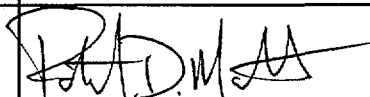
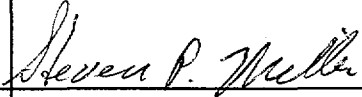



Calculation Cover Sheet

Complete only applicable items.

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1. PURPOSE

The purpose of this calculation is to document total system performance assessment modeling of Enhanced Design Alternative (EDA) Feature IV. Total System Performance Assessment (TSPA) calculations for EDA IV are based on the TSPA-VA Base Case which has been modified with a quartz sand invert, quartz sand backfill, line loading and 21 PWR waste packages that have 2-cm thick titanium grade 7 corrosion resistant material (CRM) drip shields that are placed over a 30 cm thick carbon steel (A516) waste package with an integral filler material (CRWMS M&O 1999a & 1999b). 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 IV. The performance measure for this evaluation is the expected value dose-rate history at 20 km from the repository boundary. Additional details concerning the Enhanced Design Alternative IV 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 IV modeling:

- 3.1 The base case TSPA-VA model is based on a drift spacing of 28 meters and a waste package spacing of 14 meters (CRWMS M&O 1998a). For EDA IV, the waste packages are placed 0.1 meters apart and the drift separation is increased to 56 meters occupying 740 acres, nearly the same footprint as the VA reference design (CRWMS M&O 1999a). Note that the areal loading remains unchanged because the drifts are farther apart than for the base case. The assumptions for this 'line load' configuration are inherent within the thermal hydrology data input to the TSPA model (CRWMS M&O 1999c and CRWMS M&O 1999d).
- 3.2 The basic waste package design is a 21 PWR waste package. For EDA IV the waste package

- is constructed of 30 cm thick carbon steel A516 (CRWMS M&O 1999b, Table 1). For the total system performance assessment modeling the assumptions for the waste package materials are inherent within the waste package degradation input tables (CRWMS M&O 1999c, Item #3 and CRWMS M&O 1999e).
- 3.3 A drip shield is part of the design features for EDA IV. 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, p. 15). It is assumed for the TSPA model that no flux reaches the waste packages or invert while the drip shield remains intact.
 - 3.4 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.
 - 3.5 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.
 - 3.6 Invert liquid saturation remained at 5% residual saturation (CRWMS M&O 1999d, DTN: DTN: LL990301704242.082 File: ../sandBF_85_c_j4_12_03_02_001/NUFT_input/ldth/DKMrectb12-97-afmean-j4_bfs10a) until drip shield failure. The invert saturation was calculated after drip shield failure using the relative permeability curve assuming gravity flow (Attachment I)
 - 3.7 Juvenile failure package does not see flux until drip shield failure.
 - 3.8 As part of EDA IV the waste packages contain an integral filler incorporated into their interior structure (CRWMS M&O 1999b, Table 1). One hundred percent of the integral filler mass is assumed to be available for sorption of radionuclides.

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.

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 the Technical Database tracking system under DTN: MO9807MWD RIP00.000 and are discussed in CRWMS M&O, 1998a. The files used for this calculation are provided in the DTN: MO9905MWD RIP82.000.

- a) The RIP computer code (Golder Associates, 1998) is an appropriate tool to perform the 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 (SQR), Repository Integration Program (RIP)*, 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

Software Routine Report, External Functions for the Dissolution Rate and Diffusion Coefficient Calculations within RIP for TSPA-VA, Version 1.0 (EFDR/DCC) (CRWMS M&O, 1998e), contains three DLL (dynamically linked libraries).

SFDiss, GLDiss, and EDCoef were compiled as dynamic link libraries using Visual C++ 4.0 to be used as external subroutines (sfdiss.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 nuclear 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 the Dissolution Rate and Diffusion Coefficient Calculations within RIP for TSPA-VA, Version 1.0* (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 the Dissolution Rate and Diffusion Coefficient Calculations within RIP for TSPA-VA, Version 1.0* (CRWMS M&O, 1998e).

EDCoef is a subroutine written in C programming language to calculate the effective diffusion coefficient in an unsaturated porous media 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 the Dissolution Rate and Diffusion Coefficient Calculations within RIP for TSPA-VA, Version 1.0* (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, 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: MO9807MWD RIP00.000). The specific model inputs and outputs relevant to this calculation have also been submitted to the data tracking system (DTN: MO9905MWD RIP82.000) and are discussed further in the next section.

The TSPA-VA base case RIP 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 input files to account for the effects of the design features. 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. Only changes to the model and its parameters are presented here.

