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Yucca Mountain Site Characterization Project

An Investigation of the Impact of Conceptual Model Uncertainty on the Estimated Performance of a Hypothetical High-Level Nuclear Waste Repository Site in Unsaturated, Fractured Tuff

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**AN INVESTIGATION OF THE IMPACT OF CONCEPTUAL MODEL UNCERTAINTY
ON THE ESTIMATED PERFORMANCE OF A HYPOTHETICAL HIGH-LEVEL
NUCLEAR WASTE REPOSITORY SITE IN UNSATURATED, FRACTURED TUFF**

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Abstract

Performance assessment modeling for High Level Waste (HLW) disposal incorporates three different types of uncertainty. These include data and parameter uncertainty, modeling uncertainty (which includes conceptual, mathematical, and numerical), and uncertainty associated with predicting the future state of the system. In this study, the potential impact of conceptual model uncertainty on the estimated performance of a hypothetical high-level radioactive waste disposal site in unsaturated, fractured tuff has been assessed for a given group of conceptual models. This was accomplished by taking a series of six, one-dimensional conceptual models, which differed only by the fundamental assumptions used to develop them, and conducting ground-water flow and radionuclide transport simulations. Complementary cumulative distribution functions (CCDFs) representing integrated radionuclide release to the water table indicate that differences in the basic assumptions used to develop conceptual models can have a significant impact on the estimated performance of the site. Because each of the conceptual models employed the same mathematical and numerical models, contained the same data and parameter values and ranges, and did not consider the possible future states of the system, changes in the CCDF could be attributed primarily to differences in conceptual modeling assumptions. Studies such as this one could help prioritize site characterization activities by identifying critical and uncertain assumptions used in model development, thereby providing guidance as to where reduction of uncertainty is most important.

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1.0 INTRODUCTION

The U.S. Department of Energy is responsible for the design, construction, operation, and decommissioning of a site for the deep geologic disposal of high-level radioactive waste (HLW). This necessarily involves site characterization and the use of performance assessment to demonstrate compliance with the regulations for HLW disposal set forth by the U.S. Environmental Protection Agency (EPA, 1985)¹ and the U.S. Nuclear Regulatory Commission (NRC, 1986). Within the EPA standard, the definition of "performance assessment" specifically states that the assessment will consider the associated uncertainties involved in estimating cumulative release of radionuclides to the accessible environment. In addition, the EPA Containment Requirements (40 CFR 191.13) require that a reasonable expectation that compliance with §191.13 (a) will be achieved. To provide a *reasonable* expectation through modeling, the models used in an analysis must adequately represent the real system and must consider and/or incorporate all sources of uncertainty, as practicably as possible.

Performance assessment modeling for HLW disposal incorporates three different types of uncertainty. These include data and parameter uncertainty, modeling uncertainty, and uncertainty associated with predicting the future state of the system. Traditionally, the majority of the efforts in uncertainty analysis have been directed toward treating data and parameter uncertainty; consequently, little effort has been made to treat model uncertainty. Model uncertainty includes conceptual model uncertainty, mathematical model uncertainty, and uncertainties resulting from implementing the mathematical model in a computer code (e.g., coding errors, computational limitations, user errors). Currently there is no systematic approach designed to address the uncertainty in conceptual models, nor has the impact of conceptual model uncertainty on a given regulatory performance measure been demonstrated.

1.1 Purpose

The purpose of this investigation is to take a first step at addressing conceptual model uncertainty. This will be accomplished by assessing, qualitatively, the relative impact that alternative conceptual models for a given system have on the integrated release of radionuclides at a point along a transport migration path. The source of radionuclides is a hypothetical HLW repository located in unsaturated, fractured tuff. The assessment is qualitative only in the sense that the uncertainty associated with each of the conceptual models is not quantified as part of the comparison. The results from the individual conceptual models, however, are quantitative. In general, studies such as the one presented in this report could help prioritize site characterization activities by

¹ The United States Court of Appeals, 1st Circuit, 7/17/87, vacated the EPA HLW standard 40 CFR 191 and remanded the EPA individual protection and ground water protection requirements for further consideration. While this action by the court may result in numerical criteria that differ from the EPA's original values, the content and form of the requirements are not expected to change. Therefore, the nature of the calculations made in this report and the accompanying comparisons are expected to be relevant to any revised EPA standards.

identifying critical and uncertain assumptions used in model development, thereby providing guidance as to where reduction of uncertainty is most important.

