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Calculation Cover Sheet

Complete only applicable items.

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CONTENTS

CONTENTS (continued)

1. PURPOSE

This calculation documents the total system performance assessment modeling of Enhanced Design Analyses (EDA) V. EDA V is based on the TSPA-VA base design which has been modified with higher thermal loading, a quartz sand invert, and line loading with 21 PWR waste packages that have 2-cm thick titanium grade 7 corrosion resistant material (CRM) drip shields placed over dual-layer waste packages composed of 'inside out' VA reference material (CRWMS M&O 1999a). This document details the changes and assumptions made to the VA reference Performance Assessment Model (CRWMS M&O 1998a) to incorporate the design changes detailed for EDA V. The performance measure for this evaluation is expected value dose-rate history. Time histories of dose rate are presented for EDA V and a Defense in Depth (DID) analysis base on EDA V. Additional details concerning the Enhanced Design Alternative II are provided in the "LADS 3-12 Requests" interoffice correspondence (CRWMS M&O 1999a).

2. METHOD

Total system performance assessment calculations require coupling and/or information transfer between models that represent the major components of the repository. These models, their coupling, and input parameter values used in the TSPA-VA base case are described in *Total System Performance Assessment – Viability Assessment Base Case* (CRWMS M&O, 1998a). The overall computational system remains unchanged for the design feature assessments presented in this report. However, the implementation of specific components of the base case total system model have been changed to account for the effects of the design features. The specific changes to the base case model are described in the following sections of this document.

3. ASSUMPTIONS

The assumptions that formed the basis for the TSPA-VA base case model described in *Total System Performance Assessment – Viability Assessment Base Case* (CRWMS M&O, 1998a) are entirely applicable to this calculation with any exceptions detailed below.

Assumptions for EDA V modeling:

3.1 The base case TSPA-VA model is based on a drift spacing of 28 meters and with point loading. For EDA V, the waste packages are placed in a line load and the drift separation is increased to 40 meters with an increased thermal loading of 150 MTU per acre (CRWMS M&O 1999a, p. 17-18). With increased thermal loading the repository design requires 420 acres of the proposed repository block. The assumptions for this 'line load' configuration are inherent within the thermal hydrology data input to the TSPA model (CRWMS M&O 1999d, Item 2). It is also assumed that the same number of waste packages will be used as in the base case.

3.2 Fifty percent of the VA percolation flux was used for the thermal hydrology (CRWMS M&O 1999d, Item 2). This is appropriate based on the TSPA-VA percolation fluxes (CRWMS

M&O 1998f, p. T2-33, Table 40, and the area fraction of the repository). The inputs to the thermal hydrology and EDA-V calculations are reasonable and consistent.

3.3 With the change in the repository footprint, there are associated changes to repository regions. Unlike the TSPA-VA base case in which six repository regions are defined, the EDA V repository is divided into four distinct regions for the total system model. These regions differ from the base case regions and thus have new properties. Changes to the model to account for the new regions include new average percolation fluxes for each region, new waste package distributions, and changes to definition of capture regions within the unsaturated and saturated zone models to account for the placement of the repository regions.

3.4 The basic waste package design is a 21 PWR waste package. For EDA V the waste package is constructed of two materials in an 'inside out' VA configuration. The inner material is A516 carbon steel, approximately 10 cm thick, and the outer material is approximately 2 cm thick Alloy-22 (CRWMS M&O 1999a, p. 18). For the total system performance assessment modeling the base case waste package and EBS geometry was modified to account for the new waste package dimensions. All other assumptions for the waste package materials are inherent within the waste package degradation input tables (CRWMS M&O 1999d, Item 3).

3.5 A drip shield is part of the design feature for EDA V. The drip shields are assumed to have a "mail-box" (inverted U-shaped) configuration and to be placed over the waste packages with a gap between the drip shields and the waste packages to avoid direct contact (CRWMS M&O 1999a). The drip shields are 2-cm thick and are composed of titanium grade 7. It is assumed for the TSPA model that no flux reaches the waste packages or invert while the drip shield remains intact.

3.6 After drip shield failure it is assumed that the flux into the waste package is scaled to the lesser of the available patch area of the drip shield or the waste package.

3.7 Quartz sand was assumed to be the invert material. The invert dimensions remained identical to the base case configuration. Invert Kd values were assumed to be equal to 0 for quartz sand.

3.8 Invert saturation remained at 0.05 residual saturation (DTN: LL990301804242.083 File: ./noBF_1_50_c_j4_17_03e_03_0_preClose/ NUFT_input/ ldth/ DKMrcktb12-97-afmean-j4_bfs10a) until drip shield failure. The invert saturation was calculated after drip shield failure by using the relative permeability curve assuming gravity flow. The flux into the drift was used for this calculation.

4. USE OF COMPUTER SOFTWARE AND MODELS

4.1 SOFTWARE APPROVED FOR QA WORK

The software used for modeling different components of the repository system in the TSPA-VA total system model are listed in this section. The FEHM software (TBV 564) has not been verified at the time of the calculations and the results from these calculations should be considered TBV (to be verified). The software used for the analyses presented in this document include the same software used for the TSPA-VA base case calculation (CRWMS M&O, 1998a). No new software was used for the design feature analyses.

WAPDEG and NUFT are used to produce waste package degradation and thermal hydrology inputs to the total system model. These two software programs are mentioned several times in the calculation section of this document but are not described in this software section. This is appropriate because WAPDEG and NUFT are only used to create tabular input for the total system model and are not executed during the total system calculation (Section 5.3 & Section 5.4).

4.1.1 RIP Version 5.19.01, CSCI: 30055

Installed on a multi-processor Intel Pentium II x86 computer under the Windows NT 4.0 operating system. M&O CPU Tag Numbers: 115783; 115784; 115785; 115786; 111591; 112378; 114227; 112380; 11369; 113067; and 111593.

Since RIP is used as the integrating shell for combining the different components of the repository system, all the input/output files required for running the TSPA-VA total system model are listed in MO9807MWDRIP00.000 and are discussed in CRWMS M&O, 1998a. Files that were changed are provided in the DTN: MO9906MWDRIP83.005.

a) The RIP computer code (Golder Associates, 1998) is an appropriate tool to perform the following functions that are part of the total system performance assessment calculations.

b) This software has been validated over the range it was used. (*Software Qualification Report, Repository Integration Program*, Version 5.19.01, DI: 30047-2003, Rev. 2, CRWMS M&O, 1998c)

c) This software was obtained from Software Configuration Management (SCM) in accordance with the appropriate procedures.

4.1.2 FEHM Version 2.0.0, CSCI: N/A (TBV 564)

FEHM Version 2.0.0 was compiled as a dynamic link library (DLL) with Digital Visual Fortran 5.0 and is used as an external subroutine (fehmn.dll) to RIP 5.19.01. This DLL was installed on a multi-processor Intel Pentium II x86 computer under the Windows NT 4.0 operating system. M&O CPU Tag Numbers: 115783; 115784; 115785; 115786; 111591; 112378; 114227; 112380; 11369; 113067; and 111593.

a) The FEHM computer code is an appropriate tool to perform mass transport simulations in the saturated and unsaturated zones below the potential Yucca Mountain repository (Zyvoloski et.al., 1997, p. 16).

b) This software has not been validated over the range it was used.

c) This software was not obtained from SCM in accordance with the appropriate procedures.

4.2 SOFTWARE ROUTINES

4.2.1 SZ_Convolute, Version 1.0, CSCI: 30038

SZ_Convolute was compiled as a dynamic link library using Digital Visual Fortran 5.0 and is used as an external subroutine (szconv.dll) to RIP. This DLL was installed on a multi-processor Intel Pentium II x86 computer under the Windows NT 4.0 operating system.

The program written in FORTRAN programming language uses a convolution integral technique to combine concentration breakthrough curves based on unit releases with transient radionuclide mass flux at the water table to determine radionuclide concentrations at a specified downstream boundary for which the concentration breakthrough curves were derived. The underlying assumptions in using convolution are: (1) the transport processes and flow fields from the unsaturated zone model and the saturated zone model are independent of one another, (2) the transport processes in the saturated zone model are linear, and (3) steady-state flow is valid for the saturated zone. More information on the formulation and inputs can be found in *Software Routine Report for SZ_Convolute* (CRWMS M&O, 1998d).

4.2.2 EFDR/DCC, CSCI: 30065 V1.0

External Functions for the Dissolution Rate and Diffusion Coefficient Calculations within RIP (EFDR/DCC) (CRWMS M&O, 1998e), contains three DLLs (dynamically linked libraries).

SFDiss, GLDiss, and EDCoef were compiled as dynamic link libraries using Visual C++ 4.0 to be used as external subroutines (sfdis.dll, gldiss.dll, and edc.dll) to RIP. These DLL's were installed on a multi-processor Intel Pentium II x86 computer under the Windows NT 4.0 Operating system. M&O CPU Tag Numbers: 115783; 115784; 115785; 115786; 111591; 112378; 114227; 112380; 11369; 113067; and 111593.

SFDiss is a subroutine written in C programming language to calculate the commercial spent nulcear fuel dissolution rate based on the equation developed from experimental data. More details on the formulas used and inputs for this subroutine can be found in Software Routine Report, *External Functions for Dissolution Rate and Diffusion Coefficient Calculations within RIP for TSPA-VA* (CRWMS M&O, 1998e).

GLDiss is a subroutine written in C programming language to calculate the glass dissolution rate based on the equation developed from experimental data. More details on the formulas used and inputs for this subroutine can be found in Software Routine Report, *External Functions for Dissolution Rate and Diffusion Coefficient Calculations within RIP for TSPA-VA* (CRWMS M&O, 1998e).

EDCoef is a subroutine written in C programming language to calculate the effective diffusion coefficient in an unsaturated porous medium based on the equation developed from experimental data. More details on the formulas used and inputs for this subroutine can be found in Software Routine Report, *External Functions for Dissolution Rate and Diffusion Coefficient Calculations within RIP for TSPA-VA* (CRWMS M&O, 1998e).