The RIP base case TSPA-VA model remains unchanged in respect to design features which include: 1) 'line-loading'; 2) repository footprint; 3) repository geometry; 4) invert geometry; and 5) the total number of waste packages. These EDA design features are incorporated into the process level modeling prior to inclusion within the total system model (CRWMS M&O, 1999c, Items #1, 2, and 3, CRWMS M&O, 1999d and CRWMS M&O 1999e) and therefore no changes to the TSPA-VA base case model were required. Detailed below are only the changes to the base case total system model that were necessary to evaluate the system performance of the design alternative.

Additionally, it was requested that a Defense in Depth (DID) analysis be conducted on EDA IV. A

neutralized waste package case was run for EDA IV. Details of these modifications are outlined in Section 5.6.

5.1 DRIP SHIELD MODIFICATIONS

For EDA IV a drip shield is part of the design features. 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 & 1999b). Table *.t38 (*denotes the file prefix for each unique simulation) contains the drip shield failure time history used as input for EDA IV. The WAPDEG input file used for table 38 was NE1a5s5EDA4-ds.rip (CRWMS M&O 1999e and DTN: MO9904MWDWAP72.002). It is assumed for the TSPA model that no flux reaches the waste packages or invert while the drip shield remains intact (Assumption 3.3). 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 3.4). 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 3.3)

Modifications were made to the base case file to incorporate Assumption 3.3, no flux through the waste package or through the invert until drip shield failure. The following parameters within the RIP frontend were modified 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) QDRIP parameters were modified as follows:

$$\text{QDRIP1} = \text{if}(\text{PATDSH} \leq 0, 0, \text{ZDRIP1})$$

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

5.1.2 Flux Scaled to the minimum of the patch area (Assumption 3.4)

The following parameters were created or modified :

TPATWP = total patches for a waste package = 1271 (Assumption 3.16 in CRWMS M&O 1999e, p. 10)

TPATDS = total patches for a drip shield = 1102 (Assumption 3.4 in CRWMS M&O 1999e, p. 7)

PATDSH = Average number of patches on a drip shield (CRWMS M&O 1999e, DTN:MO9904MWDWAP72.002) = table(03,time,38)

WPPAFR = waste package patch fraction = $\text{PATB05}/\text{TPATWP}$

DSPA FR = drip shield patch fraction = $\text{PATDSH}/\text{TPATDS}$

ZPATCH = selector for minimum patches (waste package or drip shield) =
 $\text{if}((\text{DSPAFR} < \text{WPPAFR}), \text{DSPAFR}, \text{WPPAFR})$

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

$$\text{FRACPA} = \text{ZPATCH} * \text{UPATCH},$$

Since $\text{FACPAT} = \text{FRACPA}$ 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 (Assumption 3.7)

The base case parameter QPAS7 was modified to eliminate the flux through the package for a juvenile failed package until the drip shield has failed.

$$\text{QPAS7} = \text{if}(\text{PATDSH} \leq 0, 0, \text{QDRIP3} * ((1 * \text{PAAREA}) / \text{SFAREA}) * \text{UPATCH})$$

5.2 INVERT MODIFICATIONS

For EDA IV, the concrete invert was replaced with a quartz sand invert (Assumption 3.5). Modifications had to be made to the base case file to remove the sorptive capacity of the concrete, and modify the physical parameter of the base case invert to the properties of the quartz sand. The K_d values of the INVERT media were set equal to zero for all radionuclides (Assumption 3.5). The porosity of the invert was set to 0.4 based upon thermal hydrology input (DTN: LL990301704242.082 File: ../sandBF_85_c_j4_12_03_02_001/NUFT_input/ldth/DKMrcktb12-97-afmean-j4_bfs10a). The residual saturation of the invert was set 0.05 (DTN: LL990301704242.082) until drip shield failure, after which it was calculated from the relative permeability curve assuming gravity flow (Assumption 3.6). To implement this the following parameters were created or modified:

- 1) UDRIP1 through UDRIP6 to create a parameter for the flux per unit area (m/yr):

$$\text{UDRIP1} = \text{QDRIP1} / 75 \text{ (m}^2\text{, CRWMS M\&O 1998g)}$$
- 2) SINSF1-6 and SINHL1-6 were modified as follows: $\text{SINSF1} = \text{table}(2, \text{UDRIP1}, 39)$
- 3) Table 39 was created to calculate the invert saturation (see Attachment for details on this table)

5.3 WASTE PACKAGE DEGRADATION

The basic waste package design is a 21PWR waste package. For EDA IV the waste package is constructed of carbon steel A516 (CRWMS M&O 1999a, p. 14 & 1999b, Table 1). The waste package degradation was modeled using the WAPDEG code (CRWMS M&O 1999e and DTN: MOL.199904MWDWAP72.002) and output files of the waste package degradation time histories were supplied as input for this calculation. Table 5.1 outlines the modification made to the base case file to incorporate the new waste package dimensions and waste package failure histories (CRWMS M&O 1999e and DTN: MOL.199904MWDWAP72.002). For carbon steel waste packages, always dripping and no drip waste package groups have identical waste package failure histories (CRWMS M&O 1999e and DTN: MOL.199904MWDWAP72.002).

