



Department of Energy

Office of Civilian Radioactive Waste Management
Yucca Mountain Site Characterization Office
P.O. Box 364629
North Las Vegas, NV 89036-8629

QA: N/A

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OVERNIGHT MAIL

Janet R. Schlueter, Chief
High-Level Waste Branch
Division of Waste Management
Office of Nuclear Materials Safety
and Safeguards
U.S. Nuclear Regulatory Commission
Two White Flint North
Rockville, MD 20852

TRANSMITTAL OF REPORT ADDRESSING KEY TECHNICAL ISSUE (KTI) AGREEMENT ITEM
UNSATURATED AND SATURATED ZONE FLOW UNDER ISOTHERMAL CONDITIONS
(USFIC) 6.01

Reference: Ltr, Brocoum to Reamer, dtd 2/2/01

This letter transmits a report entitled *Matrix Diffusion Sensitivity Analysis* which provides information to support completion of the subject KTI agreement. Specifically, the KTI agreement states:

USFIC 6.01: "The DOE will provide the final sensitivity analysis on matrix diffusion (for UZ) in the TSPA-SR, Rev. 0. Due date: December 2000. The saturated zone information will be available in TSPA-SR, Rev 1, expected to be available in June 2001."

This agreement includes two parts: unsaturated zone (UZ) and saturated zone (SZ) matrix diffusion. Matrix diffusion for the UZ was addressed in Total System Performance Assessment-Site Recommendation (TSPA-SR) Revision 00, ICN 01, which was submitted with the referenced letter. The enclosure to this letter addresses the second and final part of the agreement. It includes a discussion of the matrix diffusion sensitivity analyses performed for the SZ. Although TSPA 6.01 stated that the information would be documented in TSPA-SR, Revision 01, the information to satisfy this agreement item has been provided in this report as discussed at the April 15-16, 2002, U.S. Nuclear Regulatory Commission/U.S. Department of Energy Technical Exchange and Management Meeting on KTIs.

There are no new regulatory commitments in the body or enclosure to this letter. Please direct any questions concerning this letter and its enclosure to Timothy C. Gunter at (702) 794-1343 or Drew H. Coleman at (702) 794-5537.

William Boyle for
Joseph D. Ziegler
Acting Assistant Manager, Office of
Licensing and Regulatory Compliance

OL&RC:TCG-1515

Enclosure:
Matrix Diffusion Sensitivity Analyses

JUL 30 2002

cc w/encl:

J. W. Andersen, NRC, Rockville, MD
D. D. Chamberlain, NRC, Arlington, TX
R. M. Latta, NRC, Las Vegas, NV
S. H. Hanauer, DOE/HQ (RW-2), Las Vegas, NV
B. J. Garrick, ACNW, Rockville, MD
Richard Major, ACNW, Rockville, MD
Budhi Sagar, CNWRA, San Antonio, TX
W. C. Patrick, CNWRA, San Antonio, TX
J. R. Egan, Egan & Associates, McLean, VA
J. H. Kessler, EPRI, Palo Alto, CA
Steve Kraft, NEI, Washington, DC
W. D. Barnard, NWTRB, Arlington, VA
R. R. Loux, State of Nevada, Carson City, NV
Marjorie Paslov-Thomas, State of Nevada, Carson City, NV
Alan Kalt, Churchill County, Fallon, NV
Irene Navis, Clark County, Las Vegas, NV
George McCorkell, Esmeralda County,
Goldfield, NV
Leonard Fiorenzi, Eureka County, Eureka, NV
Andrew Remus, Inyo County, Independence, CA
Michael King, Inyo County, Edmonds, WA
Mickey Yarbro, Lander County, Battle Mountain, NV
Lola Stark, Lincoln County, Caliente, NV
L. W. Bradshaw, Nye County, Pahrump, NV
David Chavez, Nye County, Tonopah, NV
Josie Larson, White Pine County, Ely, NV
Arlo Funk, Mineral County, Hawthorne, NV
R. I. Holden, National Congress of American
Indians, Washington, DC
Allen Ambler, Nevada Indian Environmental Coalition,
Fallon, NV
CMS Coordinator, BSC, Las Vegas, NV
G. L. Smith, DOE/YMSCO, Las Vegas, NV
OL&RC Library

cc w/o encl:

L. L. Campbell, NRC, Rockville, MD
C. W. Reamer, NRC, Rockville, MD
N. K. Stablein, NRC, Rockville, MD
S. L. Wastler, NRC, Rockville, MD
Margaret Chu, DOE/HQ (RW-1), FORS
S. E. Gomberg, DOE/HQ (RW-52), FORS
R. A. Milner, DOE/HQ (RW-2), FORS
N. H. Slater-Thompson, DOE/HQ (RW-52), FORS
R. B. Murthy, DOE/OQA (RW-3), Las Vegas, NV
Richard Goffi, BAH, Washington, DC
N. H. Williams, BSC, Las Vegas, NV

JUL 30 2002

cc w/o encl: (continued)

S. J. Cereghino, BSC, Las Vegas, NV
Donald Beckman, BSC, Las Vegas, NV
R. B. Bradbury, MTS, Las Vegas, NV
R. P. Gamble, MTS, Las Vegas, NV
R. C. Murray, MTS, Las Vegas, NV
R. D. Rogers, MTS, Las Vegas, NV
E. P. Opelski, NQS, Las Vegas, NV
W. J. Boyle, DOE/YMSCO, Las Vegas, NV
J. R. Dyer, DOE/YMSCO, Las Vegas, NV
T. C. Gunter, DOE/YMSCO, Las Vegas, NV
C. L. Hanlon, DOE/YMSCO, Las Vegas, NV
G. W. Hellstrom, DOE/YMSCO, Las Vegas, NV
D. G. Horton, DOE/YMSCO, Las Vegas, NV
S. P. Mellington, DOE/YMSCO, Las Vegas, NV
C. M. Newbury, DOE/YMSCO, Las Vegas, NV
R. E. Spence, DOE/YMSCO, Las Vegas, NV
J. T. Sullivan, DOE/YMSCO, Las Vegas, NV
M. C. Tynan, DOE/YMSCO, Las Vegas, NV
J. D. Ziegler, DOE/YMSCO, Las Vegas, NV
C. A. Kouts, DOE/YMSCO (RW-2), FORS
R. N. Wells, DOE/YMSCO (RW-60), Las Vegas, NV
Records Processing Center = "6"
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MATRIX DIFFUSION SENSITIVITY ANALYSES

July 2002

Preparation:

Stephanie Kuzio for Bill Arnold
B.W. Arnold, Principal Investigator, Saturated Zone Department