4.3 MODELS

The TSPA-VA Base Case conceptual model and computer software used in this calculation are described in detail within *Total System Performance Assessment – Viability Assessment Base Case* (CRWMS M&O, 1998a). The data tracking numbers for the base case model inputs and outputs as well as the documentation sources for this model are contained in the TSPA-VA REV 01 base case calculation (CRWMS M&O, 1998a) (DTN: MO9807MWDRIP00.000). The specific model inputs and outputs relevant to this calculation have also been submitted to the data tracking system (DTN: MO9906MWDRIP83.005) and are discussed further in the next section.

The TSPA-VA base case total system model was selected for use in this calculation because it was specifically designed to calculate total system performance (and the modeling process may be adapted to calculate EDA features) in a manner consistent with the information requirements for the LA Design Selection EDA's.

5. CALCULATION

The TSPA-VA base case model and parameters were used with only minor changes to the RIP, FEHM and SZ_Convolute input files to account for the effects of the design feature. The base case model and parameters are presented in the *Total System Performance Assessment-Viability Assessment Base Case* (CRWMS M&O, 1998a). Components of the base case calculation that were not changed for the design feature analyses are not discussed in this document. Detailed below are only the changes to the base case model that were necessary to evaluate the system performance of EDA V.

In addition to the total system model evaluation with the "inside-out" waste package, a Defense in

Depth (DID) analysis was conducted for EDA V by neutralizing the waste packages.

5.1 DRIP SHIELD MODIFICATIONS

For EDA V a drip shield is part of the design feature. The drip shields are assumed to have a "mail-box" (inverted U-shaped) configuration and to be placed over the waste packages with a gap between the drip shields and the waste packages to avoid direct contact (CRWMS M&O 1999a). The drip shields are 2-cm thick and are composed of titanium grade 7. Table *.t38 (* denotes the file prefix for each unique simulation) contains the drip shield failure time history used as input for EDA V. The WAPDEG input file was NE1a5s5EDA5-ds.rip (DTN MO9904MWDWAP73.001). It is assumed for the TSPA model that no flux reaches the waste packages or invert while the drip shield remains intact (Assumption 3.5). In addition, after drip shield failure, the flux through the waste package is assumed to be scaled to the smaller of the patch area on either the drip shield or the waste package (Assumption 3.6). The following modifications were made to the TSPA-VA base case total system model to implement the drip shield design feature:

5.1.1 No flux through waste packages or invert until drip shield failure (Assumption 3.5)

Modifications were made to the base case file to incorporate Assumption 3.5, no flux through the waste package or through the invert until drip shield failure. The following parameters were modified within the RIP front end to implement this assumption:

1) QDRIP1 through QDRIP6 were copied as ZDRIP1 through ZDRIP6.
2) QDRIP1-6 were replaced with ZDRIP1-6 within the 48 defined environments
3) QDRIP1-6 parameters were modified as follows:
   QDRIP1 = if(PATDSH < =0, 0, ZDRIP1)

Effectively, since QPAT1-6 (flux through the patches) = QDRIP1-6 * FACPAT, and PATDSH = average number of patches on the drip shield (see below), QDRIP1-6 = 0 until drip shield fails, therefore QPAT1-6 = 0 until drip shield fails, and thus no flux through the waste package or invert.

5.1.2 Flux Scaled to the minimum of the patch area (Assumption 3.5)

The following parameters were created or modified:

TPATWP = total number of patches for a waste package = 889 (CRWMS M&O 1999b, Item 1, p. 9)
TPATDS = total number of patches for a drip shield = 965 (CRWMS M&O 1999b, Item 1, p. 7)
PATDSH = Average number of patches on a drip shield (DTN MO9904MWDWAP73.001) = table(03,time,38)
WPPAFR = waste package fraction failed by patches = PATB05/TPATWP

DSPAFR = drip shield fraction failed by patches = PATDSH/TPATDS
ZPATCH = selector for minimum patches (waste package or drip shield) =
if((DSPAFR <= WPPAFR), DSPAFR, WPPAFR)

ZPATCH selects the minimum of the patches available for flux. To implement this within the base case total system model the parameter FRACPA was modified as follows:

FRACPA = ZPATCH * UPATCH,

Since FACPAT = FRACPA for values of FRACPA less than or equal to 1 and QPAT (flux through the patches) = QDRIP (flux into the drift) * FACPAT, therefore the flux through the waste package is effectively scaled to the minimum of the available patches.

5.1.3 Juvenile Failure Flux

The base case parameter QPASF7 was modified to eliminate the flux through the package for a juvenile failed package until the drip shield has failed.

QPASF7 = if(PATDSH <= 0, 0, QDRIP3*((1*PAAREA)/SFAREA)*UPATCH)

5.2 INVERT MODIFICATIONS

For EDA V, the base case concrete invert was removed and replaced with a quartz sand invert (Assumption 3.7). The following modifications have been made to implement the effect of the sand invert: The Kd values of the INVERT media were set equal to zero for all radionuclides (Assumption 3.6). The porosity of the invert was set to 0.4 based upon thermal hydrology input (DTN: LL990301804242.083 File: ./noBF_1_50_c_j4_17_03e_03_0_preClose/ NUFT_input/ ldth/ DKMrcktb12-97-afmean-j4_bfs10a). The residual saturation of the invert was set to 0.05 until drip shield failure, then invert saturation is scaled to the flux through the quartz sand invert (see Attachment I) (Assumption 3.7). To implement this the following parameters were created or modified:

1) UDRIP1 through UDRIP6 to create a parameter for the unit area flux:
UDRIP1 = QDRIP1 / 75 (m^2, CRWMS M&O 1998f, Section 2.5.2.3)
2) SINSF1-6 and SINHL1-6 were modified as follows:
SINSF1 = table(2,UDRIP1,39) = SINHL1, etc.
3) Table 39 (*.t39, * denotes the file prefix for each unique simulation) was created to calculate the invert saturation based on the relative permeability curve assuming gravity flow (see Attachment I for details on this table)

5.3 WASTE PACKAGE DEGRADATION

An 'inside out VA' waste package is used for EDA V. Each waste package was modeled using the WAPDEG code (CRWMS M&O 1999b, Item 1) and output files of the waste package degradation time histories were supplied as input for this calculation. Table 5.1 outlines the modifications made to the base case file to incorporate the new waste package dimensions and waste package failure histories.

Table 5.1: Waste Package Dimensions and Input Tables for Failure Time Histories (CRWMS M&O 1999f, Item 1, p 3 of 34; DTN MO9904MWDWAP73.001)

Parameter/Table	**Description**	**EDA V ('inside-out VA') Value**
LENSF[1]	CSNF package length	5.275 – 0.45 = 4.825 (21-PWR all)
LENHLW[1]	HLW package length	5.367 – 0.45 = 4.917 (5-HLW/DOE long)
SWPRAD	CSNF package radius	0.782 (21-PWR all)
HWPRAD	HLW package radius	1.015 (5-HLW/DOE long)
Table 20 (always drip) *.t20	Waste package degradation history for always dripping packages	NE1a5s5EDA5-wp.rip
Table 35 (no drip) *.t35	Waste package degradation history for no drip packages	NE0a5s6EDA5-wp.rip

[1]For each waste package the length was adjusted to remove the 'skirt', which is used for handling during emplacement and not evaluated in the total system model.
* denotes the file prefix for each unique simulation

5.4 THERMAL HYDROLOGY INPUTS

Thermal Hydrology calculation results are used to replace table 02 (*.t02) and table 05 (*.t05). These tables contain time histories of temperatures for CSNF and HLW/DOE packages. The temperature time histories are different than the base case because of the change in the repository configuration. The temperature profiles for the repository were modeled for EDA V and the results can be found in (DTN: LL990301804242.083, MO9906SPATHRIP.000). The temperature values are used for matrix dissolution rate calculations for the total system model.

5.5 NEW REPOSITORY REGIONS

With the increase in thermal loading (150 MTU per acre) there is an associated decrease in repository area. The repository footprint has also been moved to the northeast of the base case footprint (CRWMS M&O, 1999c). To account the change in repository area, the four repository regions are modified (see assumption 3.3). The change in repository regions creates a change in the average percolation flux for each region, the distribution of packages in the repository and changes to the defined capture regions within the unsaturated and saturated zone models to account for the new locations of the regions. The following sections describe the changes made to account for new repository regions.

5.5.1 Percolation Flux

New percolation flux values were calculated for the new repository regions. The average percolation fluxes were computed from results from the TOUGH2 site scale models (see Attachment II) for current dry (DRY), long term average (LTA) and superpluvial (SP) climates. For details of this calculation, see Attachment II. Table 5.2 shows the values used for the calculation. The parameters PERD1 to 4, PERL1 to 4 and PERS1 to 4 were modified within the RIP front end for the expected value infiltration (INFMTR=2).

Table 5.2 Expected Value Percolation Flux (mm/yr) for EDA V

	DRY (PERD1 to 4)	LTA (PERL1 TO 4)	SP (PERS1 to 4)
Region 1 (A)	1.53396	20.33244	126.3416
REGION 2 (B)	1.63897	22.72911	118.8644
Region 3 (C)	2.4807	25.59147	95.58013
Region 4 (D)	3.10067	31.37456	108.4336

5.5.2 Distribution of Waste Packages

As part of the average percolation calculation (see section 5.5.1 and Attachment II), the fractional area of each repository region was also determined. These fractional areas are used to redistribute the waste packages in the regions for EDA V. As with the base case model, there are 7760 CSNF packages, 1663 HLW packages and 2546 DOESF package (see assumption 3.1). Table 5.3 shows the distribution of the waste packages based on the new fractional areas.

Table 5.3 Regional Waste Package Distribution for EDA V

	Fractional Area	CSNF Packages	HLW Packages	DOESF Packages
Region 1 (A)	0.182938	1420	304	466
Region 2 (B)	0.208171	1615	346	530
Region 3 (C)	0.301401	2339	501	767
Region 4 (D)	0.30749	2386	512	783
Total	1	7760	1663	2546

5.5.3 UZ Modifications

The UZ model was modified to account for the changes in the repository areas. With the new repository areas, the location that particles enter and leave the UZ model were modified. The nodes associated with the repository and water table were changed for each region. The new set of nodes for each region (repository and water table regions) were modified in the FEHM input file 'fmQb.zone6'. Details of the methodology used to select the new nodes at the repository and water table are described in CRWMS M&O 1999e.