1.2 Background

A knowledge of previously developed conceptual models is important in assessing the impact of conceptual model uncertainty. A number of investigators have recognized the existence of numerous alternative conceptual models, but few have intercompared results from the models. Parsons et al. (1989) reviewed and evaluated several conceptual models for ground water flow and solute transport at a HLW repository site located in unsaturated, fractured tuff formations. Their evaluations concentrated primarily on the fundamental assumptions made in the development of the conceptual models and the possible implications those assumptions could have on performance assessment modeling. However, because many of the specific assumptions and the modeling intentions of each of the conceptual models were different, a meaningful comparison of results from the models was difficult. Parsons et al. also reviewed existing information on flow and transport in unsaturated and saturated, fractured rock (much of which was specific to Yucca Mountain), and recognized that, given the existing information, a single defensible conceptual model for such a system does not exist. Rather, several alternative conceptual models are plausible.

Many investigators have realized the importance of conceptual model uncertainty and the fact that quantifying and reducing this uncertainty will increase confidence in the analysis (Bonano and Cranwell, 1988; Davis et al., 1990; de Marsily, 1990). International cooperative studies, such as INTRACON (INTRACON, 1986), INTRAVAL (INTRAVAL, 1987), HYDROCON (NRC, 1988; SKI, 1990), and GEOVAL (Davis and Goodrich, 1990), have implicitly recognized the problem of model uncertainty and, in principle, provide approaches to reducing model uncertainty (including conceptual, mathematical, and numerical model uncertainty) through the process of model validation and verification.

1.3 Scope

A conceptual model is defined here as the set of assumptions and simplifications that describe the physical system and the behavior of the system. In this study, the uncertainty in conceptual models is assessed by taking a number of alternative conceptual models for a single site and graphically comparing flow and transport results from each. That is, in this sensitivity-analysis-type approach, the impact of fundamental assumptions used to develop unique conceptual models is qualitatively assessed by plotting and comparing the quantitative flow and transport simulation results of each conceptual model.

This investigation is not intended to be exhaustive in terms of the conceptual models

chosen; rather, the emphasis was placed on elucidating the potential impact of uncertainty in conceptual models on the results of a performance assessment. In fact, only a limited number of conceptual models could be assessed because, although numerous conceptual models are conceivable, time constraints and existing mathematical and numerical techniques precluded the quantitative analysis of many of them. Although the range of conceptual models was limited in this investigation by the aforementioned constraints, in a real performance assessment one must consider all plausible conceptual models, independent of mathematical and numerical modeling capabilities.

Some important qualifications should be noted for this analysis. These are listed below, and are due mainly to the limited scope of this investigation, and also to the numerical and mathematical limitations of the calculational tools applied.

- A limited number (6) of conceptual models were analyzed.
- The analysis was confined to one-dimensional models.
- All of the models were based on a continuum approach. Ground water flow models assumed Darcy's Law to be valid.
- The analysis assumed steady-state ground water flow fields.
- A limited number of single-membered radionuclide chains were transported.
- Radionuclide transport was modeled using an advective/dispersion equation with constant, K_d -based retardation factors.
- Gas phase transport was not included in the analysis.
- The analysis assumed the system could be treated as isothermal.
- Uncertainty in transport parameters only was assumed when generating the complementary cumulative distribution functions (CCDF).
- No attempt was made to quantify the uncertainty in the fundamental assumptions made. That is, conceptual model uncertainty was not quantified.
- Integrated release of radionuclides to the water table was the only performance measure used for comparison of alternative conceptual models.
- Only "present condition" realizations were simulated. That is, disruptive or alternative scenarios were not considered.

- The investigation is preliminary and based on limited data; therefore, the results should not be taken as representative of a potential repository located at Yucca Mountain, Nevada.

1.4 Procedure to Assess Impact of Alternative Conceptual Models

A number of plausible, alternative conceptual models were defined based on a general understanding of observations made at the potential HLW disposal site at Yucca Mountain, Nevada and at other unsaturated, fractured tuff sites. For this investigation, liberal interpretations of any observations were allowed. That is, unless there existed outright, conclusive evidence that a given conceptual model could not exist, then that model was considered plausible. However, the probability of each conceptual model was not estimated and the uncertainty associated with each model was not quantified.

For the most part, each of the alternative conceptual models in this investigation are based on the same system geometry, boundary conditions, and parameter values, but are differentiated by fundamentally different assumptions of the flow and transport mechanisms in the system. Quantitative analysis of ground water flow and radionuclide transport for each of the conceptual models was conducted. Flow simulations were conducted using the DCM3D code (Updegraff and Lee, 1991). The resulting ground water flow velocities were used in the NEFTRAN II code (Olague et al., 1991) to simulate transport of radionuclides from the repository to the water table. Transport parameters (such as dispersivity and retardation factors) were assumed to have some uncertainty associated with them. As a result, transport simulations of radionuclide release to the water table could be expressed probabilistically in terms of a CCDF of total integrated release. This CCDF was the performance measure used in this study to compare alternative conceptual models with each other.