7-30-02
Date

Stephanie Kuzio
S.P. Kuzio, Principal Investigator, Saturated Zone Department

7-30-02
Date

Approval:

A.A. Eddebban
A.A. Eddebban, Department Manager, Saturated Zone

7-30-02
Date

Paul Dixon
P.R. Dixon, Subproject Manager, Natural Systems

7-30-02
Date

Reviewed by:

Thom Booth
Thom Booth, License Application Project

7-30-02
Date

ENCLOSURE

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ACRONYMS AND ABBREVIATIONS

ACRONYMS

DOE	U.S. Department of Energy
KTI	key technical issue
MTC	mass transfer coefficient
NRC	U.S. Nuclear Regulatory Commission
SZ	saturated zone
TSPA	Total System Performance Assessment
TSPA-SR	Total System Performance Assessment for Site Recommendation
USFIC	unsaturated and saturated flow under isothermal conditions
UZ	unsaturated zone

ABBREVIATIONS

km	kilometer
m	meter
ml/g	milliliter per gram
Np-237	neptunium-237
Tc-99	technetium-99

1. BACKGROUND

The subject of this report, *Matrix Diffusion Sensitivity Analyses*, presents part of the technical basis for closure of the key technical issue (KTI) agreement: Unsaturated and Saturated Flow Under Isothermal Conditions Subissue 6 Agreement 1 (USFIC 6.01). This report provides the analyses pertaining to the saturated zone (SZ).

The interest in the sensitivity analyses described in this report originated with requests by the U.S. Nuclear Regulatory Commission (NRC) under USFIC Subissue 6 (Matrix Diffusion). Specifically, the U.S. Department of Energy (DOE) agreed to provide the NRC with final results of the matrix diffusion sensitivity analyses when they became available. In an October 31 through November 2, 2000, technical exchange (Reamer and Williams 2000), the request addressed in this report was formalized in an NRC/DOE agreement.

2. APPLICABLE NUCLEAR SAFETY STANDARDS, REQUIREMENTS, AND GUIDANCE

2.1 APPLICABLE REQUIREMENTS

The Yucca Mountain disposal regulations include requirements for evaluating postclosure performance of the repository, including multiple barriers (10 CFR 63.113) and a description of the capabilities of the natural and engineered barriers (10 CFR 63.115). The sensitivity analyses presented in this report provide further demonstration of the characterization of the SZ barrier, which is part of the multiple barrier system.

2.2 KTI AGREEMENTS

This report addresses the following KTI agreement:

USFIC 6.01: The DOE will provide the final sensitivity analysis on matrix diffusion (for UZ) in the TSPA-SR, Rev. 0. Due date: December 2000. The saturated zone information will be available in TSPA-SR, Rev.1, expected to be available in June 2001.

The requested information pertains to the matrix diffusion sensitivity analyses. The sensitivity analyses for the unsaturated zone (UZ) were documented in *Total System Performance Assessment for the Site Recommendation* (CRWMS M&O 2000a), and this report provides the sensitivity analyses for the SZ. While the original agreement indicated that these analyses would be provided in a revision to *Total System Performance Assessment for the Site Recommendation*, the DOE believes that this report contains the information necessary to satisfy the agreement.

2.3 STATUS OF AGREEMENTS

DOE considers this report to fully address the agreement, and, pending the NRC review and acceptance, recommends that the agreement be closed.

3. MATRIX DIFFUSION SENSITIVITY ANALYSES

3.1 INTRODUCTION

The migration of radionuclides within fractured volcanic rocks of the SZ at Yucca Mountain may potentially be slowed by molecular diffusion from groundwater in the fractures into the pore water of the rock matrix. The process of matrix diffusion in volcanic media at Yucca Mountain has been investigated at both the laboratory and field scales (CRWMS M&O 2000b). Based on the conclusions of these studies, matrix diffusion has been incorporated into the SZ site-scale flow and transport model for the simulation of radionuclide transport in the SZ (CRWMS M&O 2000c).

This report provides the sensitivity analyses on matrix diffusion in the SZ. Sensitivity analyses are reported at both the subsystem modeling level and at the total-system level. The SZ site-scale flow and transport model supporting Total System Performance Assessment for the Site Recommendation (TSPA-SR) (CRWMS M&O 2000a) is used to examine the bounding cases of matrix diffusion relative to the expected-case behavior (BSC 2001a) of the SZ transport system. In addition, the range of uncertainty in parameters affecting matrix diffusion and SZ model results used in TSPA analyses are presented. Finally, results of a sensitivity analysis on the impacts of SZ matrix diffusion with the TSPA model used in the *FY01 Supplemental Science and Performance Analyses, Volume 1: Scientific Bases and Analyses* and *Volume 2: Performance Analyses* (BSC 2001b; BSC 2001c) are documented.

Four model cases are referred to in this report: two expected-case models, nominal case, and base case. Section 3.3 and corresponding figures cite the expected-case SZ model as defined in the *Saturated Zone Transport-Time Analyses Letter Report* (BSC 2001a). This report re-evaluates the conservatism of the SZ input parameters used in TSPA-SR, providing a more realistic treatment of the SZ input parameters. Section 3.4 and corresponding figures cite the expected-case model from the *Input and Results of the Base Case Saturated Zone Flow Model* (BSC 2001d). This report defines a conservative expected-case model based on the parameter inputs used in the SZ Base Case Flow Model for TSPA-SR. Section 3.5 and corresponding figures cite the TSPA-SR nominal case. The nominal case includes the concept of uncertainty in key SZ model parameters and conceptual models, which were provided as breakthrough curves to the TSPA-SR calculation. Section 3.6 and corresponding figures cite the TSPA-SR base-case calculation. The base case defined in this section is the TSPA-SR nominal scenario calculation for the mean annual dose (CRWMS 2000a, Figure 4.1-5).

3.2 MATRIX DIFFUSION IN THE SZ SITE-SCALE MODEL

The conceptual model of transport in fractured media used in the current SZ transport calculations consists of individual flowing fractures that transmit fluid and radionuclides, as illustrated in Figure 1. The surrounding rock matrix contains immobile water, but radionuclides can diffuse into and out of the rock matrix and sorb within the rock matrix. Therefore, radionuclide migration is attenuated with respect to the transport velocities within the fractures.