5.5.4 SZ Breakthrough Curves

With the change in the repository area, the saturated zone breakthrough curves were modified to account for new capture area at the water table. The scaling factor at the top of the SZ curve files was modified for all of the stream tubes to account for the change in water table area for each region. Details of the calculation are described in Attachment III.

5.6 DID MODIFICATIONS

A single Defense in Depth scenarios was run for the EDA V model by neutralizing the waste package. This calculation is provided to determine the robustness of the total system by removing an important barrier to radionuclide release. This section provides details about the changes made to the model to account for the neutralization of the waste package.

Neutralizing the waste package assumes that the entire inventory is available for transport at time zero. For each source term group the primary failure mode was set to degenerate with a probability equal to 1 at time zero. The juvenile failure source term group SF5 was deleted packages within this source term group were moved to region 4 (SF4). With no waste packages, diffusive releases were assumed to occur through an area equal to half the surface area of the package (either HLW/DOESF or SF package).

ADIFPI = 0 (diffusive area through pits)
FACPIT= 0 (pit fraction)
WPAHLW = Pi * HWPRAD * LENHLW
WPASF = Pi * SWPRAD * LENSF

Flux through the waste form was scaled to the patch area of the drip shield. Prior to drip shield failure, there is no advective flux through the waste form.

For high level waste and DOESF pathways the area for diffusion through patches (ADIFPA) was set equal to WPAHLW, and for spent fuel pathways ADIFPA was set to WPASF. Advective release was scaled to the flux able to pass through the drip shield. ZPATCH was set equal to the DSPAFR, the drip shield patch fraction. In addition, the following parameters were modified:

VWSF = VWRNS * PORWF * SATWF
VWRNS = VRODSF
VWHLW=VWRNH * PORWF * SATWF
VWRNH = VGLSHL
VWDSF = VWRND * PORWF * SATWF
VWRND = VRODDS

5.7 CORRECTION OF INPUT FORMATTING ERROR FROM INITIAL RESULTS

After completion of the "check copy" of this document, a mistake was discovered in the format of the temperature input files (*.t02 and *.t05, see section 5.4 for description of these files). The results became part of the record for the QAP 3-12 Input Design Transmittal for *"Enhanced Design Alternatives I,II, IIIa, IIIb,IV, and V. Best available data from NUFT (Thermal Hydrology), WAPDEG (Waste Package Degradation) and RIP (Total System Performance Assessment) computations"* (CRWMS M&O 1999d). The temperature inputs affect the matrix dissolution rate. With the incorrect format, the temperature values for repository regions 3 and 4 were 0 degrees Celsius after 5,000 years while regions 1 and 2 were provided with the histories for regions 3 and 4 after 5000 years. The correction of the temperature input file should have little effect on the total system results. Results from using both the correct and incorrect temperature input files are provided in Section 6 for completeness.

6. RESULTS

Since unqualified inputs were used in the development of the results presented in this section, they should be considered TBV. This document will not directly support any construction, fabrication, or procurement activity, and therefore, the inputs and outputs are not required to be procedurally controlled as TBV. However, any use of the data from this analysis for inputs into documents supporting construction, fabrication, or procurement is required to be controlled as TBV in accordance with appropriate procedures.

EDA V results are presented for 10,000 year and 1,000,000 year total system performance assessment model simulations. Figures 6.1 and 6.2 contain dose rates per year for the EDA V case and DID waste package neutralization case. The dose rate for the neutralized waste package case is several orders of magnitude higher than the EDA V case for the first 10,000 years following repository closure (Figure 6.1). The dose rate for the DID case is higher than the waste package case for the first 400,000 years (Figure 6.2). Both cases have a similar dose rate after

400,000 years, except around the second SP climate (around 750,000 years after repository closure) were the DID dose rate is nearly an order of magnitude higher than the case with a waste package.

Figures 6.3 and 6.4 show the results using the incorrect format for the temperature input files (see Section 5.7 above). These results were provided in CRWMS M&O 1999d. The results are very similar to the results presented in Figure 6.1 and 6.2 and any conclusions that were made about EDA V based on the initial incorrect results should not be changed.

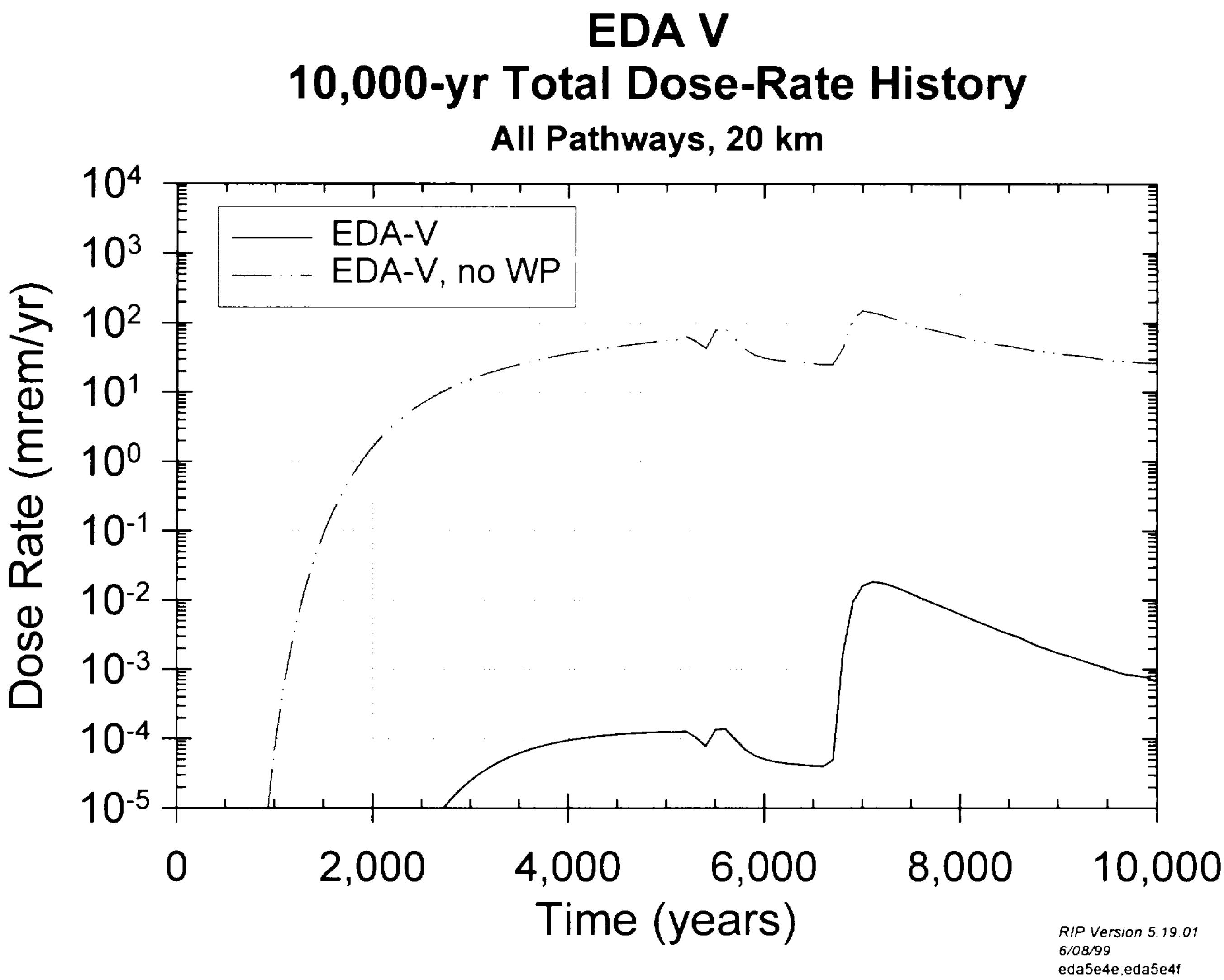

Figure 6.1 10,000-Year Dose Rate Histories for EDA V Analyses.