2.0 DEFINITION OF ALTERNATIVE CONCEPTUAL MODELS

2.1 Conceptual Models and Conceptual Model Uncertainty

Flow and transport models used in performance assessment are, without exception, built upon a set of fundamental assumptions and simplifications of a physical system and on how that system behaves. This set of assumptions and simplifications is referred to as the "conceptual model" of the system. The development of a conceptual model generally involves simplifying the real system so that it can be represented with a tractable mathematical model that, in turn, can be solved using analytical and/or numerical techniques. The conceptual model, therefore, provides a description of the geometry of the system, the boundary and initial conditions associated with the system, the physical and chemical processes occurring within the system, and a description of how those processes occur (i.e., the variables and parameters chosen to represent those processes).

Because models are by definition, simplifications of reality, uncertainty is inherent within them. The large degree of uncertainty associated with a conceptual model for an HLW repository site is generally the result of the large spatial and temporal scales of interest and the inability to test the performance of a real site under post-waste-emplacement conditions over regulatory time frames. In addition, the "real" system is often poorly characterized, making the development of a defensible conceptual model a difficult task.

Large uncertainties imply that only limited information is available to support or refute alternative conceptual models. Consequently, a number of alternative conceptual models may be plausible for a single site. Furthermore, it is not clear whether the uncertainty associated with each conceptual model can be quantified with an adequate degree of confidence or how that uncertainty would be represented. As a result, performance assessment would have to acknowledge in some manner all the plausible conceptual models to ensure that all the possible realizations of a given site's behavior have been considered. In this investigation, conceptual model uncertainty is represented in terms of a number of alternative conceptual models; the alternative models are treated as mutually exclusive and are evaluated independently.

2.2 Approach to Choosing Alternative Conceptual Models

A simple, but systematic approach for choosing and defining conceptual models is illustrated in Figure 2.1. An approach such as this provides a way to define alternative conceptual models, so that the fundamental assumptions that segregated the models are explicit, and therefore, can easily be articulated. Note that although some of the fundamental assumptions illustrated in Figure 2.1 apply to both flow and transport (e.g., dimensionality), the figure does not explicitly include some transport assumptions (e.g., matrix diffusion). A more generalized flow chart that included transport could be developed based on the same idea. In practice, the flow chart should be much more

Figure 2.1. Generalized Flow Chart of the Major Assumptions Needed to Develop a Conceptual Model for an Unsaturated, Fractured Flow System

detailed in order to allow for the consideration of all the assumptions, both implicit and explicit, that need to be made.

Although Figure 2.1 depicts a sequential decision-making process for developing the conceptual model, this is not necessarily the case. For example, the decision of whether flow is fracture dominated, matrix dominated, or a combination of the two does not depend on the dimensionality of the model. Rather, several of the modeling assumptions are made in parallel and not in series. The assumption of whether or not there exists resistance to flow and transport across the fracture/matrix interface, though, obviously requires a prior assumption that both fracture and matrix play a role in flow and transport. The use of a flow chart provides a systematic method for documenting assumptions.

Specifically, some of the key assumptions that go into the development of flow and transport conceptual models for HLW disposal in unsaturated, fractured media are

- dimensionality (one-, two-, or three-dimensional);
- steady-state or transient flow conditions;
- isothermal versus nonisothermal;
- single phase or multiphase flow and transport;
- matrix and/or fracture flow and transport;
- degree of interaction between the matrix and the fractures (for example, do fracture coatings impact matrix/fracture transfer for flow and transport);
- interconnectedness of fracture networks;
- structural features (e.g., faults);
- stratigraphy (i.e., number of hydrogeologic units and dip);
- boundary and initial conditions; and
- solute retardation mechanisms.

This is by no means a complete list of all the considerations that go into the development of a conceptual model. The assumptions that go into each conceptual model will be not only site specific, but also purpose specific. Note that this list does not include assumptions concerning parameter values and their distributions because these are really beyond our definition of conceptual model. Also, some of these

assumptions are generic for the development of flow and transport modeling in any medium and not just unsaturated and fractured media.