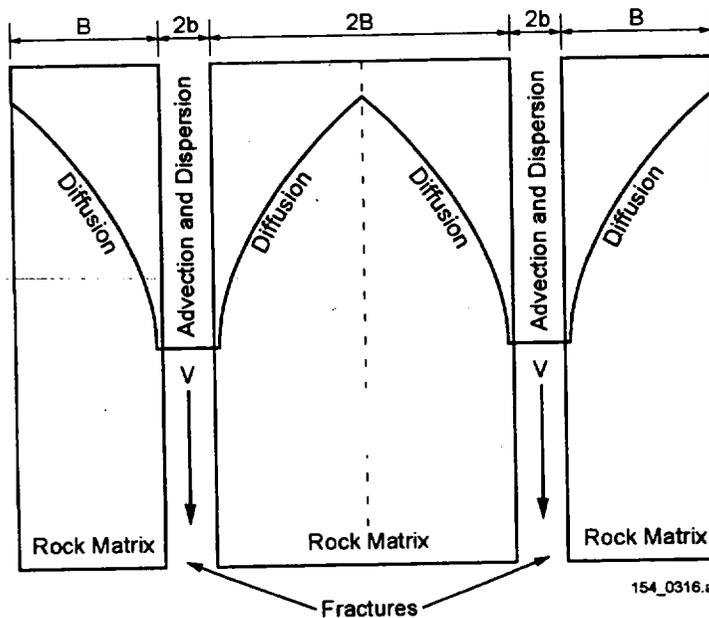


Figure 1. Schematic Diagram of the Matrix Diffusion Model

The abstracted model consists of equally spaced fractures (spacing = $2B$), each carrying fluid at the same velocity. The FEHM particle-tracking model employs an analytical solution of Sudicky and Frind (1982) to impart delays to each particle traveling within the fractured volcanic tuffs so that the diffusion-delayed transport time distribution predicted by the analytical solution is obtained. The fracture aperture ($2b$) represents the mean distance across the fracture, which, in reality, is a rough-walled discontinuity of variable aperture. The flow porosity of the medium is, through geometric considerations, b/B . This porosity is distinguished from the matrix porosity, which corresponds only to the porosity in the medium surrounding each flowing fracture.

The fracture spacing parameter is obtained from the analysis of field investigations identifying the distance between flowing fractures in boreholes at the site (CRWMS M&O 2000d). This parameter, combined with estimates of the fracture porosity (CRWMS M&O 2000d), allows the mean fracture aperture to be calculated. Unfortunately, borehole logs cannot be used to distinguish between single fractures and fracture zones; therefore, each flowing interval is modeled as a single fracture. It is possible that a flowing interval actually represents a zone of closely spaced fractures rather than an individual fracture.

The migration of sorbing radionuclides within the rock matrix is also controlled by sorption onto mineral grains of the matrix. An equilibrium, linear isotherm sorption model is used in which diffusive migration within the matrix is retarded by the factor, R_f :

$$R_f = 1 + \rho_b K_d / \phi \quad (\text{Eq. 1})$$

where

ρ_b is the matrix dry bulk density

K_d is the sorption coefficient

ϕ is the matrix porosity

The sorption process within the rock matrix tends to delay the migration of radionuclides within the matrix and provides significantly greater storage capacity for radionuclides within the matrix.

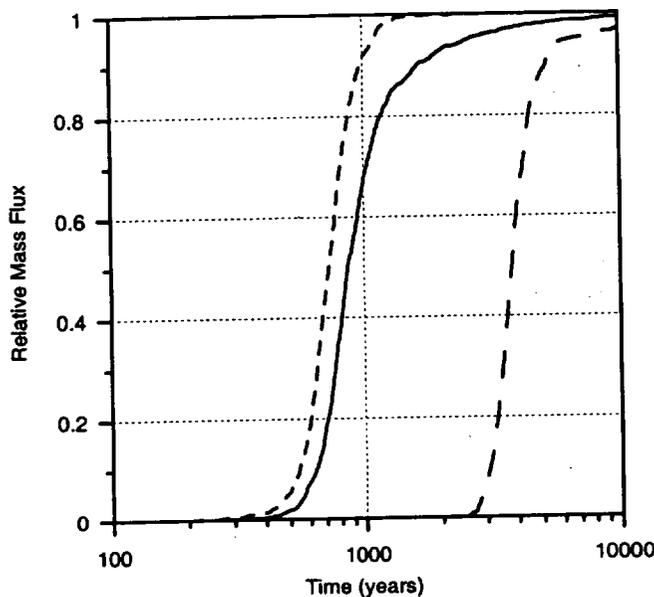
Numerical implementation of this conceptual model is done in the FEHM software code (LANL 1999) and is used in the SZ site-scale flow and transport model for the simulation of radionuclide transport documented in this report, the TSPA-SR (CRWMS M&O 2000a), and the *Supplemental Science and Performance Analyses* (BSC 2001b; BSC 2001c). The dual-porosity matrix diffusion conceptual model is applied to the fractured volcanic units in the SZ site-scale model, as described in BSC (2001d). Radionuclide transport within hydrogeologic units along the flow paths from the repository that behave as porous media (i.e., the valley-fill alluvium) is simulated using the porous medium approach.

3.3 SENSITIVITY IN THE EXPECTED-CASE SZ MODEL

One method to examine the sensitivity of the SZ flow and transport model with regard to matrix diffusion is to perform simulations that illustrate the bounding behavior of the system (i.e., minimal diffusion into the rock matrix and maximum diffusion). These simulations are compared to the expected-case breakthrough curves for several representative radionuclides in this portion of the sensitivity analysis. The representative radionuclides are selected for the sensitivity analyses based both on illustration of processes (i.e., relative sorption or nonsorption in different units) and on their importance to simulated dose in the TSPA-SR (CRWMS M&O 2000a).

The calibrated three-dimensional SZ site-scale flow and transport model (BSC 2001e; BSC 2001d) supporting the TSPA-SR (CRWMS M&O 2000a) is used to perform these simulations. The parameter values in these deterministic cases are taken from the expected-case model, as defined in BSC (2001a). The simulation results shown in Figures 2 to 4 are for radionuclide transport to the hypothetical location of the reasonably maximally exposed individual, as defined by 10 CFR 63.312(a). It should be noted that none of the breakthrough curves and transport time analyses shown in this report include radioactive decay to facilitate interpretation with regard to matrix diffusion. All results are for radionuclides with relatively long half-lives.

