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

SCIENTIFIC NOTEBOOK

170-12E

12.1 TPA CODE VERSION 5.0DEVELOPMENT FOR SCR-382 [entry made by R. Benke on April 4, 2002]

For those TPA input parameters that were effected by this code change, the TPA input parameters were identified with the corresponding symbolic variables used in the forthcoming descriptions. **Before the change SCR-382**, the inhalation dose per year (rem/yr) in DCAGS for the i^{th} radionuclide was calculated as:

$$D_{inh,i}(t) = B \cdot I_i \cdot \eta_i \cdot f_e \cdot f_R(t) \cdot \left[(S_0 - S_\infty) \exp(-\lambda_r t) + S_\infty \right] \tag{1}$$

where

B = breathing rate (m^3/yr),
I_i = Inhalation-to-dose conversion factor for the i^{th} radionuclide (rem/Ci),
f_e = occupancy factor for time fractions the individual is exposed to indoor and outdoor contaminated air (-),
$f_R(t)$ = time-dependent fraction of resuspended mass that emanated from the contaminated volcanic layer (-), equal to the ratio of the ash blanket thickness as a function of time to the thickness of the resuspendable layer, (Note: no code changes were made to this variable, and therefore, it is not described further)
η_i = activity per mass of ash for the i^{th} radionuclide (Ci/g)
S_0 = airborne mass load above fresh ash blanket in the year following deposition (g/m^3) = AirborneMassLoadAboveFreshAshBlanket[g/m3],
S_∞ = airborne mass load at long times after the event (g/m^3) = AirborneMassLoadAboveSoil[g/m3], and
λ_r = rate of reduction of airborne mass load (1/yr) = OccupancyFactorForVolcanismDoseCalculation[-].

After the change SCR-382 to add categories of indoor and outdoor mass loading for heavy and light disturbance, the inhalation dose per year (rem/yr) in DCAGS for the i^{th} radionuclide was calculated as follows:

$$D_{inh,i}(t) = B \cdot I_i \cdot \eta_i \cdot \left\{ \begin{array}{l} \left[f_{out-H}\left(S_{ash-H} - S_{out-H}\right) + f_{out-L}\left(S_{ash-L} - S_{out-L}\right) \right] \cdot f_R(t) \cdot \exp(-\lambda_r t) \\ + \left[f_{out-H} S_{out-H} + f_{out-L} S_{out-L} \right] + \left[f_{in-H} S_{in-H} + f_{in-L} S_{in-L} \right] + \left[f_{offsite} S_{offsite} \right] \end{array} \right\} \tag{2}$$

where

S_{ash-H} = mass load above fresh ash deposit with heavy disturbance (g/m^3) = AirborneMassLoadAboveFreshAshBlanketHeavyDisturbance[g/m3],
S_{ash-L} = mass load above fresh ash deposit with light disturbance (g/m^3) = AirborneMassLoadAboveFreshAshBlanketLightDisturbance[g/m3],
S_{out-H} = outdoor mass load for dust with heavy disturbance (g/m^3) = AirborneMassLoadOutsideHeavyDisturbance[g/m3],
S_{out-L} = outdoor mass load for dust with light disturbance (g/m^3) = AirborneMassLoadOutsideLightDisturbance[g/m3],
S_{in-H} = indoor mass load for dust with heavy disturbance (g/m^3) = AirborneMassLoadInsideHeavyDisturbance[g/m3],
S_{in-L} = indoor mass load for dust with light disturbance (g/m^3) = AirborneMassLoadInsideLightDisturbance[g/m3],
$S_{offsite}$ = offsite mass load (g/m^3) = AirborneMassLoadOffsite[g/m3],
f_{out-H} = fraction of time receptor spends outdoors with heavy disturbance = OccupancyFractionOutsideHeavyDisturbance[-],
f_{out-L} = fraction of time receptor spends outdoors with light disturbance = OccupancyFractionOutsideLightDisturbance[-],
f_{in-H} = fraction of time receptor spends indoors with heavy disturbance = OccupancyFractionInsideHeavyDisturbance[-],
f_{in-L} = fraction of time receptor spends indoors with light disturbance = OccupancyFractionInsideLightDisturbance[-], and
$f_{offsite}$ = fraction of time receptor spends offsite = OccupancyFractionOffsite[-].

12.2 TPA 5.0 BetaB Testing [entry made by R. Benke on December 13, 2002]

12.2.1 TEST

The TPA 5.0 BetaB mean value input file (tpa.inp) was obtained and modified in the following ways:
(1) the simulation time was set to 100,000 yr;
(2) the receptor distance was set to 20 km; and
(3) the output option was set to all outputs.