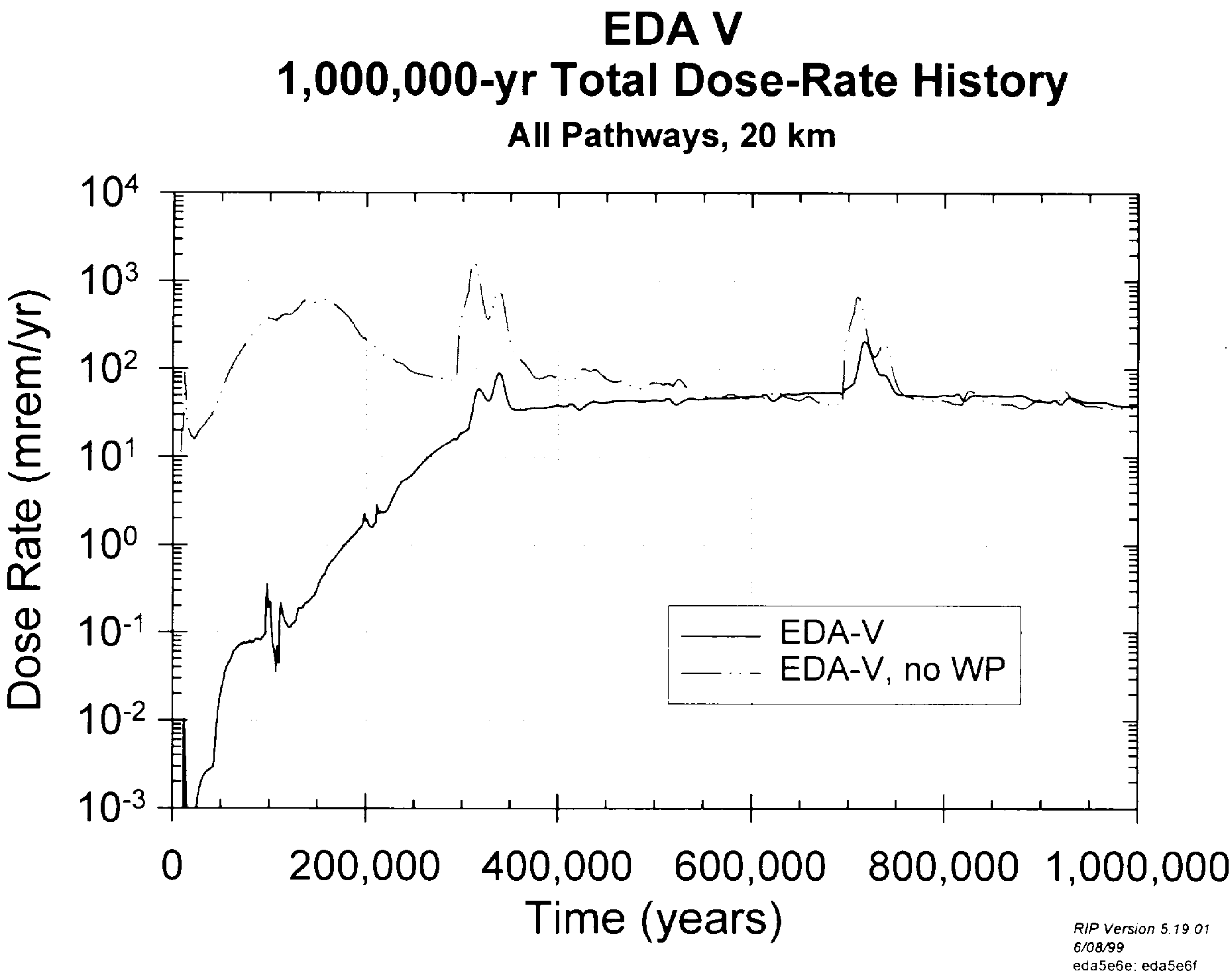

Figure 6.2 1,000,000-Year Dose Rate Histories for EDA V Analyses.

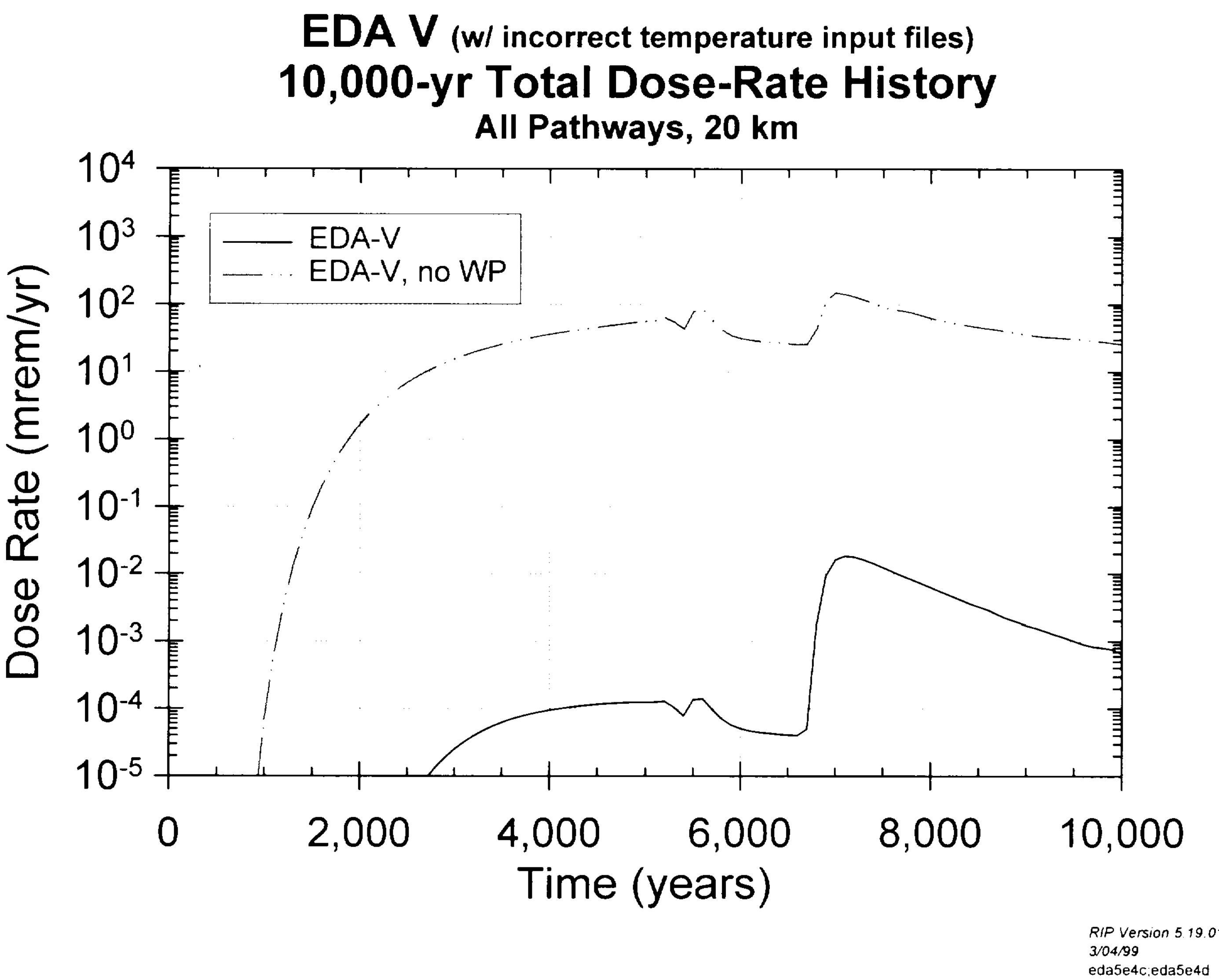

Figure 6.3 Initial 10,000-Year Dose Rate Histories for EDA V Analyses Using Incorrect Temperature Input Files.

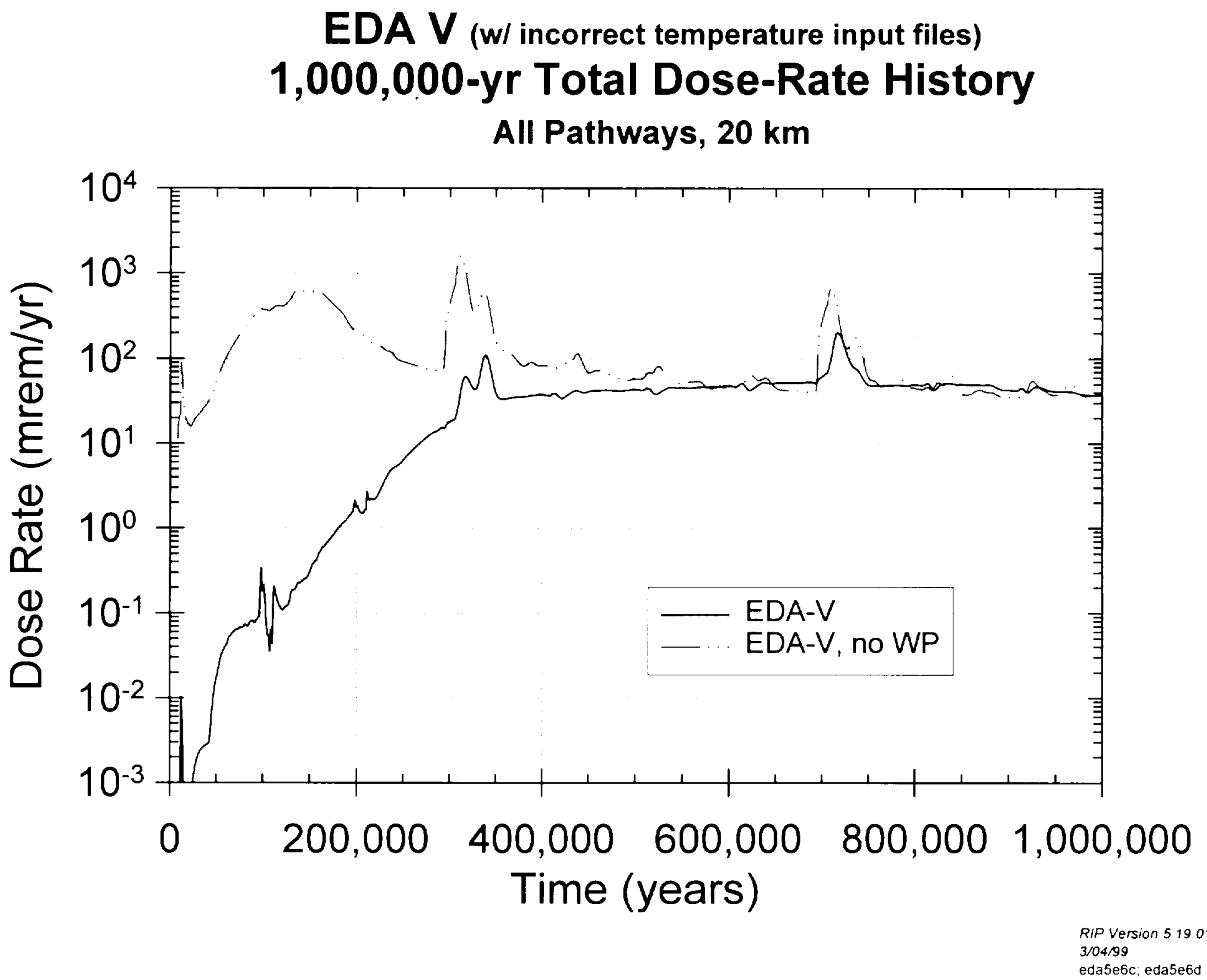

Figure 6.4 Initial 1,000,000-Year Dose Rate Histories for EDA V Analyses Using Incorrect Temperature Input Files.