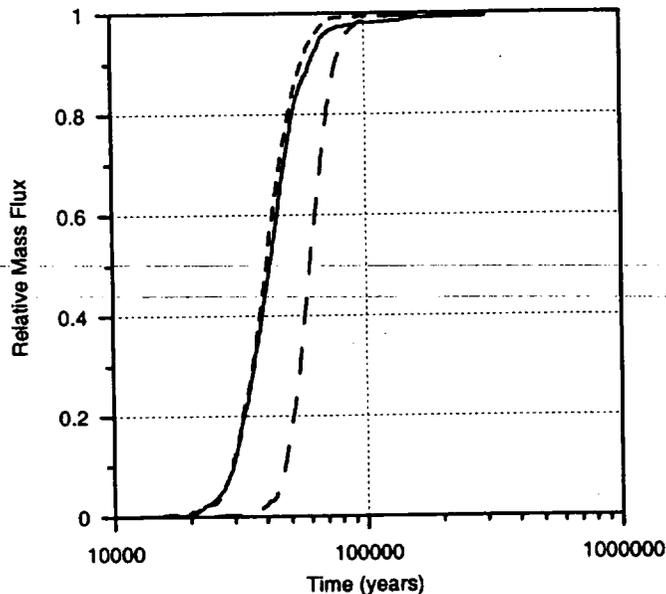
Simulation results for Tc-99, Np-237, and uranium are shown in Figures 2, 3, and 4, respectively. Each figure shows the mass breakthrough curve for the expected-case model as the solid line, the no-matrix-diffusion model with the short dashed line, and the maximum matrix-diffusion model as the long dashed line. The simulations with no matrix diffusion are performed by increasing the flowing interval spacing parameter by three orders of magnitude relative to the expected case. This approach numerically allows some very minor matrix diffusion, but for this model, the results are indistinguishable from purely advective transport in the fractures. The simulations with maximum matrix diffusion are performed by decreasing the fracture aperture by three orders of magnitude.



NOTE: The solid line shows the expected-case model results, the short dashed line shows results with no matrix diffusion, and the long dashed line shows results with maximum matrix diffusion.

Figure 2. Simulated Mass Breakthrough Curves for Tc-99 at 18-km Distance

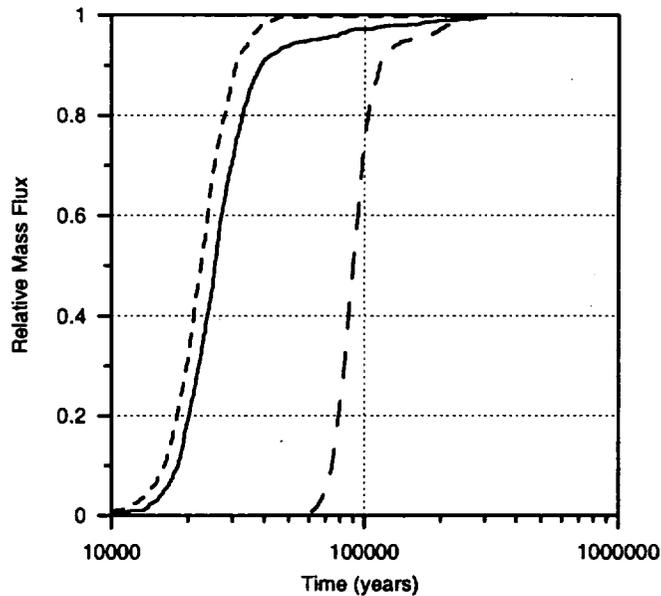
Figure 2 shows the results of the sensitivity analysis for Tc-99, which does not sorb in the volcanic tuff units nor in the alluvium of the SZ site-scale model. The breakthrough curve for the no-matrix-diffusion case represents relatively rapid transport through the volcanic units and slower transport in the portion of the flow path through alluvium. Most of the transport time in this breakthrough curve is accounted for by transport through the porous medium of the alluvium. The breakthrough curve for the maximum matrix-diffusion case represents full participation of the solute storage capacity of the volcanic rock matrix in the transport process, resulting in significantly longer transport time through the SZ system. These two cases constitute a bounding "envelope" of the behavior of the SZ expected-case model with regard to matrix diffusion for a nonsorbing species. As illustrated by the expected-case model breakthrough curve, there is a significant, but limited, contribution of matrix diffusion to transport times in the expected behavior of the system. However, if there were complete diffusive transfer between the fractures and matrix, the transport times of nonsorbing radionuclides in the SZ could be greater than 2,000 years longer.



NOTE: The solid line shows the results of the expected-case model, the short dashed line shows results with no matrix diffusion, and the long dashed line shows results with maximum matrix diffusion.

Figure 3. Simulated Mass Breakthrough Curves for Np-237 at 18-km Distance

Figure 3 shows a similar set of mass breakthrough curves for Np-237, which has a relatively small sorption coefficient in the volcanic rock matrix (0.5 ml/g) and a moderate sorption coefficient in the alluvium (18.2 ml/g). The transport times for all cases are significantly longer than those for Tc-99 in Figure 2 due to the sorption of Np-237 in both the volcanic units and the alluvium. The expected-case model breakthrough curve indicates that there is a relatively small amount of delay due to matrix diffusion and sorption on the volcanic rock matrix, relative to the no-diffusion case. However, it is interesting to note the delays for Tc-99 and Np-237 at the midpoints of the breakthrough curves in absolute terms. The delay for Tc-99 in the expected case relative to the no-diffusion case at the midpoint of the breakthrough curve in Figure 2 is 136 years; whereas, the delay for Np-237 in the expected case shown in Figure 3 is about 1,300 years.



NOTE: The solid line shows the results of the expected-case model, the short dashed line shows results with no matrix diffusion, and the long dashed line shows results with maximum matrix diffusion.

Figure 4. Simulated Mass Breakthrough Curves for Uranium at 18-km Distance

Figure 4 shows a similar set of mass breakthrough curves for uranium isotopes, which have a somewhat larger sorption coefficient in the volcanic rock matrix (2.0 ml/g) and a somewhat smaller sorption coefficient in the alluvium (10 ml/g), relative to Np-237. The bounding envelope of breakthrough with regard to matrix diffusion is significantly wider for uranium than for Np-237 because of the relatively larger value of the sorption coefficient in the volcanic rock matrix. This example illustrates the relatively more significant role of matrix diffusion for radionuclides that experience even moderate sorption in the matrix of the fractured units. The expected-case model breakthrough curve for uranium shown in Figure 4 is much closer to the response for the case with no diffusion than the maximum diffusion case.

3.4 PARAMETER UNCERTAINTY IN THE SZ MATRIX DIFFUSION MODEL

Significant uncertainty exists for several of the parameters that influence matrix diffusion in fractured volcanic tuffs, as described in CRWMS M&O (2000d). The uncertainty parameters in the SZ site-scale flow and transport model that affect dual-porosity matrix diffusion are effective diffusion coefficient, flowing interval spacing, fracture porosity, and groundwater specific discharge.