A mean value run was performed using TPA 5.0 BetaB using the modified tpa.inp file. The input and output files supporting this test are located at /net/spock/home/rbenke/figure316. The spreadsheet and Word Perfect files are located at /net/spock/home/rbenke/figure316/FilesAndPlots.

12.2.2 RESULTS

The Tc-99 and Np-237 release rates from the engineering barrier system (EBS), unsaturated zone (UZ), and saturated zone (SZ) were obtained by subarea and time from the TPA output files (ebsrel.rlt, uzft.rlt, and szft.rlt, respectively) and are plotted in spreadsheets (Tc99ebsrel-rlt.xls and Np237ebsrel-rlt.xls; Tc99uzft-rlt.xls and Np237uzft-rlt.xls; Tc99szft-rlt.xls and Np237szft-rlt.xls, respectively).

12.2.3 COMPARISON

The plots from TPA 5.0 BetaB were compared to the plots in Figure 3-16 of the draft "System-Level Performance Assessment of the Proposed Repository at Yucca Mountain using the TPA Version 4.1 Code" (CNWRA2002-05) [see Figure3-16.wpd]. The TPA 5.0 BetaB total release rate (summation of all ten subareas) was compared to the TPA 4.1j result at five times: 10,000 yr; 30,000 yr; 50,000 yr; 80,000 yr; and 100,000 yr. The ratio of the release rates from the two versions for each time was used to quantify the difference in the versions. To allow for a better visual comparison, the total release rates from TPA 4.1j (corresponding to Figure 3-16) were added to each plot noted in the Results section.

EBS (Tc-99)
For the Tc-99 release rate from the EBS, the two versions were within a factor of about 5.
EBS (Np-237)
For the Np-237 release rate from the EBS, the two versions were within a factor of about 5.

UZ (Tc-99)
For the Tc-99 release rate from the UZ, the two versions were within a factor of about 5.
UZ (Np-237)
For the Np-237 release rate from the UZ, the two versions were within a factor of about 9.

SZ (Tc-99)
For the Tc-99 release rate from the SZ, the two versions were within a factor of about 5.
SZ (Np-237)
For the Np-237 release rate from the SZ, the TPA 5.0BetaB version resulted in an earlier releases from the SZ (arrival at the biosphere). A release rate exceeding 10^{-6} Ci/yr was realized after 5,000 yr in TPA 5.0 BetaB and after about 30,000 yr in TPA 4.1j. The second increase in the release rate also occurred about 20,000 years sooner in TPA 5.0 BetaB (before 70,000 yr in TPA 5.0 BetaB compared to after 90,000 yr in TPA 4.1j), but was slightly more gradual (an increase 1 order of magnitude in the release rate required about 30,000 yr in TPA 5.0 BetaB compared to less than 10,000 yr in TPA 4.1j). Because of the differences in timing of the second increase in the release rate, the release rate at 80,000 yr for TPA 5.0 BetaB was a factor of about 14 greater than the release rate at 80,000 yr for TPA 4.1j. At 100,000 yr, the release rates were within a factor of 1.5.

12.3 Testing the UZFLOW module using TPA 5.0BetaM

[entry made by R. Benke on February 12, 2003]

12.3.1 Robustness testing on UZFLOW inputs in *tpa.inp*

To test the code for robustness, UZFLOW input values were changed in the tpa.inp file. The intermediate output from UZFLOW, namely the *infilper.res* file, was also examined for qualitative consistency with the inputs (i.e., reasonableness check). Errors in executing the TPA code and anomalies in the intermediate outputs from these input changes are documented in Table 12.3-1. Three files were saved for each test run: (i) *tpa.inp*, (ii) *infilper.res*, and (iii) *tpa.out*. As shown in Table 12.3-1, the files from each test run were stored in separate folders within the directory *net/spock/home/rbenke/UZFLOWtest5.0.*

Table 12.3-1. Documentation of the robustness testing on *UZFLOW* inputs using TPA 5.0BetaM.

Test Name (same as folder)	Input values changed from the nominal input file, *tpa.inp*	Notes and Error Messages
Mode 1 Nominal Input	none	
Mode 1 Const Infiltration Values	constant ArealAverageMeanAnnualInfiltrati onAtStart[mm/yr] 9.99 ** constant MeanAnnualPrecipitationMultiplie rAtGlacialMaximum 1.0 ** constant MeanAnnualTemperatureIncreaseAtG lacialMaximum[degC] 0	
Mode 2 Const Infiltration Only	iconstant UZFLOWSampleMode 2 ** constant ArealAverageMeanAnnualInfiltrati onAtStart[mm/yr] 7.77	
Mode 2 Const Infiltration-HydProp	iconstant UZFLOWSampleMode 2 ** constant ArealAverageMeanAnnualInfiltrati onAtStart[mm/yr] 7.77 ** constant UZFLOWHydraulicPropertyUncertain tyDeviation[N(0,1)] 0.0	
Mode 3 Const HydProp-MAP-MAT 1	iconstant UZFLOWSampleMode 3 ** constant ArealAverageMeanAnnualInfiltrati onAtStart[mm/yr] 1.23 ** constant UZFLOWHydraulicPropertyUncertain tyDeviation[N(0,1)] 0.0 ** constant MeanAnnualPrecipitationMultiplie rAtGlacialMaximum 1.0 ** constant MeanAnnualTemperatureIncreaseAtG lacialMaximum[degC] 0	