2.3 Summary of Conceptual Models Chosen

As stated earlier, each of the alternative conceptual models in this investigation is based on the same system geometry, boundary conditions, and parameter values (i.e., material properties), but is differentiated from the rest by fundamentally different assumptions of the flow and transport mechanisms in the system. A schematic illustrating the basic stratigraphy and boundary conditions is presented in Figure 2.2. All of the conceptual models chosen assume a spatially and temporally uniformly distributed flux at the repository horizon equal to 0.1 mm/yr. Steady-state ground water flow through a one-dimensional system, from the base of the repository to the water table, was assumed. Five of the six models assumed the fifteen hydrogeologic layers or units shown in Figure 2.2. The sixth model assumed an equivalent four-layer stratigraphy based on average properties from the fifteen-layer case. Only four radionuclide species (^{99}Tc , ^{129}I , ^{135}Cs , and ^{237}Np) were released from the repository and transported. The transport model assumes a single, dominant, nonbranching transport path. Radionuclide retardation factors were based on the distribution coefficient (K_d) for each radionuclide. No other chemical reactions were included. Gas phase transport was also not included. The final result of the simulations was total integrated release of radionuclides at the water table.

The conceptual models chosen are nominally distinguished in terms of one or two fundamental assumptions. These alternative conceptual models were chosen because they address some fundamental assumptions of flow and transport that are considered critical to site performance for a site located in an unsaturated, fractured medium. The different conceptual models are described below.

(1) Matrix-dominated flow and transport

This is a single-continuum model that assumes that all the ground water flux through the system occurs only in the porous matrix. This implicitly assumes that either any water that enters fractures is immediately imbibed by the matrix or that water never enters the fractures. The former case would require that the resistance to flow across the fracture face into the matrix be negligible, and that no transfer is allowed from the matrix to the fracture. Given certain materials, these assumptions may be reasonable for low fluxes; under such conditions, water can be held in the unsaturated matrix by capillary suction forces. Also, under low infiltration conditions, pulses of infiltrating water may be dampened spatially and temporally before they reach the repository horizon. As a result of these flow assumptions, solutes in the liquid phase can only be transported through the matrix.

(2) Fracture-dominated flow and transport

This is another single-continuum model; however, this model assumes that all the ground water flux through the system occurs only in the fractures. If the model does not include

Figure 2.2. Basic Stratigraphy and Boundary Conditions Assumed for Alternative Conceptual Models

an interacting matrix, then it implicitly assumes that none of the water that enters fractures is imbibed by a matrix. Because the system is not fully saturated throughout, this assumption implies that the resistance to flow across the fracture face into the matrix is extremely large. This could be the result of coatings on the fracture face or the inability of water to wet the matrix rock (i.e., capillary suction is not present if water does not wet the surface). Fracture dominated flow could also be conceptualized for a system in which a given flux through the fractures had been established and then the net flux from fracture to matrix was equal to zero. This would probably only occur in a system that was effectively saturated. This model also implicitly assumes that the fractures in the system are connected throughout. This conceptual model assumes that transport of radionuclides occurs only in the fractures. Also retardation of radionuclides was assumed not to occur in the fracture continuum (that is, fracture retardation factors were set equal to 1).

(3) Fracture dominated flow and transport, but with matrix diffusion of radionuclides

The ground water flow mathematical model is identical to the second model described above. However, conceptually, immobile matrix water is assumed to play a role in radionuclide transport in this model. The presence of the immobile phase provides a storage volume for which solutes can diffuse in and out of (termed "matrix diffusion"). Radionuclides may also be sorbed onto the matrix rock and consequently be retarded whereas they are conceptualized as not being retarded in the fractures. Transport of radionuclides in and out of the matrix is modeled as a linear function of the concentrations in the fracture and matrix water, and is assumed directly proportional to a mass-exchange coefficient. The mass-exchange coefficient is a measure of the resistance to transport across the fracture/matrix interface.

(4) Simultaneous matrix and fracture flow and either matrix or fracture transport

This is a dual-continuum flow model assuming that the flux through the system occurs in both the fractures and the matrix simultaneously. The amount of water that transfers from fracture to matrix (or matrix to fracture) is a function of the pressure difference across the fracture/matrix interface and a transfer factor that indicates either the propensity or resistance to flow across this interface. Note that the flow transfer factor is not the same parameter as the transport mass exchange coefficient. Solute transport at any given point along the transport path, however, only occurs in either the fracture or the matrix, but not both simultaneously. Transport can switch from fracture to matrix (or matrix to fracture), from one point to the next along the path. Transport is assumed to occur in the medium (fracture or matrix) that has the highest pore velocity. For transport modeling, the medium (fracture or matrix) in which no transport is occurring is considered immobile. However, transfer of dissolved radionuclides from the mobile liquid to the immobile liquid (as in model 3) is not considered in this model. Again, retardation is assumed not to occur in the fractures.