Table 5.1: Waste Package Dimensions and Input Tables for Failure Time Histories (CRWMS M&O 1999a, 1999b, & 1999e and DTN: MOL.199904MWDWAP72.002)

Parameter/Table	EDA IV (A516)
LENSF ¹ (length of SF waste package)	5.635 – 0.45 = 5.185
LENHLW ¹ (length of HLW and DOESF waste package)	5.667 – 0.45 = 5.217
SWPRAD (spent fuel waste package radius)	1.012
HWPRAD (HLW and DOESF waste package radius)	1.24
Table 20 (always dripping) *.t20 (waste package degradation time history)	NE1a5s5EDA4-wp.rip
Table 35 (no drip) *.t35 (waste package degradation time history)	NE1a5s5EDA4-wp.rip

¹For 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.

5.4 THERMAL HYDROLOGY INPUTS

Waste package surface temperature used as input for waste form degradation models are updated based on thermal hydrology calculations. The average waste package surface temperature (T_{wp}) in each of the six repository regions and for both commercial spent nuclear fuel (CSNF) and high level waste (HLW) are fed into RIP using multi-dimensional tables. Thermal Hydrology calculation results for EDA IV are used to replace table 02 (*.t02) and table 05 (*.t05) of the base case total system model (*denotes the file prefix for each unique simulation). The temperature profiles for the repository were modeled for EDA IV and the results can be found in (CRWMS M&O 1999d and DTN: LL990301704242.082).

5.5 FILLER MATERIALS

A feature of EDA IV is the use of an integral filler (CRWMS M&O 1999a, p. 14 and CRWMS M&O 1999b, Table 1). To account for the retardation of radionuclide transport through the waste package due to the waste package filler material the following adjustments were made to incorporate the sorptive effects of the filler. A new material (media) called FILLER was added to the RIP model to take credit for the sorption of the basket corrosion materials and fillers. New parameters were

added for the partition coefficients (LANL, 1997, p136, table 25):

KDCBA = partition coefficient of Carbon = $0.055 \text{ m}^3/\text{kg}$
 KDNPBA = partition coefficient of Neptunium = $0.75 \text{ m}^3/\text{kg}$
 KDPUBA = partition coefficient of Plutonium = $3.0 \text{ m}^3/\text{kg}$
 KDUBA = partition coefficient of Uranium = $0.55 \text{ m}^3/\text{kg}$
 KDPABA = partition coefficient of Protactinium = $0.75 \text{ m}^3/\text{kg}$
 KDSEBA = partition coefficient of Selenium = $0.03 \text{ m}^3/\text{kg}$

The mass of the material was added to each of the waste package cells using the following parameters:

BASSF = total mass of steel basket material and filler for available for commercial spent nuclear fuel (CSNF)

BASHLW = total mass of basket material and filler available for high level waste (HLW)

BASDF = total mass of basket material and filler available for DOE spent fuel (DOESF)

The total mass used for each of these parameters are defined below (CRWMS M&O 1998f, Tables 6.1.1 and 6.2.1):

CSNF = 10021 kg (mass of basket material) + 8460.1 kg (mass of filler material) = 18481.1 kg

HLW = 7629.6 kg (mass of basket material) + 18759.6 kg (filler material) = 26389.2 kg

DOESF = 8797.4 kg (basket + filler materials)

For DOESF and HLW co-disposal packages the total mass fraction for each waste type must be calculated assuming for each co-disposal package 5/6 of the mass is HLW, and 1/6 DOESF. The following adjustments must be made:

BASHLW = $26389.2 \text{ kg} * 5/6 = 21991 \text{ kg}$

BASDF = $(26389.2 \text{ kg} * 1/6 * (1663 \text{ co-disposal packages}/2546 \text{ packages total}) + (8497.4 * (883 \text{ DOESF packages}/2546 \text{ packages total})) = 5923.9 \text{ kg}$

BASSF = 18481 kg

5.6 DEFENSE IN DEPTH MODIFICATIONS

The DID analyses evaluate the effects of the different barriers on the total system performance by neutralizing the respective barriers, rendering them ineffective to the retardation of flow and transport of radionuclides. The DID case was run in addition to the 'base case' EDA IV model. For EDA IV DID modifications were made only to neutralize the waste package performance. The modifications to the EDA IV base case are outlined as follows:

5.6.1 Neutralized Waste Packages

Neutralizing the waste package assumes that the entire radionuclide 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 SF7 was removed and a single package was added to the total for the source term in region 3 (SF3). With no waste packages, diffusive releases were assumed to occur through half the surface area of the package (either HLW or SF package).

$$ADIFPI = 0 \text{ (diffusive area through pits)}$$

$$FACPIT = 0 \text{ (pit fraction)}$$

$$WPAHLW = P_i * HWPRAD * LENHLW$$

$$WPASF = P_i * SWPRAD * LENSF$$

The flux through the waste form was scaled to the patch area on the drip shield (see Section 5.1).

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 passing through the drip shield. ZPATCH was set equal to the DSPAFR, the drip shield patch fraction. In addition, the following parameters were modified:

$$VWSF = VWRNS * PORWF * SATWF$$

$$VWRNS = VRODSF$$

$$VWHLW = VWRNH * PORWF * SATWF$$

$$VWRNH = VGLSHL$$

$$VWDSF = VWRND * PORWF * SATWF$$

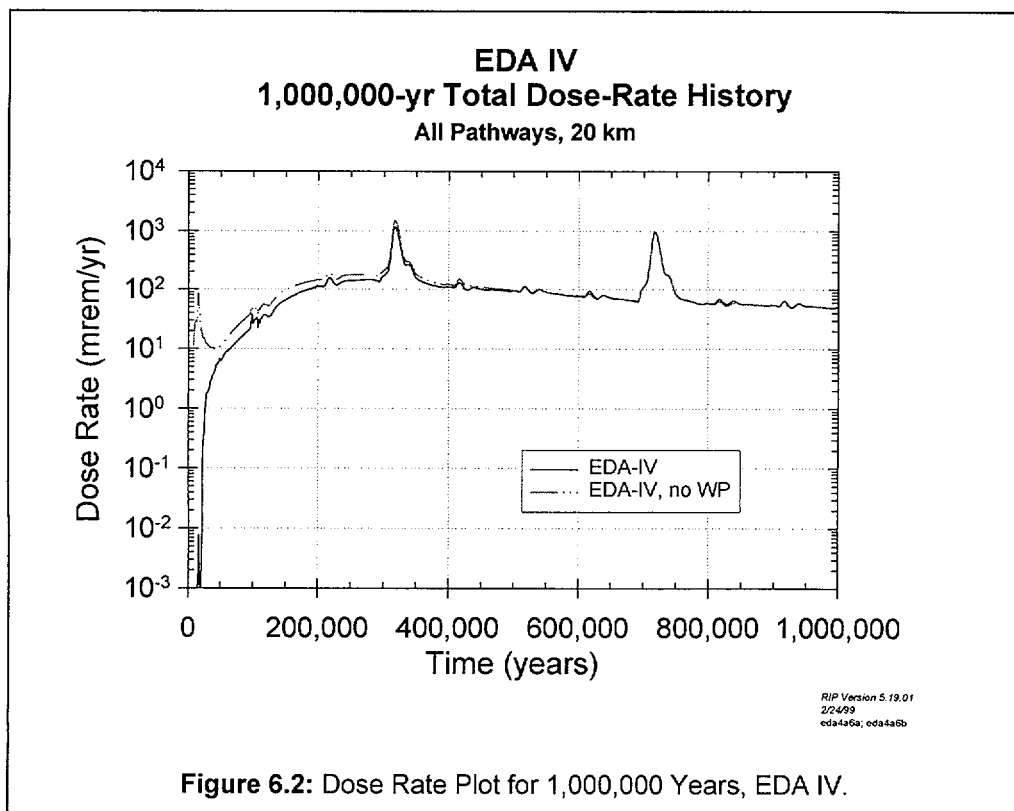
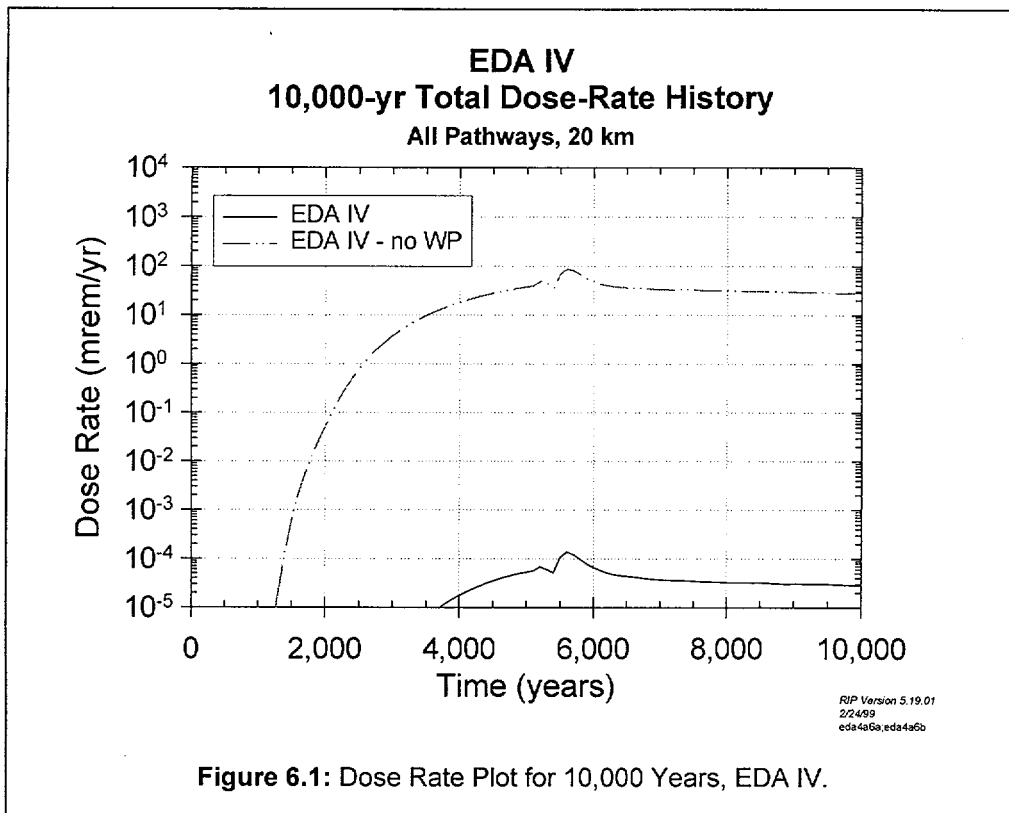
$$VWRND = VRODDS$$