7. REFERENCES

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8. ATTACHMENTS

I	Calculation of Invert Saturation Under Dripping Conditions
II	Calculation of Average Percolation Rates for Designated Repository Sub-Areas of EDA-V
III	Modification of Saturated Zone Breakthrough Curves

Attachment I

Calculation of Invert Saturation Under Dripping Conditions

Calculation of Invert Saturation Under Dripping Conditions

Introduction

Liquid saturation in the invert material is used to determine the diffusion coefficient (*Fitting of the Data for Diffusion Coefficients in Unsaturated Porous Media*, CRWMS M&O, 1998b), required for calculating the diffusive transport of radionuclides through the invert. For total system performance assessment (TSPA) calculations done in support of the Enhanced Design Alternatives (EDA) study, the liquid saturation of the invert material is assumed to be at the residual level (S_r) till the breach of the dripshield. After the failure of the dripshield, the flux entering the drift is assumed to be in contact with the invert material and the liquid saturation in the invert material corresponding to gravity flow is used for the diffusion coefficient calculation. This is done by equating the hydraulic conductivity of the invert material to the flux entering the drift and calculating the saturation corresponding to this hydraulic conductivity value.

Calculation

All the equations and numerical calculations used to calculate the saturation in the invert under dripping conditions are presented in this section.

The relative hydraulic conductivity (K_r) is defined as (Mualem, 1976, equation 1):

$$K_r = \frac{K}{K_{sat}} \quad \textbf{(1)}$$

$$K = K_r \cdot K_{sat} \quad \textbf{(2)}$$

where hydraulic conductivity K, is a function of the saturation and K_{sat} is the hydraulic conductivity in saturated conditions.

Effective saturation S_e , is defined as (Mualem, 1976, equation 2):

$$S_e = \frac{S - S_r}{S_{max} - S_r} \quad \textbf{(3)}$$

$$S = (S_{max} - S_r)S_e + S_r \qquad (4)$$

where S is the actual saturation, S_r is the residual saturation and S_{max} is the maximum saturation.

Further, relative hydraulic conductivity is defined as (van Genuchten, 1980, equation 8):

$$K_r = S_e^{1/2}[1-(1-S_e^{1/m})^m]^2 \qquad (5)$$

$$m = 1 - \frac{1}{\beta} \qquad (0 < m < 1) \qquad (6)$$

where m and β are the van Genuchten pore size distribution parameters.

Using intrinsic permeability, saturated hydraulic conductivity can be calculated as (de Marsily, 1986, page 60)

$$K_{sat} = \frac{k_{sat} \cdot g}{\nu} \qquad (7)$$

where g is the acceleration due to gravity and ν is the kinematic viscosity.

From thermal hydrology calculations (CRWMS M&O 1999g and DTN: LL990301804242.083), m = 0.7636, S_r = 0.05, S_{max} = 1.0 and intrinsic permeability (k_{sat}) = 1.6E-11 m^2.

k_{sat} = 1.6 x 10^{-11} m^2
g = 9.81 m/s^2 (de Marsily, 1986, p. 412)
ν = 10^{-6} m^2/s (de Marsily, 1986, p. 413, Table A.2.4)

K_{sat} = 1.6 x 10^{-4} m/s

Combining the above information with equations 2, 4, 5 and 6:

$$S = 0.95 \cdot S_e + 0.05 \qquad (8)$$

$$K = (1.6\times10^{-4})\cdot(S_e^{1/2}[1-(1-S_e^{1.31})^{0.7636}]^2) \qquad (9)$$

Using Microsoft Excel-97, a series of effective saturation (S_e) values was generated from 0 to 0.1 at an interval of 0.001 (see Table 1). Using equation 8, saturation values for the corresponding effective saturation values was calculated in the second column. Hydraulic conductivity in *m/s* is calculated using equation 9 (third column). The last column contains the hydraulic conductivity values in *m/yr*. Assuming gravity flow, the flux into the drift was equated to the hydraulic conductivity value and the corresponding saturation value (second column) was used for diffusion coefficient calculation.

Table 1 Hydraulic conductivity vs. saturation values

Effective Saturation	**Saturation**	**Hydraulic Conductivity**	**Hydraulic Conductivity**
S_e	***S***	***K* (m/s)**	***K* (m/yr)**
0	0.0500	0.00E+00	0.00E+00
0.001	0.0510	4.07E-14	1.28E-06
0.002	0.0519	3.54E-13	1.12E-05
0.003	0.0529	1.25E-12	3.96E-05
0.004	0.0538	3.08E-12	9.71E-05
0.005	0.0548	6.18E-12	1.95E-04
0.006	0.0557	1.09E-11	3.44E-04
0.007	0.0567	1.76E-11	5.57E-04
0.008	0.0576	2.68E-11	8.44E-04
0.009	0.0586	3.87E-11	1.22E-03
0.01	0.0595	5.37E-11	1.69E-03
0.011	0.0605	7.23E-11	2.28E-03
0.012	0.0614	9.49E-11	2.99E-03
0.013	0.0624	1.22E-10	3.84E-03
0.014	0.0633	1.54E-10	4.84E-03
0.015	0.0643	1.90E-10	6.00E-03
0.016	0.0652	2.33E-10	7.34E-03
0.017	0.0662	2.81E-10	8.87E-03
0.018	0.0671	3.36E-10	1.06E-02
0.019	0.0681	3.98E-10	1.26E-02
0.02	0.0690	4.67E-10	1.47E-02
0.021	0.0700	5.44E-10	1.72E-02
0.022	0.0709	6.29E-10	1.98E-02

0.023	0.0719	7.23E-10	2.28E-02
0.024	0.0728	8.26E-10	2.60E-02
0.025	0.0738	9.38E-10	2.96E-02
0.026	0.0747	1.06E-09	3.34E-02
0.027	0.0757	1.19E-09	3.76E-02
0.028	0.0766	1.34E-09	4.21E-02
0.029	0.0776	1.49E-09	4.70E-02
0.03	0.0785	1.66E-09	5.23E-02
0.031	0.0795	1.84E-09	5.79E-02
0.032	0.0804	2.03E-09	6.40E-02
0.033	0.0814	2.23E-09	7.04E-02
0.034	0.0823	2.45E-09	7.73E-02
0.035	0.0833	2.68E-09	8.46E-02
0.036	0.0842	2.93E-09	9.24E-02
0.037	0.0852	3.19E-09	1.01E-01
0.038	0.0861	3.47E-09	1.09E-01
0.039	0.0871	3.76E-09	1.19E-01
0.04	0.0880	4.07E-09	1.28E-01
0.041	0.0890	4.40E-09	1.39E-01
0.042	0.0899	4.74E-09	1.50E-01
0.043	0.0909	5.10E-09	1.61E-01
0.044	0.0918	5.48E-09	1.73E-01
0.045	0.0928	5.88E-09	1.86E-01
0.046	0.0937	6.30E-09	1.99E-01
0.047	0.0947	6.74E-09	2.13E-01
0.048	0.0956	7.20E-09	2.27E-01
0.049	0.0966	7.68E-09	2.42E-01
0.05	0.0975	8.18E-09	2.58E-01
0.051	0.0985	8.70E-09	2.74E-01
0.052	0.0994	9.25E-09	2.92E-01
0.053	0.1004	9.81E-09	3.09E-01
0.054	0.1013	1.04E-08	3.28E-01
0.055	0.1023	1.10E-08	3.47E-01
0.056	0.1032	1.17E-08	3.68E-01
0.057	0.1042	1.23E-08	3.89E-01
0.058	0.1051	1.30E-08	4.10E-01
0.059	0.1061	1.37E-08	4.33E-01
0.06	0.1070	1.45E-08	4.56E-01
0.061	0.1080	1.52E-08	4.80E-01
0.062	0.1089	1.60E-08	5.05E-01
0.063	0.1099	1.68E-08	5.31E-01
0.064	0.1108	1.77E-08	5.58E-01

0.065	0.1118	1.86E-08	5.86E-01
0.066	0.1127	1.95E-08	6.15E-01
0.067	0.1137	2.04E-08	6.44E-01
0.068	0.1146	2.14E-08	6.75E-01
0.069	0.1156	2.24E-08	7.06E-01
0.07	0.1165	2.34E-08	7.39E-01
0.071	0.1175	2.45E-08	7.72E-01
0.072	0.1184	2.56E-08	8.07E-01
0.073	0.1194	2.67E-08	8.43E-01
0.074	0.1203	2.79E-08	8.79E-01
0.075	0.1213	2.91E-08	9.17E-01
0.076	0.1222	3.03E-08	9.56E-01
0.077	0.1232	3.16E-08	9.96E-01
0.078	0.1241	3.29E-08	1.04E+00
0.079	0.1251	3.42E-08	1.08E+00
0.08	0.1260	3.56E-08	1.12E+00
0.081	0.1270	3.70E-08	1.17E+00
0.082	0.1279	3.84E-08	1.21E+00
0.083	0.1289	3.99E-08	1.26E+00
0.084	0.1298	4.15E-08	1.31E+00
0.085	0.1308	4.30E-08	1.36E+00
0.086	0.1317	4.46E-08	1.41E+00
0.087	0.1327	4.63E-08	1.46E+00
0.088	0.1336	4.80E-08	1.51E+00
0.089	0.1346	4.97E-08	1.57E+00
0.09	0.1355	5.15E-08	1.62E+00
0.091	0.1365	5.33E-08	1.68E+00
0.092	0.1374	5.51E-08	1.74E+00
0.093	0.1384	5.70E-08	1.80E+00
0.094	0.1393	5.90E-08	1.86E+00
0.095	0.1403	6.10E-08	1.92E+00
0.096	0.1412	6.30E-08	1.99E+00
0.097	0.1422	6.51E-08	2.05E+00
0.098	0.1431	6.72E-08	2.12E+00
0.099	0.1441	6.94E-08	2.19E+00
0.1	0.1450	7.16E-08	2.26E+00

Attachment II

Calculation of Average Percolation Rates for Designated Repository Sub-Areas of EDA-V

Calculation of Average Percolation Rates
for Designated Repository Sub-Areas of EDA-V:

1. Purpose:

The objective of this calculation is to provide average percolation rates for the designated repository sub-areas of enhanced design alternative (EDA) V.