One way to examine the aggregate uncertainty in the parameters affecting matrix diffusion is to define a “lumped” parameter that combines impacts of the underlying parameters in a manner consistent with the diffusive process. The mass transfer coefficient (MTC) is a parameter that embodies the favorability of the medium for mass transfer between the fractures and rock matrix (Reimus et al. 1999). The MTC is defined as:

$$MTC = \frac{\phi_m \sqrt{D_e}}{b} = \frac{\phi_m \sqrt{D_e}}{\phi_f B} \quad (\text{Eq. 2})$$

where

ϕ_m is the matrix porosity

D_e is the effective diffusion coefficient

b is the half fracture aperture

ϕ_f is the flow (fracture) porosity

B is the half flowing interval spacing (see Figure 1)

High values of the MTC correspond to a relatively high potential for matrix diffusion. It should be noted that the MTC is a property of the medium, and the process of matrix diffusion is affected by the rate of groundwater flow in the fractures. The impact of uncertainty in groundwater flow rate is, thus, not evaluated through the use of the MTC parameter.

Figure 5 shows a histogram of the values of the MTC from 300 realizations of the parameter values for the SZ site-scale flow and transport model for the TSPA-SR (CRWMS M&O 2000a). It is apparent from this plot that there is a great deal of aggregate uncertainty (over five orders of magnitude in the MTC) in matrix diffusion represented in the model. The value of the MTC from the SZ expected-value model (BSC 2001d) is also shown in Figure 5 for comparison to the suite of values considered in Monte Carlo analyses. A majority of the realizations of the SZ system have lower values of the MTC than the expected case, indicating a lower potential for matrix diffusion.

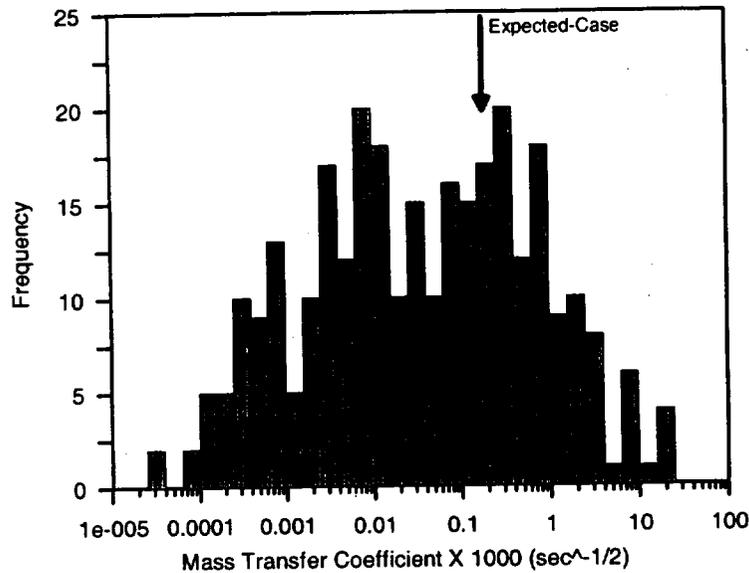


Figure 5. Histogram of MTC Values for SZ Transport

3.5 SENSITIVITY IN THE SZ TRANSPORT MODEL FOR TSPA

The sensitivity of the SZ site-scale flow and transport model to matrix diffusion within the context of overall uncertainty in SZ flow and transport is investigated in this section of the report. The multiple realizations of SZ transport for the nominal case that are used in the TSPA-SR (CRWMS M&O 2000a) incorporate uncertainty in many parameters in the SZ site-scale model (BSC 2001d). Alternative cases for no matrix diffusion and enhanced matrix diffusion have been defined, and 100 Monte Carlo simulations have been produced for each case (BSC 2001b).

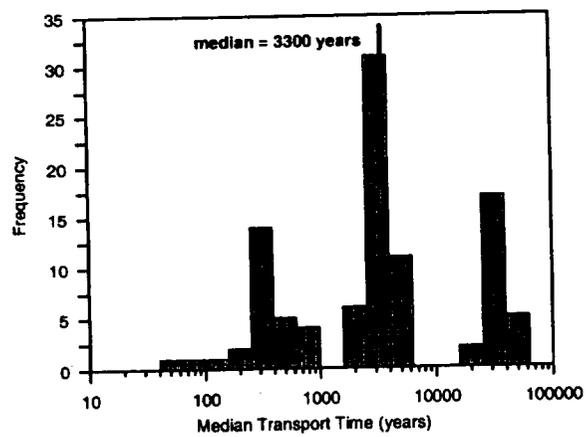
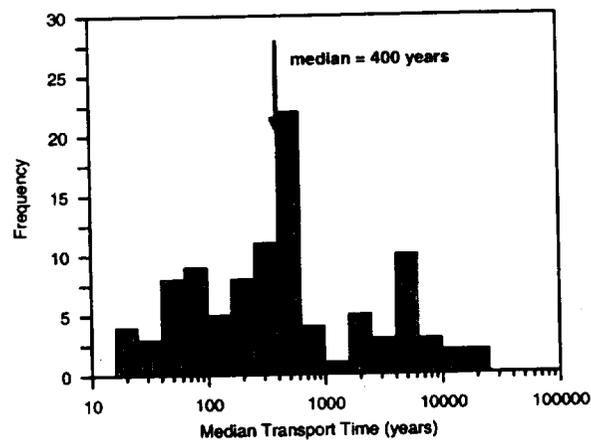
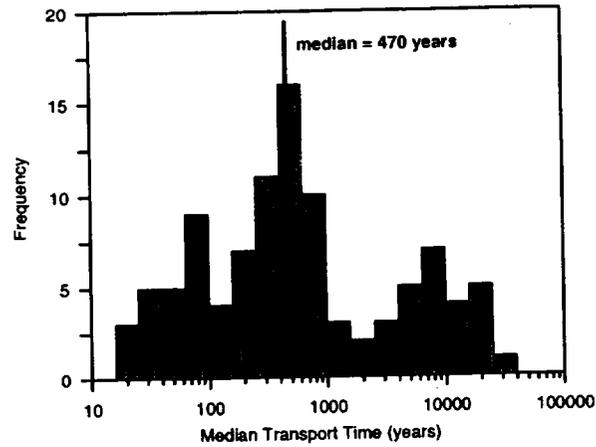
The sensitivity analysis for the no-matrix-diffusion case is implemented in the SZ site-scale flow and transport model by reducing the value of the effective matrix diffusion coefficient by 10 orders of magnitude in all realizations. This large reduction in the matrix diffusion coefficient effectively renders the simulated radionuclide mass delay to matrix diffusion insignificant. Other stochastic parameters for the SZ have the same values for the sensitivity analysis as the nominal case analysis (BSC 2001d).