(5) Simultaneous matrix and fracture flow and equivalent-porous-medium transport

This ground water flow conceptual model is identical to the dual-continuum model used in the fourth model described above. However, radionuclide transport is described using

an equivalent-porous-medium approximation. The equivalent-porous-medium approximation uses single, equivalent (combined) values for the matrix and fracture transport velocities and retardation factors. That is, matrix and fracture velocities at each point along the migration path are combined to produce a single, equivalent velocity at that point. The model assumes that a concentration equilibrium always exists between the matrix and fracture and that there exists zero resistance to transport across the matrix/fracture interface. Retardation factors for the fractures were assumed to equal to 1. Erickson et al. (1986) and Dudley et al. (1988) provide some guidance for the conditions under which an equivalent-porous-medium approach is applicable. Leigh (1991) has demonstrated the use of the equivalent-porous-medium approach for transport modeling using the NEFTRAN code.

(6) An alternative stratigraphic representation of the hydrogeologic system different from the stratigraphy used in the five prior conceptual models

A dual-continuum ground water flow model similar to the fourth model described above was assumed, but with a simplified hydrogeologic stratigraphic representation of the system. The distance from the repository to the water table remained the same; however, the fifteen hydrogeologic units used in the previous five conceptual models were combined to form four "equivalent" units. The properties in the four equivalent layers were derived as arithmetic averages of the properties in the layers from which they were composed. Radionuclide transport was treated in the same manner as in the fourth conceptual model.

A schematic representation of the alternative conceptual models is presented in Figure 2.3.

0.1 mm/yr Infiltration Rate

- 1) All Matrix
- 3) Fracture w/ Matrix Diffusion
- 5) Equivalent Porous Medium

- 2) All Fracture
- 4) Dual Continuum
- 6) Four-Layer Stratigraphy

Figure 2.3. Schematic Representation of Conceptual Models Tested

an equivalent-porous-medium approximation. The equivalent-porous-medium approximation uses single, equivalent (combined) values for the matrix and fracture transport velocities and retardation factors. That is, matrix and fracture velocities at each point along the migration path are combined to produce a single, equivalent velocity at that point. The model assumes that a concentration equilibrium always exists between the matrix and fracture and that there exists zero resistance to transport across the matrix/fracture interface. Retardation factors for the fractures were assumed to equal to 1. Erickson et al. (1986) and Dudley et al. (1988) provide some guidance for the conditions under which an equivalent-porous-medium approach is applicable. Leigh (1991) has demonstrated the use of the equivalent-porous-medium approach for transport modeling using the NEFTRAN code.

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A schematic representation of the alternative conceptual models is presented in Figure 2.3.

0.1 mm/yr Infiltration Rate

Figure 2.3. Schematic Representation of Conceptual Models Tested

3.0 PROCEDURE FOR ANALYSES

3.1 Mathematical and Numerical Models

Quantitative analysis of ground water flow and radionuclide transport for each of the conceptual models was conducted using the DCM3D (Updegraff and Lee, 1991) ground water flow and NEFTRAN II (Olague et al., 1991) radionuclide transport computer codes. A description of each of these mathematical/numerical models is provided below along with information specific to these conceptual models.

3.1.1 Ground Water Flow Analysis

DCM3D (Dual Continuum Model 3D) (Updegraff and Lee, 1991) was used to simulate the flow field for all the conceptual models described in Section 2.3. DCM3D is a computer code designed to model three-dimensional ground-water flow in an unsaturated, fractured, porous medium. The model implemented in DCM3D uses a dual-continuum concept to model flow. One continuum represents the fractures and the other represents the porous matrix. Flow in the two continua are coupled by a transfer term which depends on the pressure head difference between the two continua, the saturated and relative hydraulic conductivity of the porous matrix, the fracture specific surface, and the fracture spacing.

DCM3D solves the following ground-water flow equations for the porous matrix and fracture continua, respectively:

$$C_m \frac{\partial h_m}{\partial t} = \nabla \cdot (\mathbf{K}_m (\nabla h_m + \nabla z)) - \Gamma + Q_m \quad (3-1)$$

and

$$C_f \frac{\partial h_f}{\partial t} = \nabla \cdot (\mathbf{K}_f (\nabla h_f + \nabla z)) + \Gamma + Q_f \quad (3-2)$$

where

h_m	=	pressure head in the porous matrix continuum
h_f	=	pressure head in the fracture continuum
C_m	=	specific storage coefficient of the porous matrix continuum
C_f	=	specific storage coefficient of the fracture continuum
$\mathbf{K}_m$	=	hydraulic conductivity tensor for the porous matrix continuum
$\mathbf{K}_f$	=	hydraulic conductivity tensor for the fracture continuum
Q_m	=	volumetric porous matrix continuum source term per unit volume of continua

Q_f	=	volumetric fracture continuum source term per unit volume of continua
Γ	=	porous matrix continuum to fracture continuum transfer term
z	=	direction distance
t	=	time.