2. Method:

Step 1. Using as input a given list of FEHM node identifiers of the repository nodes and their designated zones, a computer program identifies the corresponding TOUGH2 node identifiers (only TOUGH2 column identifiers for the TOUGH2 grid are needed, because the elevation is the repository horizon).

Step 2. Using as inputs the TOUGH2 node identifiers, TOUGH2 connection data at the repository horizon (between layer 'm' and layer 'n' in the TOUGH2 UZ grid), and the water flux at these connections (extracted from TOUGH2 outputs), a computer program calculates the average percolation rates for the designated repository sub-areas.

3. Assumptions:

N/A.

4. Computer Programs:

Two programs have been used in the calculations:

(1) The computer program used in Step 1 described above is named as 'fehm-tough_node5.f', version 1.0. Two input files are needed; one is a list of FEHM node identifiers, the coordinates and the zone associations, and the other is a standard ELEME input section for TOUGH2. The output file contains, in a format required by 'hgram_eda5.f' (see below), the TOUGH2 identifiers for each of the designated zones. The transition from FEHM identifiers to TOUGH2 identifiers are based on comparisons of coordinates.

A code listing of this program and example input and output files are provided in Appendix I. This is a program performing rather straightforward procedures, therefore, no version control is necessary.

The executable of this program has been obtained by using the HP FORTRAN 90/S700 compiler (version: B.10.20.00).

The program has been verified via visual inspections.

(2) The computer program used in Step 2 described above is named as 'hgram_eda5.f', version 1.0.

This program performs calculation procedures essentially identical to the program, 'hgram.f' (CSCI: 30066 V 1.0). It differs from 'hgram.f' only in a few comment lines about the specifications of two parameters and a requirement on the compatibility of flux file and connection file, and in a calculation and printout of 'total repository area currently counted'. Since the procedures used in 'hgram.f' has been verified, the program 'hgram_eda5.f' needs no further verification.

A code listing of this program is given in Appendix II.

The executable of this program has been obtained by using the HP FORTRAN 90/S700 compiler (version: B.10.20.00).

5. Calculation:

(1). Input and output files used for identifying TOUGH2 node identifiers from designated FEHM identifiers:

Input files:

* eda5node.dat:
A typical line contains zone identifier for a node, x, y, z coordinates, FEHM node identifier.

Total number of zones = 4, identified as A, B, C, and D.

* elem_bas_dkm.dat:
A typical ELEME section of input for the TOUGH2 UZ grid (DTN: LB971100001254.001).

Output file:

* column_ed5.dat:
For each of the zones, list of the column identifiers of those TOUGH2 nodes that correspond to the designated FEHM nodes in 'eda5node.dat'; each list is ended with '&&&'.

(2). Input and output files for calculating the average percolation rates for the designated zones:

Input files:

* column_ed5.dat:

For each of the zones, list of the column identifiers of those TOUGH2 nodes that correspond to the designated FEHM nodes in 'eda5node.dat'; each list is ended with '&&&'.

* repof_bas.con:
A typical CONNE section of input for the TOUGH2 base-case UZ grid (DTN: LB971100001254.001).

* repof_f1.con:
A typical CONNE section of input for the TOUGH2 long-term average UZ grid (DTN: LB971100001254.001).

* repof_f2.con:
A typical CONNE section of input for the TOUGH2 super pluvial UZ grid (DTN: LB971100001254.001).

* mnaqb_p.rep (DTN: LB971212001254.001):
This file is obtained by extracting the flux data from the TOUGH2 TSPA-VA base-case present-day-infiltration output, which is identified with the DTN given in the parentheses. Ignore the first 4 columns; the last column contains the fluxes (at the repository horizon, in kg/sec) listed in the exact same order as the corresponding connections given in 'repof_bas.con', where these fluxes are defined.

* mnaqbf1.repfract (DTN: LB971212001254.001):
Similar to 'mnaqb_p.rep', but for the long-term average climate.

* mnaqbf2.repfract (DTN: LB971212001254.001):
Similar to 'mnaqb_p.rep', but for the super pluvial climate.

6. Results:

* mnaqb_p_rep.out: the results including the average percolation rates for 'mnaqb_p.rep'.

```
flux filename=mnaqb_p.rep
******* domain ID=domA
number of blocks in the domain= 14
area-total for the domain (m*m) = 365340.0
area-fraction of total repository = 0.182938
average percolation flux (mm/yr) = 1.53396
total repository area currently counted= 365340.0
sum of current dom-area fractions: sum_tot= 0.182938
******* domain ID=domB
number of blocks in the domain= 64
area-total for the domain (m*m) = 415733.0
area-fraction of total repository = 0.208171
```

average percolation flux (mm/yr) = 1.63897
total repository area currently counted= 781073.0
sum of current dom-area fractions: sum_tot= 0.391109
******* domain ID=domC
number of blocks in the domain= 19
area-total for the domain (m*m) = 601921.0
area-fraction of total repository = 0.301401
average percolation flux (mm/yr) = 2.4807
total repository area currently counted= 1382994.
sum of current dom-area fractions: sum_tot= 0.69251
******* domain ID=domD
number of blocks in the domain= 11
area-total for the domain (m*m) = 614080.0
area-fraction of total repository = 0.30749
average percolation flux (mm/yr) = 3.10067
total repository area currently counted= 1997074.
sum of current dom-area fractions: sum_tot= 1.0

* mnaqbf1_p_rep.out: the results including the average percolation rates for 'mnaqbf1.repfract'.

flux filename=mnaqbf1.repfract
******* domain ID=domA
number of blocks in the domain= 14
area-total for the domain (m*m) = 365340.0
area-fraction of total repository = 0.182938
average percolation flux (mm/yr) = 20.33244
total repository area currently counted= 365340.0
sum of current dom-area fractions: sum_tot= 0.182938
******* domain ID=domB
number of blocks in the domain= 64
area-total for the domain (m*m) = 415733.0
area-fraction of total repository = 0.208171
average percolation flux (mm/yr) = 22.72911
total repository area currently counted= 781073.0
sum of current dom-area fractions: sum_tot= 0.391109
******* domain ID=domC
number of blocks in the domain= 19
area-total for the domain (m*m) = 601921.0
area-fraction of total repository = 0.301401
average percolation flux (mm/yr) = 25.59147
total repository area currently counted= 1382994.
sum of current dom-area fractions: sum_tot= 0.69251
******* domain ID=domD
number of blocks in the domain= 11
area-total for the domain (m*m) = 614080.0

area-fraction of total repository = 0.30749
average percolation flux (mm/yr) = 31.37456
total repository area currently counted= 1997074.
sum of current dom-area fractions: sum_tot= 1.0

* mnaqbf2_p_rep.out: the results including the average percolation rates for 'mnaqbf2.repfract'.

flux filename=mnaqbf2.repfract
******* domain ID=domA
number of blocks in the domain= 14
area-total for the domain (m*m) = 365340.0
area-fraction of total repository = 0.182938
average percolation flux (mm/yr) = 126.3416
total repository area currently counted= 365340.0
sum of current dom-area fractions: sum_tot= 0.182938
******* domain ID=domB
number of blocks in the domain= 64
area-total for the domain (m*m) = 415733.0
area-fraction of total repository = 0.208171
average percolation flux (mm/yr) = 118.8644
total repository area currently counted= 781073.0
sum of current dom-area fractions: sum_tot= 0.391109
******* domain ID=domC
number of blocks in the domain= 19
area-total for the domain (m*m) = 601921.0
area-fraction of total repository = 0.301401
average percolation flux (mm/yr) = 95.58013
total repository area currently counted= 1382994.
sum of current dom-area fractions: sum_tot= 0.69251
******* domain ID=domD
number of blocks in the domain= 11
area-total for the domain (m*m) = 614080.0
area-fraction of total repository = 0.30749
average percolation flux (mm/yr) = 108.4336
total repository area currently counted= 1997074.
sum of current dom-area fractions: sum_tot= 1.0

7. References:

N/A.

8. Appendix I: Code Listing of fehm-tough_node5.f, version 1.0, and Example Input and Output Files.

(1) Code Listing:

```
c
c     To find the corresonding TOUGH nodes for given FEHM nodes defined
c     into subregions. For the TOUGH2 nodes, only column identifiers
c     are output to a file.
c
c     Before each run, provide the input file name for unit-11,
c     the output file name for unit-21,
c     and the parameter: node_end, the last node in the input file.
c
      parameter (num_dkm=37604*2,node_end=36101)
      parameter (dist_min=0.5, delev_min=1.0, dy_min=1.0, dx_min=1.0)
      character dom_id*1,dom_id_old, elem*5,ma1*3,ma2*2

      open(11, file='eda5node.dat', status='old')
      open(12, file='elem_bas_dkm.dat', status='old')

      open(21, file='column_eda5.dat')

      read(11,*)
      read(11,*)
      dom_id_old=' '
1000  read(11,*) dom_id, x1, y1, z1, node1
      write(6,'(a1,3(f15.3),i10)') dom_id, x1, y1, z1, node1
      if(dom_id.ne.dom_id_old.and.dom_id.ne.'A') write(21,'(a3)') '&&&'
      if(dom_id.ne.dom_id_old) write(21,'(a3,a1)') 'dom',dom_id
      dom_id_old=dom_id
      rewind(12)
      read(12,*)
      do 200 i=1,num_dkm
        read(12,1499) elem,ma1,ma2,evol,aht,x2,y2,z2
        if((elem(1:1).eq.'M').or.(abs(z2-z1).gt.delev_min)
     + .or.(abs(y2-y1).gt.dy_min).or.(abs(x2-x1).gt.dx_min)) goto 200
 1499     FORMAT(A5,10X,A3,A2,2E10.4,10x,3f10.3)
          dist=sqrt((x2-x1)**2+(y2-y1)**2+(z2-z1)**2)
          if(dist.le.dist_min) goto 300
 200  continue
 300  write(21,'(a3)') elem(3:5)
      if(node1.ne.node_end) goto 1000
      write(21,'(a3)') '&&&'
      close(21)
      stop
      end
```