The sensitivity analysis for the enhanced matrix-diffusion case is implemented by reducing the flowing interval spacing by two orders of magnitude for all realizations. This reduces the geometric mean of the flowing interval spacing from about 20 m to 0.2 m, which is a relatively small distance for matrix diffusion at the length and time scales of SZ flow and transport simulations. Other stochastic parameters for the SZ have the same values for the sensitivity analysis as the base-case analysis (BSC 2001d).

The simulated radionuclide breakthrough curves from the no-matrix-diffusion analysis have somewhat shorter transport times than for the nominal case, on a realization-by-realization basis. The differences in the transport time between the no-matrix-diffusion case and the nominal case are greater for those radionuclides that experience significant sorption in the volcanic matrix. The simulated radionuclide breakthrough curves from the enhanced matrix-diffusion analysis have longer transport times than for the nominal case.

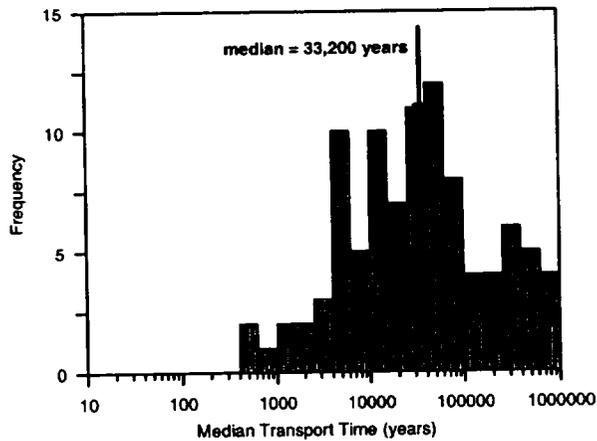
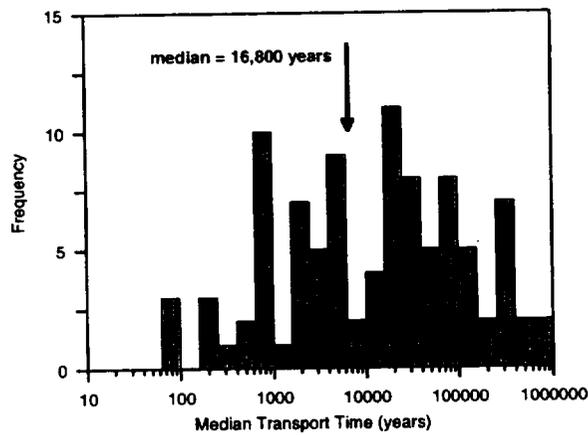
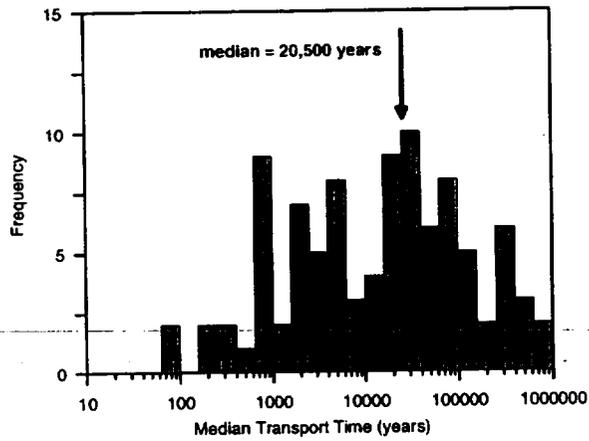
The histograms of median transport time (i.e., the time at the midpoint of the breakthrough curve) for Tc-99 are compared for the nominal case, the no-matrix-diffusion case, and the enhanced matrix-diffusion case in Figure 6. As expected, the distribution of median transport times for the no-matrix-diffusion case is shifted toward shorter transport times, with the median of the midpoints of the breakthrough curves shifted from 470 years in the nominal case to 400 years in the no-matrix-diffusion case (upper and middle plots in Figure 6). The distribution of median transport times for the enhanced matrix-diffusion case is shifted toward significantly longer transport times relative to the nominal case, with the median of the midpoints of the breakthrough curves shifted to 3,300 years (upper and lower plots in Figure 6). Interestingly, removing the effects of uncertainty in the matrix diffusion for the enhanced matrix-diffusion case produces a more distinct tri-modal distribution of median transport times shown in the lower plot of Figure 6, reflecting the separation among the low, medium, and high specific discharge cases used in the SZ transport model for TSPA. It should be noted that the overall uncertainty in the median transport time, as represented by the width of the histograms, is much larger than the shift in median transport times from the nominal case to the no-matrix-diffusion case and the enhanced matrix-diffusion case.

The histograms of median transport time for Np-237 are compared for the nominal case, the no-matrix-diffusion case, and the enhanced matrix-diffusion case in Figure 7. Similar trends in the distributions of median transport time to those noted for Tc-99 are present in the plots for Np-237, but all of the distributions are shifted toward longer transport times because of the sorbing nature of this radionuclide. The median of the midpoints of the breakthrough curves for the nominal case is 20,500 years, compared to 16,800 years for the no-matrix-diffusion case and 33,200 years for the maximum matrix-diffusion case. As with Tc-99, the overall uncertainty in the median transport time, as represented by the width of the histograms, is much larger than the shift in median transport times from the nominal case to the no-matrix-diffusion case and the enhanced matrix-diffusion case.



NOTE: Results for the nominal case, no-diffusion case, and maximum diffusion case are shown in the top, middle, and bottom plots, respectively.

Figure 6. Median Transport Times for Tc-99 at 18-km Distance



NOTE: Results for the nominal case, no-diffusion case, and maximum diffusion case are shown in the top, middle, and bottom plots, respectively.

Figure 7. Median Transport Times for Np-237 at 18-km Distance

3.6 SENSITIVITY IN THE TSPA MODEL RESULTS

The sensitivity analysis of matrix diffusion described in the previous section was carried forward to TSPA simulations of dose as documented in *Supplemental Science and Performance Analyses* (BSC 2001c). The base-case results of the TSPA model are compared to the results of the no-matrix-diffusion case and the maximum (enhanced) matrix-diffusion case.