The porous matrix and fracture continua hydraulic conductivities are related to the saturated and relative hydraulic conductivities as follows:

$$\underline{\mathbf{K}}_m = \underline{\mathbf{K}}_{sm} K_{rm}(h_m) \quad (3-3)$$

and

$$\underline{\mathbf{K}}_f = \underline{\mathbf{K}}_{sf} K_{rf}(h_f) \quad (3-4)$$

where

$\underline{\mathbf{K}}_{sm}$	=	saturated hydraulic conductivity tensor of the porous matrix continuum
$\underline{\mathbf{K}}_{sf}$	=	saturated hydraulic conductivity tensor of the fracture continuum
K_{rm}	=	relative hydraulic conductivity of the porous matrix continuum
K_{rf}	=	relative hydraulic conductivity of the fracture continuum

The porous matrix and fracture continua relative hydraulic conductivities are defined by the van Genuchten relationships (see Equation 3-7 and Equation 3-8) and, therefore, depend on the porous matrix and fracture continua pressure head, respectively. The porous matrix and fracture continua specific storage coefficients are defined, respectively, as:

$$C_m = n_m S_m \beta + S_m \alpha_{b_m} (1 - n_m) + n_m \frac{\partial S_m}{\partial h_m} \quad (3-5)$$

and

$$C_f = n_f S_f \beta + S_f \alpha_{b_f} (1 - n_f) + n_f \frac{\partial S_f}{\partial h_f} \quad (3-6)$$

where

S_m	=	porous matrix continuum degree of saturation
S_f	=	fracture continuum degree of saturation
n_m	=	porous matrix continuum porosity
n_f	=	fracture continuum porosity
α_{b_m}	=	porous matrix continuum compressibility
α_{b_f}	=	fracture continuum compressibility
β	=	water compressibility.

The porous matrix and fracture degrees of saturation are defined by the van Genuchten relationship (see Equation 3-7) and, therefore, are dependent on the pressure head in the porous matrix and fractures, respectively.

DCM3D uses the van Genuchten equations (van Genuchten, 1980) to define the saturation and relative hydraulic conductivity characteristic curves for both the matrix and fractures. These equations are:

$$S_e = \frac{S - S_r}{1 - S_r} = \left(\frac{1}{1 + (\alpha h_c)^n} \right)^m \quad (3-7)$$

and

$$k_r = \sqrt{S_e} \left(1 - \left(1 - S_e^{1/m} \right)^m \right)^2 \quad (3-8)$$

where

- S is the degree of saturation;
- S_e is the effective saturation;
- S_r is the residual saturation;
- h_c is the capillary head;
- k_r is the relative hydraulic conductivity.

m , n , and α are parameters where m is related to n by $m = 1 - 1/n$. The van Genuchten equations are assumed applicable for both matrix and fractures.

The transfer term (Γ) depends on the fracture specific surface (A_s), a pseudo-length between the matrix centroid and the fractures (l), the matrix saturated hydraulic conductivity (K_{sm}), the matrix relative hydraulic conductivity (K_{rm}) and the difference between the matrix pressure head (h_m) and the fracture pressure head (h_f) (Updegraff and Lee, 1991). The transfer term is estimated as:

$$\Gamma = A_s \frac{K_{sm} K_{rm}}{l} (h_f - h_m) \quad (3-9)$$

There is a lack of data on the fracture specific surface and the pseudo-length parameter. Specific surface is defined as surface area per unit volume. If a block with dimensions $\Delta x \Delta y \Delta z$ has f vertical fractures per unit length (e.g. fractures per meter), then the fracture specific surface becomes:

$$A_s = \frac{2(f \Delta x) \Delta y \Delta z}{\Delta x \Delta y \Delta z} = 2f \quad (3-10)$$

where

$$\begin{aligned}\Delta x \Delta y \Delta z &= \text{the volume of the block} \\ \Delta y \Delta z &= \text{the area of one side of the fracture} \\ f \Delta x &= \text{the number of vertical fractures in the block.}\end{aligned}$$

The number "2" enters into the equation because flow across both sides of the fracture must be considered.