Mode 3 Const HydProp-MAP-MAT 2	iconstant UZFLOWSampleMode 3 ** constant ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] 32.1 ** constant UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)] 0.0 ** constant MeanAnnualPrecipitationMultiplierAtGlacialMaximum 1.0 ** constant MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC] 0	(Note, more than one realization required to see an effect. `UZFLOWHydraulicPropertyUncertaintyDeviation` affects uncertainty between different realizations.)
Mode 3 Const MAP-MAT Zero HydPropUncert	iconstant NumberOfRealizations 5 ** iconstant UZFLOWSampleMode 3 ** constant ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] 32.1 ** constant UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)] 0 ** constant MeanAnnualPrecipitationMultiplierAtGlacialMaximum 1.0 ** constant MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC] 0	(Note, more than one realization required to see an effect. `UZFLOWHydraulicPropertyUncertaintyDeviation` affects uncertainty between different realizations.)
Mode 3 Const MAP-MAT Small HydPropUncert	iconstant NumberOfRealizations 5 ** iconstant UZFLOWSampleMode 3 ** constant ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] 32.1 ** normal UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)] -2,2 ** constant MeanAnnualPrecipitationMultiplierAtGlacialMaximum 1.0 ** constant MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC] 0	(Note, more than one realization required to see an effect. `UZFLOWHydraulicPropertyUncertaintyDeviation` affects uncertainty between different realizations.)

Mode 3 Const MAP-MAT Large HydPropUncert	iconstant NumberOfRealizations 5 ** iconstant UZFLOWSampleMode 3 ** constant ArealAverageMeanAnnualInfiltrationAtStart[mm/yr] 32.1 ** normal UZFLOWHydraulicPropertyUncertaintyDeviation[N(0,1)] -10,10 ** constant MeanAnnualPrecipitationMultiplierAtGlacialMaximum 1.0 ** constant MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC] 0	(More than one realization required to see an effect. UZFLOWHydraulicPropertyUncertaintyDeviation affects uncertainty between different realizations.)
MAP Multiplier Large 10	constant MeanAnnualPrecipitationMultiplierAtGlacialMaximum 10.0	
MAT Diff Small -5	constant MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC] -5	
MAT Diff Large -30	constant MeanAnnualTemperatureIncreaseAtGlacialMaximum[degC] -30	
No Loss	AnnualInfiltrationLossMode(0=NoLoss,1=LossCalculated) 0	***>>> error in UZFT <<<*** Matrix infiltration is too low for the Van Genuchten curve from DCM3D infil(itime)= 0. time= 0. NSTEP= 1 KMAT(NSTEP)= 0. SATM(N)= 0. N= 1 lmedia(N)= 1.0000000000000 Note: IEEE floating-point exception flags raised: Inexact; Division by Zero; Underflow; See the Numerical Computation Guide, ieee_flags(3M)
Time Step Small 50y	TimeStepForClimate[yr] 50.0	
Time Step Large 2000y	TimeStepForClimate[yr] 2000.0	
MAP Std Dev Small 3	StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 3.0	(smaller effect than MAT Std Dev)
MAP Std Dev Large 10	StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 10.0	
MAT Std Dev Small 2	StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 2.0	(larger effect than MAP Std Dev)