(2) Example Input Files:

eda5node.dat:

```
Sub-Region  East(X)        North(Y)         Z             node
12345678901234567890123456789012345678901234567890123456789012345678901
A      171700.016   233675.797  1008.970     23356
A      171700.281   234040.656  1024.780     23425
A      171719.016   233840.797  1030.340     23559
A      171800.281   233940.656  1018.010     23869
A      171900.281   233600.656  1025.610     24231
A      172017.141   233734.984  1016.700     24653
```

A	172020.625	233940.953	1016.680	24695
A	172057.750	233882.203	1015.860	24848
A	172103.875	233505.938	1007.730	25000
A	172119.266	233752.484	1014.500	25037
A	172187.063	233628.875	1003.400	25205
A	172213.406	233825.656	1005.880	25327
A	172261.016	233690.516	1000.320	25521
A	171583.781	234102.719	1010.650	35599
B	171482.016	234491.703	1007.220	3499
B	171510.109	234405.344	1008.610	3581
B	171524.156	234362.188	1007.990	3605
B	171535.281	234232.656	1035.440	3628
B	171538.188	234319.000	1005.300	3652
B	171560.578	234450.094	1004.280	3676
B	171665.188	234442.484	1029.440	23174
B	171674.938	234231.188	1028.910	23242
B	171680.578	234370.094	1030.020	23286
B	171705.344	234316.734	1027.890	23517
B	171705.766	234402.281	1027.500	23538
B	171728.172	234204.281	1023.950	23580
B	171730.563	234350.516	1026.340	23624
B	171732.125	234573.188	1023.200	23645
B	171740.563	234375.516	1025.190	23692
B	171772.156	234283.719	1022.190	23780
B	171794.156	234323.438	1021.140	23824
B	171815.656	234155.844	1016.370	23937
B	171820.641	234240.984	1018.140	24001
B	171850.641	234274.984	1017.430	24044
B	171860.641	234200.281	1015.070	24086
B	171875.281	234080.656	1013.580	24129
B	171890.625	234314.703	1016.680	24173
B	171890.641	234235.281	1015.070	24194
B	171903.625	234260.703	1015.330	24274
B	171920.125	234140.828	1013.570	24340
B	171940.625	234300.703	1014.660	24361
B	171947.125	234186.828	1014.680	24406
B	171958.266	234018.672	1015.430	24493
B	171969.125	234226.547	1015.330	24514
B	171990.625	234058.953	1016.280	24558
B	171991.109	234266.266	1014.010	24579
B	172020.609	234118.391	1017.970	24674
B	172056.594	234178.109	1016.680	24827
B	172060.625	234070.953	1017.520	24869
B	172078.594	234217.828	1012.950	24913
B	172090.625	234010.953	1018.040	24958
B	172122.094	234089.953	1016.720	25058
B	172135.625	233940.953	1014.330	25100
B	172144.094	234129.672	1013.570	25121
B	172166.078	234169.375	1010.350	25163
B	172180.594	233980.063	1012.860	25184
B	172209.578	234041.516	1010.730	25283
B	172231.563	234081.219	1007.450	25416
B	172253.563	234120.938	1004.200	25458
B	172297.063	233993.063	1004.780	25601
B	172300.063	233920.063	1004.100	25661
B	172319.047	234032.781	1002.270	25682
B	172340.563	233865.188	1001.390	25724
B	172406.547	233984.344	996.420	25971
B	172428.531	234024.063	994.850	25992
B	172472.031	233896.188	1044.300	26075
B	172494.016	233935.906	1042.250	26160

```
B       172515.516  233768.297  1044.080     26240
B       172516.016  233975.609  1040.530     26261
B       172559.516  233847.734  1039.740     26297
B       172581.500  233887.453  1038.070     26318
B       172603.500  233927.172  1036.890     26390
B       171625.281  234232.656  1029.090     35640
B       171621.953  234331.703  1030.620     35681
B       171622.578  234377.094  1010.710     35723
B       171622.578  234420.094  1011.380     35764
B       171615.438  234495.297  1010.330     35807
B       171571.625  234549.203  1012.830     35848
C       171648.719  234646.156  1029.970     23102
C       171766.203  234487.844  1020.050     23736
C       171800.047  234900.047  1033.930     23845
C       171816.156  234363.156  1019.990     23958
C       171860.125  234442.594  1017.520     24065
C       171905.844  234670.609  1017.380     24295
C       171947.625  234394.156  1013.100     24427
C       172122.578  234297.266  1006.220     25079
C       172283.047  234342.313  1040.660     25558
C       172324.047  234566.047  1033.710     25702
C       172450.047  234260.047  1038.990     26012
C       172472.516  234103.484  1042.440     26096
C       172600.047  234500.047  1027.070     28877
C       172602.203  234326.516  1027.870     28898
C       172647.484  234006.609  1036.020     29068
C       172650.047  234150.047  1034.940     29110
C       171559.250  234730.375  1018.230     35891
C       171563.891  234885.281  1025.370     35934
C       171615.734  235027.625  1020.830     35978
D       171803.797  235214.594  1012.270     23914
D       171945.297  235450.109  1012.420     24383
D       171990.047  235080.047  1013.330     24535
D       172067.672  234869.906  1006.850     24890
D       172211.891  235111.922  1002.950     25304
D       172250.047  234750.047  1039.870     25436
D       172450.047  235075.047  1040.840     26033
D       172506.203  234781.391  1032.890     26219
D       171615.938  235237.531  1017.420     36022
D       171631.984  235537.094  1018.470     36066
D       171700.047  235575.047  1015.810     36101
```

elem _bas_dkm.dat:

```
ELEME
Fi   1          tswF10.1206E+030.1000E+01       168400.500 229900.000 1044.6900
Mi   1          tswM10.1352E+070.0000E+00       168400.000 229900.000 1044.6900
Fj   1          tswF20.1046E+040.1000E+01       168400.500 229900.000 1030.5200
Mj   1          tswM20.8111E+070.0000E-00       168400.000 229900.000 1030.5200
Fk   1          tswF30.1703E+040.1000E+01       168400.500 229900.000  994.0800
Mk   1          tswM30.1622E+080.0000E-00       168400.000 229900.000  994.0800
...
...
...
BT428           botbd0.2521E+550.0000E+00       172081.760 232401.650  730.4200
BT451           botbd0.2548E+550.0000E+00       172170.760 232500.650  730.4900
BT469           botbd0.2789E+550.0000E+00       172243.900 232630.170  730.5800
BT498           botbd0.2809E+550.0000E+00       172343.780 232847.080  730.6900
BT515           botbd0.3767E-550.0000E+00       172405.800 233019.850  730.6700
BT527           botbd0.3106E-550.0000E+00       172453.630 233243.630  730.8100
```

(2) Example Output File:

column_eda5.dat:

```
domA
310
314
320
344
371
4 8
410
424
433
435
453
461
476
273
&&&
domB
246
256
262
263
264
269
3 1
3 4
3 7
318
319
321
323
324
326
332
337
350
354
359
361
364
368
369
373
376
385
388
393
395
4 0
4 1
4 9
423
425
427
```

(2) Example Output File:

column_eda5.dat:

```
domA
310
314
320
344
371
4 8
410
424
433
435
453
461
476
273
&&&
domB
246
256
262
263
264
269
3 1
3 4
3 7
318
319
321
323
324
326
332
337
350
354
359
361
364
368
369
373
376
385
388
393
395
4 0
4 1
4 9
423
425
427
```

430
436
445
446
450
452
459
468
472
482
486
489
496
516
517
530
537
544
545
554
559
567
293
290
291
292
286
272
&&&
domC
297
330
342
351
360
374
389
437
479
490
523
531
564
566
576
578
268
270
287
&&&
domD
347
387
399
426
460
471
524
543
G38
G83

```
311
&&&
```