If it is assumed that fractures are equally spaced and that the centroid between two fractures is where the porous matrix pressure occurs, then

$$l = \frac{1}{2f} \quad (3-11)$$

Therefore,

$$\frac{A_s}{l} = 4f^2 \quad (3-12)$$

and has dimensions of length⁻². Finally, Equation 3-12 can be substituted into Equation 3-9 to yield:

$$\Gamma = 4f^2 K_{sm} K_{rm} (h_f - h_m) \quad (3-13)$$

The fracture frequency, f , is provided in Barnard and Dockery (1991). The term $A_s K_{sm} / l$, or $4f^2 K_{sm}$, is called the transfer factor and is tabulated in Table 3.1. The same result as Equation 3-12 can be obtained for horizontal fractures.

General. Flow in a vertical, one-dimensional column was modeled. Data are based on measurements of USW G-4 drill hole core from Yucca Mountain (see Barnard and Dockery, 1991). The modeled column extended from the water table (elevation 730.6 m above mean sea level) to the bottom of the repository (elevation 960.0 m). The elevation difference between the water table and the repository bottom was 229.4 m. In all the models, the downward direction was considered as the positive direction.

All conceptual models were run through a transient solution to go from an initially zero water-flux condition to steady-state. Steady-state was assumed when the total Darcy flux through the matrix and fractures was equal to the recharge rate of 0.1 mm/yr.

The same boundary conditions and initial conditions were used for all the conceptual model simulations. Water was injected at the repository boundary at a rate of 0.1 mm/yr to simulate recharge. The matrix and fracture pressure heads were set at 0.0 m at the water table; that is, saturated conditions in both the matrix and fractures

at the water table. The initial pressure head in each grid block was set to the negative of the distance of the grid block center above the water table. This initial pressure head caused a zero water flux throughout the column at the beginning of the simulation.

For purposes of this study, fifteen distinct stratigraphic layers exist between the water table and the repository. These layers are distinct because of their matrix hydrologic properties rather than their fracture ones. Their names, elevations, and hydrologic properties are summarized in Table 3.1. The data were taken from the base case specification for this problem (see Barnard and Dockery, 1991).

Matrix-dominated flow model. Thirteen stratigraphic layers were used in the matrix-dominated flow model. Layer 3, Layer 4, and Layer 5 were combined into one layer and assigned the matrix hydrological properties of Layer 4. This was done to ease the computational burden of the problem.

The computational problems were caused by two factors. First, Layer 4 had such a high matrix saturated hydraulic conductivity compared to Layer 3 and Layer 5. Second, because Layer 3's saturated hydraulic conductivity was less than the recharge rate, an inverted (perched) water table formed there. In order to move the water table, DCM3D used very small time steps and this required large amounts of computer time. In order to reduce the computer time, the three layers were combined. Combining the three layers into one eliminated the inverted water table problem. It was believed that assigning the hydrologic properties of Layer 4 to the combined layer would provide faster travel times because the saturated hydraulic conductivity of Layer 4 is six orders of magnitude higher than that of Layer 3 or Layer 5. Thus, it was believed the this combined layer would provide a conservative estimate of the travel time.

The grid consisted of 278 grid blocks. The grid block assignments and thicknesses are shown in Table 3.2. The finer grid spacing in Layer 5 occurs at the bottom of the layer at its boundary with Layer 6. The coarser grid spacing occurs at the top of the layer against the boundary of Layer 4.

Fracture-dominated flow model. Five stratigraphic layers were used in this model. The top two layers, Layer 1 and Layer 2, were combined into one layer. These two layers were combined because they had the same fracture hydrological properties. The bottom ten layers, Layer 6 through Layer 15 were combined into another layer for the same reason. This combining of layers was done as a matter of convenience only. Layer 3, Layer 4, and Layer 5 remained as distinct layers.

The grid consisted of 1000 grid blocks, which ranged in thickness from a minimum of 0.01 m to a maximum of 0.25 m. The smaller grid block thickness were located at the bottoms of each of the five layers. The thicknesses of the grid blocks are shown in Table 3.3.