MAT Std Dev Large 20	StandardDeviationOfMATAboutMeanI nOneTimePeriod[degC] 20.0	exec: calling uzflow UZFLOW: Uncertainty parameter: 0.0000E+00 Mean Annual Infiltration at Start(AAI0): 9.7117E+00 val = 55.639603800000 nvec = 4 vec 0. 7.3333333000000 14.666667000000 22.000000000000 out-of-bound error in table interpolation
MAT Std Dev 10	StandardDeviationOfMATAboutMeanI nOneTimePeriod[degC] 10.0	exec: calling uzflow UZFLOW: Uncertainty parameter: 0.0000E+00 Mean Annual Infiltration at Start(AAI0): 9.7117E+00 val = 36.509801900000 nvec = 4 vec 0. 7.3333333000000 14.666667000000 22.000000000000 out-of-bound error in table interpolation
MAT Std Dev 5	StandardDeviationOfMATAboutMeanI nOneTimePeriod[degC] 5.0	exec: calling uzflow UZFLOW: Uncertainty parameter: 0.0000E+00 Mean Annual Infiltration at Start(AAI0): 9.7117E+00 val = 26.944900950000 nvec = 4 vec 0. 7.3333333000000 14.666667000000 22.000000000000 out-of-bound error in table interpolation
Climate Pert Set 1	constant StandardDeviationOfMAPAboutMeanI nOneTimePeriod[mm/yr] 1.0 ** constant StandardDeviationOfMATAboutMeanI nOneTimePeriod[degC] 1.0	(Note, this is the nominal case for tests on the remaining inputs. Non-zero standard deviations were chosen because the following parameters are linked in the UZFLOW module: StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr], StandardDeviationOfMATAboutMeanInOneTimePeriod[degC], CorrelationBetweenMAPAndMAT, and ClimatePerturbationSet.)
MAP-MAT Corr Zero	constant StandardDeviationOfMAPAboutMeanI nOneTimePeriod[mm/yr] 1.0 ** constant StandardDeviationOfMATAboutMeanI nOneTimePeriod[degC] 1.0 ** CorrelationBetweenMAPAndMAT 0.0	(Note, compared to the results from Climate Pert Set 1)

MAP-MAT Corr Positive	constant StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 1.0 ** constant StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 1.0 ** CorrelationBetweenMAPAndMAT +0.8	(Note, compared to the results from Climate Pert Set 1)
Climate Pert Set 2	constant StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 1.0 ** constant StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 1.0 ** iconstant ClimatePerturbationSet 2	(Note, compared to the results from Climate Pert Set 1)
Climate Pert Set 0	ClimatePerturbationSet 0	(Note, compared to the results from Climate Pert Set 1) requested climate noise set out of range!

12.3.2 Robustness testing on external data files

To test the code for robustness, data were changed in the external data files associated with the UZFLOW module. The intermediate output from UZFLOW, namely the *infilper.res* file, was examined for qualitative consistency with the changes (i.e., reasonableness check). The results are presented in Table 12.3-2. Four files were saved for each test run: (i) *tpa.inp*, (ii) *infilper.res*, (iii) *tpa.out.*, and (iv) the modified external data file. As shown in Table 12.3-2, the files from each test run were stored in separate folders within the directory *net/spock/home/rbenke/UZFLOWtest5.0.*

Table 12.3-2. Documentation of the robustness testing on UZFLOW external data files using TPA 5.0BetaM.

Test Name (same as folder)	Description of change to external data	Input values changed from the nominal input file, *tpa.inp*	Notes
External Data Nominal	none	constant StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 0.5 ** constant StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 0.15	
External Data Climato1.dat	increased the value of each random number by one order of magnitude	constant StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 0.5 ** constant StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 0.15	

External Data Climato2.dat	zero climate effect on infiltration set for times less than 6000 yr; constant fraction of 0.9 set between 6000 yr and 10,000 yr	constant StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 0.5 ** constant StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 0.15	
External Data Maydtbl.dat	All -1.??? values were changed to 1.??? and all -2.??? values were changed to 2.???	constant StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 0.5 ** constant StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 0.15	

12.3.3 Recommendations

1. Fix error when `AnnualInfiltrationLossMode(0=NoLoss,1=LossCalculated)` is set to a value of 0.

2. (Optional) Add comment to *tpa.inp* stating that noise data are present for values of up to 2.4 for `StandardDeviationOfMATAboutMeanInOneTimePeriod[degC]`.

3. (Optional) Add comment to *tpa.inp* stating that values for the `iconstant, ClimatePerturbationSet`, should be greater than zero.

ENDING STATEMENTS [entry made by R. Benke on March 21, 2003]

Entries into Scientific Notebook No. 170-12E for pages 12-1 to 12-10 in the period between April 4, 2002 to March 21, 2003 have been made by Roland Benke. No original text entered into this Scientific Notebook has been removed.

Roland Benke — Date

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.

Gordon Wittmeyer, Element Manager — Date

External Data Climato2.dat	zero climate effect on infiltration set for times less than 6000 yr; constant fraction of 0.9 set between 6000 yr and 10,000 yr	constant StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 0.5 ** constant StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 0.15	
External Data Maydtbl.dat	All -1.??? values were changed to 1.??? and all -2.??? values were changed to 2.???	constant StandardDeviationOfMAPAboutMeanInOneTimePeriod[mm/yr] 0.5 ** constant StandardDeviationOfMATAboutMeanInOneTimePeriod[degC] 0.15	

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Roland R. Benke — March 21, 2003

Roland Benke — Date

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.

11-08-05

~~Gordon Wittmeyer, Element Manager~~ — Date

James Winterle

RB