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 inputs 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.

6.1 EDA IV RESULTS

Results of TSPA calculations for EDA IV are presented in Figures 6.1 & 6.2. The neutralized waste package case shows the highest dose release over the 10,000 year period and the EDA IV base case peak dose 6 orders of magnitude lower than the neutralized waste package. For 1,000,000 results the neutralized waste package case again shows the highest dose rate at early times. After approximately 50,000 years the dose rate begins to merge with the neutralized waste package case showing higher doses during super pluvial events.



7. REFERENCES

CRWMS M&O 1999a. *Design Input Request for LADS Phase II EDA Evaluations (c)*. Input Tracking No. LAD-SEI-99114.R. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990317.0072.

CRWMS M&O 1999b. *Design Input Transmittal for Waste Stream Information for LADS, Phase 2, EDA's*. Input Tracking No. PA-WP-99142.T. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990315.0047.

CRWMS M&O 1999c. *Design Input 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*. Input Tracking No. SSR-PA-99085.Ta. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.19990317.0363.

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8. ATTACHMENTS

I. CALCULATION OF INVERT SATURATION UNDER DRIPPING CONDITIONS

Attachment I

I. CALCULATION OF INVERT SATURATION UNDER DRIPPING CONDITIONS

I.1 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, 1998h), 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.

I.2 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):

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

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

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):

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

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

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):

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

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

where m is the van Genuchten air entry scaling parameter and β is the van Genuchten pore size distribution parameter.

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

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

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

From thermal hydrology calculations (CRWMS M&O 1999d and DTN: LL990301704242.082), $m = 0.7636$, $S_r = 0.05$, $S_{\max} = 1.0$ and intrinsic permeability (k_{sat}) = $1.6\text{E-}11 \text{ m}^2$.

$$k_{sat} = 1.6 \times 10^{-11} \text{ m}^2$$

$$g = 9.81 \text{ m/s}^2 \text{ (de Marsily, 1986, p. 412)}$$

$$\nu (@20 \text{ C}) = 10^{-6} \text{ m}^2/\text{s} \text{ (de Marsily, 1986, p. 413, Table A.2.4)}$$

$$K_{sat} = 1.6 \times 10^{-4} \text{ m/s}$$

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

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

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$$K = (1.6 \times 10^{-4}) \cdot (S_e^{1/2} [1 - (1 - S_e^{1.31})^{0.7636}]^2) \tag{9}$$

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 I.2.1). 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 I.2.1 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

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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

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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