The upper plot in Figure 8 shows the mean annual dose calculated in the TSPA-SR base case (CRWMS M&O 2000a, Figure 4.1-5,) compared with the mean annual dose calculated without the effects of matrix diffusion in the SZ. The differences between the model with matrix diffusion and the no-matrix-diffusion case model are not discernable by visual inspection of the plots. The most likely reason for this situation is as follows. Approximately half of the TSPA-SR (CRWMS M&O 2000a) realizations have little or no matrix diffusion because of a low diffusion coefficient, large flowing-interval spacing, or the high-groundwater-flux case. The mean annual dose in the TSPA-SR (CRWMS M&O 2000a) is primarily influenced by the realizations that produce the high annual dose values, particularly for Np-237, and many of the high-dose realizations include a SZ representation that has little or no matrix diffusion. Thus, reducing matrix diffusion in the half of the realizations that include significant matrix diffusion does little to increase the mean annual dose. It should also be remembered that the mean annual dose in the TSPA-SR (CRWMS M&O 2000a) is controlled by factors external to the SZ for most of the first 100,000 years after repository closure.

The lower plot in Figure 8 shows the mean annual dose calculated in the TSPA-SR base case (CRWMS M&O 2000a) compared with the mean annual dose calculated with maximum (enhanced) matrix diffusion in the SZ transport model. As shown in Figure 8, the differences in expected annual dose between the model with matrix diffusion and the model with enhanced matrix diffusion are generally less than 20 percent, and the simulated doses are somewhat lower for the model with enhanced matrix diffusion, as expected. Approximately half of the TSPA-SR (CRWMS M&O 2000a) realizations have little or no matrix diffusion because of a low diffusion coefficient or a high groundwater flux. Reducing the flowing-interval spacing does not address these other factors. The mean annual dose in the TSPA-SR (CRWMS M&O 2000a, Figure 4.1-5) is primarily influenced by the realizations that produce the high annual dose values, particularly for Np-237. The sorption coefficient for Np-237 in the volcanic matrix averages 0.5 ml/g (CRWMS M&O 2000a, Table 3.8-3). Thus, even if Np-237 does diffuse into the matrix, there is little retardation because of the relatively low sorption coefficient for this radionuclide. The combination of the high-groundwater-flux cases, low diffusion coefficient, and low Np-237 sorption coefficient tends mostly to override the effect of enhanced matrix diffusion, at least for the calculation of the mean annual dose. This sensitivity study is an example of how a change in a subcomponent model can have impact in that subcomponent model but not a large impact on the total system. Also, the TSPA-SR (CRWMS M&O 2000a) shows that the mean annual dose is controlled by factors external to the SZ for most of the first 100,000 years after repository closure.

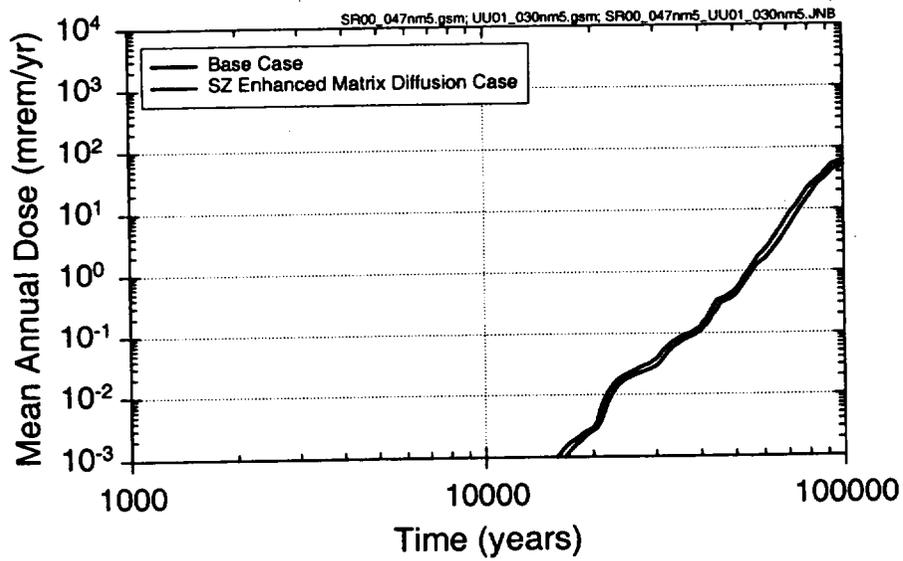
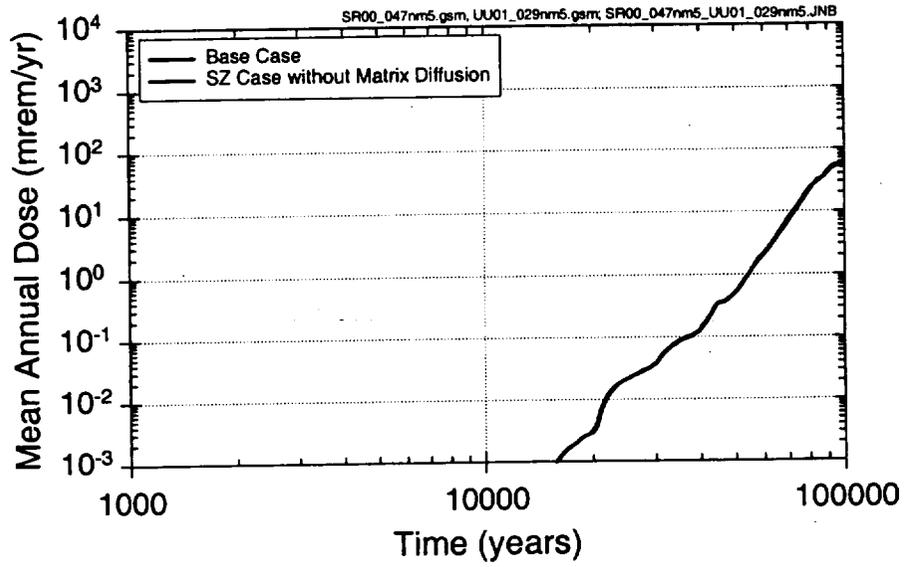


Figure 8. Simulated TSPA Dose Rates for the Base Case, the No-Matrix-Diffusion Case, and the Maximum Matrix-Diffusion (Enhanced) Case for SZ Flow and Transport

It also should be noted that climatic conditions wetter than present conditions exist for most of the time greater than 600 years in the future in the TSPA model. These wetter climatic conditions correspond to higher groundwater fluxes in the SZ and more rapid radionuclide transport through the SZ system. Accordingly, any shifts in the dose curves due to differences between the base case, the no-matrix-diffusion case, and the maximum (enhanced) matrix-diffusion case are compressed relative to the differences in transport time shown for present conditions in Figures 6 and 7. This effect tends to diminish the apparent sensitivity to matrix diffusion at the TSPA level relative to the sensitivity observed at the SZ system level.