9. Appendix II: Code Listing of hgram_eda5.f, version 1.0.

```
C
C     To produce percolation histograms & average percolcations
c     for given subdomains of the repository area at the repository
C     horizon (m & n layers) with prescribed lists of columns.
C
C     Parameters:
C       kode_his=1, calculate histograms;
C               =0, no histogram calculations.
C       serr_kg = expected sum-level (close to 1.0) for flux in kg/s;
C       serr_mm = expected sum-level (close to 1.0) for flux in mm/yr.
C       eps = tolerance for error between actual sum and expected sum.
C     Input Files:
C     column.dat --- subdomain IDs and lists of columns.
C     conne.dat --- vertical connections with area sizes.
C     qflux=filename --- containing percolation flux in the sequence
C                           of the connections.
C     Output Files:
C       phkg.out --- percolation historgrams in kg/s.
C       avg_phmm.out --- average percolation &
C                         percolation historgrams in mm/yr.
C
C     Note: numcon=numflu=1467 for f1 (long-term average climate),
C           numcon=numflu=1429 for f2 (super pluvial climate),
c           but numcon=numflu=1470 is suitable for all cases.
c           Total area = 6725763.0 for eda1.
c                      = 4626160.0 for eda2.
c                      = 1997074.0 for ead5.
c
c           'qflux' must be compatible with 'conne.dat' in terms of both
c           the total number of lines and the sequence.

      parameter (kode_his=0,serr_kg=0.000,serr_mm=0.9999,eps=0.001)
      parameter (numdom=6,numcon=1470,numflu=1470, totarea=1997074.)
      parameter (rmin_kg=0,rmax_kg=0,delt_kg=0)
      parameter (rmin_mm=0,rmax_mm=2.0,delt_mm=2.0)
      character ecol*3,EL1*2,EL2*2,NE1*3,NE2*3,dom*4
      character*40 qflux
      data qflux/'mnaqb_p.rep' /

      open(21, file='column_eda5.dat', status='old')
      open(22, file='repof_bas.con', status='old')

      open(23, file=qflux, status='old')

      open(25, file='domain.tmp')
      open(26, file='phkg.out')
      open(27, file='avg_phmm.out')

      sum_tot=0.
      area_tcur=0.
      write(27,*) 'flux filename=',qflux
1000  numd=numd+1
      area_tot=0.
```

```
      read(21,*) dom
      write(27,*) '******* domain ID=',dom
      rewind(25)
      numcol=0
2000  numcol=numcol+1
        rewind(22)
        rewind(23)
        read(22,*)
        read(23,*)
c*** read the column:
        read(21,100) ecol
100     format(A3)
        if(ecol.eq.'&&&') goto 3000
c*** find the corresponding area and its sequential number:
        do j=1,numcon
          READ(22,20) EL1,NE1,EL2,NE2,NSEQ,NAD1,NAD2,ISOT,D1,D2,AREAX,BETAX
20        FORMAT(A2,A3,A2,A3,4I5,4E10.4)
          if(NE1.eq.ecol) then
            area_col=AREAX
            area_tot=area_tot+AREAX
            nums_col=j
            goto 120
          endif
        enddo
c*** find the corresponding flux (fracture, or matrix, or total):
120     do k=1,numflu
          read(23,*) d1,d2,d3,d4,xflux
          if(k.eq.nums_col) then
            fkg_col=xflux
            fmm_col=xflux*3.1536e07/area_col
            goto 140
          endif
        enddo
c*** write ecol, area_col, fkg_col, and fmm_col to a file:
140     write(25,200) ecol, area_col, fkg_col, fmm_col
cinf        write(6,200) ecol, area_col, fkg_col, fmm_col
200     format(A3,3e15.4)
      goto 2000

C*** find the area-weighted average percolation for the domain
3000  write(25,*)
      rewind(25)
      numcol=numcol-1
      avg_per=0.
      do i=1,numcol
        read(25,200) ecol, area_col, fkg_col, fmm_col
        avg_per=avg_per+area_col*fmm_col
      enddo
      avg_per=avg_per/area_tot
      write(27,*) 'number of blocks in the domain=',numcol
      write(27,*) 'area-total for the domain (m*m) =', area_tot
      write(27,*) 'area-fraction of total repository =',area_tot/totarea
      write(27,*) 'average percolation flux (mm/yr) =', avg_per
      sum_tot=sum_tot+area_tot/totarea
      area_tcur=area_tcur+area_tot
      write(27,*) 'total repository area currently counted=',area_tcur
      if(kode_his.eq.0) goto 6000

c*** check the fkg_col & fmm_col against flux group intervals to
c*** identify the groups to which they belong, then to add their area
c*** contributions to the total area fraction of the groups:
```

```
      sum_areaf_kg=0.
      sum_areaf_mm=0.
      m=0
4000  m=m+1
       dkg1=rmin_kg+(m-1)*delt_kg
       dkg2=rmax_kg+(m-1)*delt_kg
       dmm1=rmin_mm+(m-1)*delt_mm
       dmm2=rmax_mm+(m-1)*delt_mm
       areaf_kg=0.
       areaf_mm=0.
       rewind(25)
       do i=1,numcol
        read(25,200) ecol, area_col, fkg_col, fmm_col
        if(fkg_col.gt.dkg1.and.fkg_col.le.dkg2) then
         areaf_kg=areaf_kg+area_col/area_tot
        endif
        if(fmm_col.gt.dmm1.and.fmm_col.le.dmm2) then
         areaf_mm=areaf_mm+area_col/area_tot
        endif
       enddo
       sum_areaf_kg=sum_areaf_kg+areaf_kg
       sum_areaf_mm=sum_areaf_mm+areaf_mm
       write(26,300) dkg1,dkg2,areaf_kg
       write(27,300) dmm1,dmm2,areaf_mm
300    format(3e12.4)

      if(abs(sum_areaf_kg-serr_kg).gt.eps.or.
     +       abs(sum_areaf_mm-serr_mm).gt.eps) goto 4000

      write(26,*) 'sum_areaf_kg=',sum_areaf_kg
      write(27,*) 'sum_areaf_mm=',sum_areaf_mm
6000  write(27,*) 'sum of current dom-area fractions: sum_tot=',sum_tot
      if(numd.lt.numdom) goto 1000
      stop
      end
```

10. Attachments:

All the related files, including the programs, 'fehm-tough_node5.f' and 'hgram_eda5.f', and the final output files for the results, are provided in the data associated with the DTN: MO9904MWDWAP73.001.

Attachment III

Modification of Saturated Zone Breakthrough Curves

Modification of Saturated Zone Breakthrough Curves

For these set of simulations, the transport of radionuclides in the saturated zone (SZ) was modeled following the same approach of TSPA-VA (see Chapter-8 for more details, CRWMS M&O, 1998g). One dimensional transport using streamtubes was used to calculate concentration of radionuclides 20 km downstream from the repository. Four streamtubes were used corresponding to the four source sub regions at the water table as shown in Figure III-1. Assuming the same flowpaths for the radionuclides exiting at the water table, the breakthrough curves for these streamtubes are similar to the breakthrough curves used for the expected-value TSPA-VA base case, except for the cross-sectional area of the streamtubes. Similar to TSPA-VA, the breakthrough curves generated based on a unit release for these streamtubes are used in a convolution integral program to calculate the time varying concentrations based on the mass flux at the water table. This convolution integral program (szconv.dll) is run along with the total system model.

The cross-sectional area for these streamtubes are specified as the ratio between the volumetric groundwater flow rate from each source region at the water table and the specific discharge within the streamtubes. The product of cross-sectional area and the dilution factor is input as the first line in the breakthrough curve files used as input to the convolution integral program. The cross-sectional area term in all the breakthrough curve files for the four streamtubes were modified to account for the volumetric groundwater flow rates in the four source subregions as shown in Figure III-1. The volumetric groundwater flow rates for the four regions are shown in Table III-1.

Region	Volumetric groundwater flow rate (kg/s)	Volumetric groundwater flow rate (m^3/yr)	Cross-sectional area (m^2)
A	0.041	1294.97	2158.29
B	0.225	7108.62	11847.71
C	0.156	4903.88	8173.13
D	0.273	8620.84	14368.06

Table III-1 Volumetric groundwater flow rates for EDA-V

The calculation of volumetric groundwater flow rates is discussed in CRWMS M&O, 1999h. The volumetric flux in kg/s is converted to m3/yr by dividing with the specific density of water and converting the time units to years. The cross-sectional area shown in column 4 of the table is calculated by dividing the volumetric groundwater flow rate (m^3/yr) with a specific discharge of 0.6 m/yr (Section 8.3.3, Chapter-8, CRWMS M&O, 1998g). These cross-sectional areas along with a dilution factor of 10 (CRWMS M&O 1998g, Table 8-19) are used as input to a software routine ASAP (CRWMS M&O 1999i) for the modification of the saturated zone breakthrough curves to account for the volumetric groundwater flow rates in the four source subregions for EDA-V.

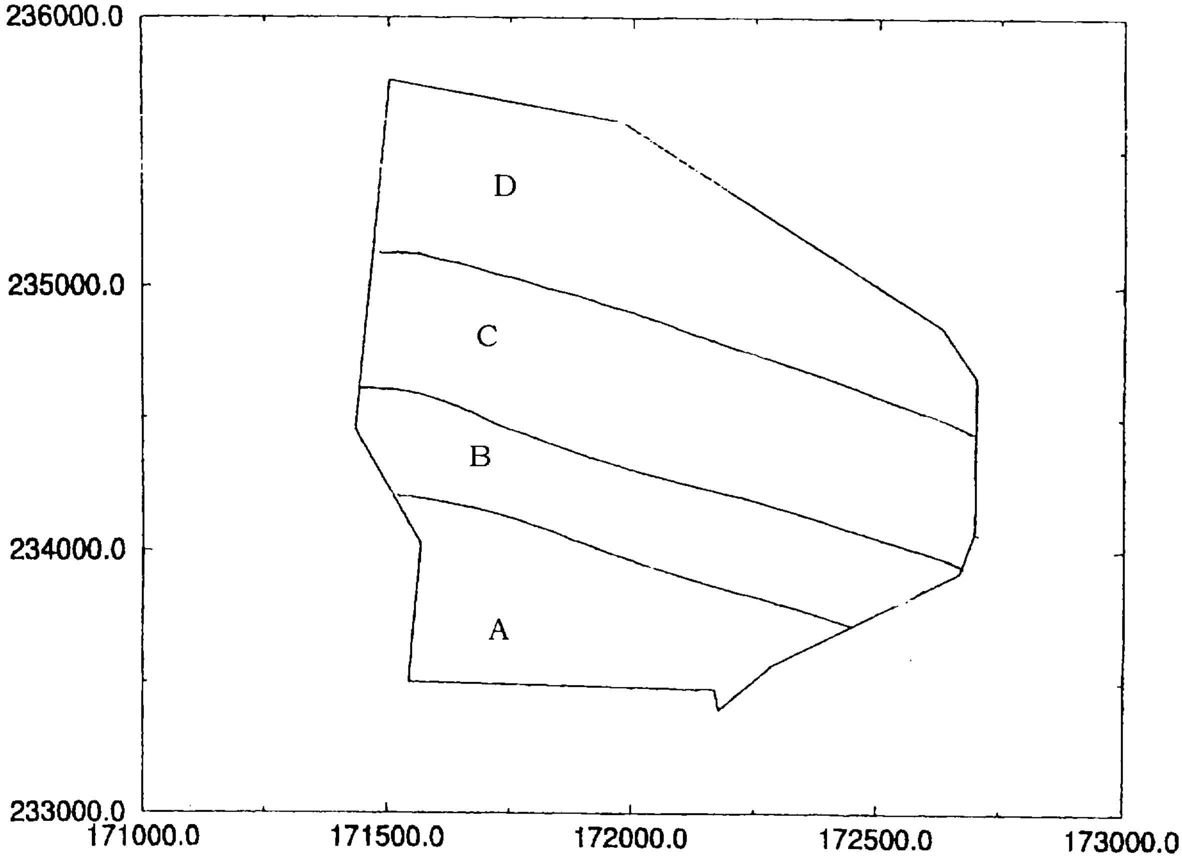

Figure III-1. Repository regions for EDA-V