was divided. Also, the number of waste packages ~~and centroid coordinates~~ GADAMS 7-25-03 were compared before and after the subarea was divided. The centroid coordinates were compared to calculated coordinates for just the first of the divided subareas.

All testing was performed on machine spock in the following directory: $HOME/svtp_e5-2.

7-28-03 PA-SCR-457 GADAMS:
The objective of this task was to perform testing of the software changes implemented under scr, PA-SCR-457.

Testing was conducted in accordance with the Test Plan for TPA SCR #457. The testing consisted of one process level test and one system level test. The process level test was designed to verify that the DSFAILT module produces the same drip shield thickness versus time in the new code version as was generated prior to the code change when Fluoride Enhancing Factor was always used. The system level test was

designed to verify that without fluoride enhancement, the DSFAIL/DSFAILT module will correctly generate a linearly decreasing drip shield thickness versus time that corresponds to the drip shield corrosion rate.

The software successfully passed the process level and system level test in accordance with the Test Plan for TPA SCR #457. For this testing, version 5.0h and 5.0m of the TPA code was used. All testing was performed on machine spock in directory: $HOME/PA-SCR-457.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

7-30-03 PA-SCR-458 GADAMS:
The objective of this task was to perform testing of the software changes implemented under scr, PA-SCR-458.

Testing was conducted in accordance with the Test Plan for TPA SCR #458. The testing consisted of 14 process level tests. Thirteen of these tests were designed to verify that an incorrectly formatted ia.dat file will cause TPA execution to stop and an appropriately formatted error message will be generated to the screen. One test verified that multiple sequential comment lines were acceptable in ia.dat.

The software successfully passed the process level tests in accordance with the Test Plan for TPA SCR #458. For this testing, version 5.0o of the TPA code was used. All testing was performed on machine spock in directory: $HOME/PA-SCR-458.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

8-1-03 PA-SCR-394 GADAMS:
A series of 6 tests was conducted on machine spock using VERSION 4.1.1CHG2B of the TPA code. These tests were the same tests conducted under entry 4-18-03 PA-SCR-394 GADAMS for tests 3 (bathtub) and 4 (flowthrough) except that solubility limits were set to constants for all radioelements. The following summarizes the 6

tests:
test1: bathtub study, solubility limits set to constant 200 kg/m3
test2: flowthrough study, solubility limits set to constant 200 kg/m3
test3: bathtub study, solubility limits set to constant 2000 kg/m3
test4: flowthrough study, solubility limits set to constant 2000 kg/m3
test5: bathtub study, solubility limits set to constant 10000 kg/m3
test6: flowthrough study, solubility limits set to constant 10000 kg/m3

These tests were conducted on machine spock in directory: $HOME/PA-SCR-394/run/TEST7-29-03.

8-8-03 TPA TEST GADAMS:
The purpose of this test was to perform a test run using the tpa4.1j code with two tpa.inp parameters set to the sample distributions used in version tpa5.0o. The sample distributions for critical relative humidity for humid air corrosion and critical relative humidity for aqueous corrosion from version 5.0o were used in version 4.1j instead of the values used in 4.1j previously. The following summarizes the values from 4.1j and 5.0o:

```
The following values are present in 4.1j originally:
**
constant
CriticalRelativeHumidityHumidAirCorrosion
0.55
**
normal
CriticalRelativeHumidityAqueousCorrosion
0.6, 0.65
**

The following values are present in 5.0o:
**
constant
CriticalRelativeHumidityHumidAirCorrosion
0.2
**
uniform
CriticalRelativeHumidityAqueousCorrosion
0.242, 0.56
**
```

The screen output peak mean dose from the test is as follows:

exec: Peak Mean Dose is 3.13658E-02 rem/yr at 52300.0 yr.

exec: Run Successfully Completed

The calculated peak mean dose for the compliance period of 10k years is as follows:

```
Peak Mean Dose of    1.60049 mrem/yr occurs at    10000.00 years.
```

This test was conducted on machine spock in directory: $HOME/test8-6-03.

Qualifications for performing this work are proficiency in developing, implementing, and maintaining FORTRAN 77 code.

8-13-03 PA-SCR-394 GADAMS:
Two tests (test1 - bathtub model, test2 - flowthrough model) were conducted on machine spock using VERSION 4.1.1CHG2B of the TPA code. These tests were the same tests conducted under entry 4-18-03 PA-SCR-394 GADAMS for tests 3(bathtub) and 4 (flowthrough) except that solubility limits were set in the range of 10,000 kg/m3 to 10,002 kg/m3.

These tests were conducted on machine spock in directory: $HOME/PA-SCR-394/run/test8-6-03.

Entries into Scientific Notebook #170-16E for pages __1__ - _10__ have been made by George Adams 3/23/05.

No original text entered into this Scientific Notebook has been removed.

9-16-2005 ~~3/23/05.~~ 9-16-2005

I have reviewed this scientific notebook and find it in compliance with QAP-001. There is sufficient information regarding methods used for conducting tests, acquiring and analyzing data so that another qualified individual could repeat the activity.

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