3.7 CONCLUSIONS

Sensitivity analyses examining matrix diffusion in the SZ radionuclide transport simulations are conducted to address the KTI agreement USFIC 6.01 between the DOE and the NRC. Sensitivity of the modeling is evaluated at the subsystem level using the SZ site-scale flow and transport model and at the system level using the TSPA model. The range of uncertainty in parameters influencing matrix diffusion is also examined in an aggregate fashion.

The bounds on the radionuclide transport times through the SZ system related to uncertainty in the matrix diffusion process span several thousand years for nonsorbing radionuclides and several tens of thousands of years for sorbing radionuclides, within the context of the expected-case model. The radionuclide breakthrough curves using the expected-case parameters for matrix diffusion are much closer to the no-matrix-diffusion bound than to the maximum matrix-diffusion bound. This result indicates that the expected behavior of the SZ system is for diffusion from fractures into the matrix to provide significant, but limited, delay in the transport of radionuclides from beneath the repository to the accessible environment. The delay afforded by matrix diffusion is much more significant in absolute terms for sorbing radionuclides than for nonsorbing radionuclides. It should be noted that limitations of the data available for the flowing interval spacing may result in underestimating matrix diffusion in the expected-case model (BSC 2001a).

Uncertainty in the individual parameters affecting matrix diffusion in the fractured volcanic units of the SZ results in a relatively large degree of aggregate uncertainty in the matrix diffusion process. The uncertainty distribution of the MTC calculated for parameter vectors used in the TSPA-SR analyses indicates several orders of magnitude uncertainty in the potential for matrix diffusion. Comparing the expected-case value of the MTC, its relation to the uncertainty distribution of MTC, and the expected-case transport times relative to the bounding transport times indicates that a large fraction of the SZ transport realizations have very little matrix diffusion.

Examination of the distributions of median SZ transport time from the multiple realizations of the SZ site-scale flow and transport model shows that the range of behavior for the nominal case more closely resembles the range for the no-matrix-diffusion case than it does the enhanced (maximum) matrix-diffusion case. The overall uncertainty in the distributions of SZ transport time is significantly greater than the uncertainty related to the matrix diffusion process, for both sorbing and nonsorbing radionuclides.

Sensitivity of the simulated dose in the TSPA model is limited with regard to matrix diffusion in the SZ. Simulations with enhanced matrix diffusion in the SZ show a shift of the mean annual dose curve to somewhat later times, relative to the nominal case and the no-matrix-diffusion case. The mean dose curves for the nominal case and the no-matrix-diffusion case are graphically indistinguishable on the plot shown in Figure 8, indicating that the nominal case is essentially at the conservative bound of the TSPA model with regard to matrix diffusion in the SZ.

In summary, the SZ site-scale flow and transport model shows significant sensitivity to matrix diffusion in the fractured volcanic units of the SZ, and the expected behavior is closer to the bounding case of no matrix diffusion. The TSPA model shows a little sensitivity to the process of matrix diffusion, with the nominal case behavior essentially equal to the case of no matrix diffusion (Figure 8). These modeling results indicate that matrix diffusion in the SZ is simulated to have some influence on radionuclide transport in the SZ, but the results are closer to the conservative bounds of behavior than they are to taking full credit for the diffusive and sorptive capacity of the volcanic rock matrix in the SZ.

4. REFERENCES

4.1 DOCUMENTS CITED

- BSC (Bechtel SAIC Company) 2001a. *Saturated Zone Transport-Time Analyses Letter Report*. MIS-MGR-HS-000001 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20020225.0092.
- BSC 2001b. *FY01 Supplemental Science and Performance Analyses, Volume 1: Scientific Bases and Analyses*. TDR-MGR-MD-000007 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010712.0062.
- BSC 2001c. *FY01 Supplemental Science and Performance Analyses, Volume 2: Performance Analyses*. TDR-MGR-PA-000001 REV 00. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010724.0110.
- BSC 2001d. *Input and Results of the Base Case Saturated Zone Flow and Transport Model for TSPA*. ANL-NBS-HS-000030 REV 00 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20011112.0068.
- BSC 2001e. *Calibration of the Site-Scale Saturated Zone Flow Model*. MDL-NBS-HS-000011 REV 00 ICN 01. Las Vegas, Nevada: Bechtel SAIC Company. ACC: MOL.20010713.0049.
- CRWMS M&O (Civilian Radioactive Waste Management System Management and Operations) 2000a. *Total System Performance Assessment for the Site Recommendation*. TDR-WIS-PA-000001 REV 00 ICN 01. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20001220.0045.
- CRWMS M&O 2000b. *Unsaturated Zone and Saturated Zone Transport Properties (U0100)*. ANL-NBS-HS-000019 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000829.0006.
- CRWMS M&O 2000c. *Saturated Zone Transport Methodology and Transport Component Integration*. MDL-NBS-HS-000010 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000824.0513.
- CRWMS M&O 2000d. *Uncertainty Distribution for Stochastic Parameters*. ANL-NBS-MD-000011 REV 00. Las Vegas, Nevada: CRWMS M&O. ACC: MOL.20000526.0328.
- LANL (Los Alamos National Laboratory) 1999. *Software Code: FEHM V2.00*. V2.00. SUN Ultra Sparc. 10031-2.00-00.
- Reamer and Williams 2000. *Summary Highlights of NRC/DOE Technical Exchange and Management Meeting on Unsaturated and Saturated Flow Under Isothermal Conditions*. ACC: MOL.20001128.0206.
- Reimus, P.W.; Adams, A.; Haga, M.J; Humphrey, A.; Callahan, T.; Anghel, I.; and Counce, D. 1999. *Results and Interpretation of Hydraulic and Tracer Testing in the Prow Pass Tuff at the*

C-Holes. Milestone Report SP32E7M4. Los Alamos, New Mexico: Los Alamos National Laboratory. TIC: 246377.

Sudicky, E.A. and Frind, E.O. 1982. "Contaminant Transport in Fractured Porous Media: Analytical Solutions for a System of Parallel Fractures." *Water Resources Research*, 18, (6), 1634–1642. Washington, D.C.: American Geophysical Union. TIC: 217475.

4.2 CODES, STANDARDS, REGULATIONS, AND PROCEDURES

10 CFR (Code of Federal Regulations) 63. Energy: Disposal of High-Level Radioactive Wastes in a Geologic Repository at Yucca Mountain, Nevada. Readily available.