Table 3-1. Matrix and Fracture Properties

Matrix Properties							vanGenuchten Parameters		
Layer Number	Layer Name	Top Elevation (m)	Bottom Elevation (m)	Thickness (m)	Porosity	Hydraulic Conductivity (m/s)	Alpha (1/m)	n	Sr
1	Tpt-TML	960.0	930.2	29.8	0.12	2.0E-11	0.010	1.70	0.05
2	Tpt-TM	930.2	868.6	61.6	0.10	2.0E-11	0.005	1.90	0.10
3	Tpt-TV	868.6	860.1	8.5	0.04	3.0E-12	0.002	1.70	0.00
4	Tpt-TNV	860.1	850.9	9.2	0.20	2.4E-06	0.030	2.20	0.15
5	Tpt-TN	850.9	841.2	9.7	0.36	3.0E-12	0.020	1.20	0.00
6	Tpt-BT	841.2	840.6	0.6	0.23	2.0E-11	0.002	1.60	0.10
7	Tcb-TN	840.6	836.0	4.6	0.36	1.0E-11	0.004	1.50	0.15
8	Tcb-BT	836.0	835.4	0.6	0.23	2.0E-11	0.002	1.60	0.10
9	Tcb-TN	835.4	829.0	6.4	0.36	1.0E-11	0.004	1.50	0.15
10	Tcb-BT	829.0	826.3	2.7	0.23	2.0E-11	0.002	1.60	0.10
11	Tcb-TN	826.3	794.6	31.7	0.36	1.0E-11	0.004	1.50	0.15
12	Tcb-BT	794.6	793.7	0.9	0.23	2.0E-11	0.002	1.60	0.10
13	Tcb-TN	793.7	750.4	43.3	0.36	1.0E-11	0.004	1.50	0.15
14	Tcb-BT	750.4	733.3	17.1	0.23	2.0E-11	0.002	1.60	0.10
15	Tcpp-TN	733.3	730.6	2.7	0.28	5.0E-12	0.001	3.00	0.20
Fracture Properties							vanGenuchten Parameters		
Layer Number	Layer Name	Fracture Frequency (1/m)	Transfer Factor (1/m-s)	Porosity	Hydraulic Conductivity (m/s)	Alpha (1/m)	n	Sr	
1	Tpt-TML	5	2.0E-09	3.0E-05	1.2E-09	1.280	4.23	0.04	
2	Tpt-TM	5	2.0E-09	3.0E-05	1.2E-09	1.280	4.23	0.04	
3	Tpt-TV	10	1.2E-09	2.0E-04	8.0E-08	1.280	4.23	0.04	
4	Tpt-TNV	3	8.6E-05	6.6E-05	2.6E-08	1.280	4.23	0.04	
5	Tpt-TN	3	1.1E-10	9.0E-05	7.2E-08	1.280	4.23	0.04	
6	Tpt-BT	3	7.2E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
7	Tcb-TN	3	3.6E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
8	Tcb-BT	3	7.2E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
9	Tcb-TN	3	3.6E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
10	Tcb-BT	3	7.2E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
11	Tcb-TN	3	3.6E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
12	Tcb-BT	3	7.2E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
13	Tcb-TN	3	3.6E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
14	Tcb-BT	3	7.2E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	
15	Tcpp-TN	3	1.8E-10	1.8E-05	5.4E-10	1.280	4.23	0.04	

Table 3-2: Grid Block Thicknesses for Matrix Flow Problem

Layer No.	Number of Grid Blocks	Thickness of Grid Block (m)	Thickness of Layering (m)
1	8	3.725000000	29.80000
2	32	1.925000000	61.60000
3	32	0.265625000	8.50000
4	16	0.575000000	9.20000
5	56	0.151562500	8.48750
	8	0.075781250	0.60625
	16	0.037890625	0.60625
6	2	0.300000000	0.60000
7	4	1.150000000	4.60000
8	4	0.250000000	1.00000
9	8	0.750000000	6.00000
10	4	0.675000000	2.70000
11	32	0.990625000	31.70000
12	4	0.225000000	0.90000
13	32	1.353125000	43.30000
14	16	1.068750000	17.10000
15	4	0.675000000	2.70000
Totals	278		229.40000

Table 3-3: Grid Block Thicknesses for Fracture Dominated Flow

Layer 1 to Layer 2		Layer 3		Layer 4		Layer 5		Layer 6 to Layer 15	
Number of Grid Blocks	Thickness of Grid Blocks (m)	Number of Grid Blocks	Thickness of Grid Blocks (m)	Number of Grid Blocks	Thickness of Grid Blocks (m)	Number of Grid Blocks	Thickness of Grid Blocks (m)	Number of Grid Blocks	Thickness of Grid Blocks (m)
360	0.25	25	0.25	32	0.25	32	0.25	434	0.25
1	0.29	1	0.23	1	0.24	1	0.22	1	0.24
1	0.23	1	0.22	1	0.19	1	0.20	1	0.20
1	0.18	1	0.19	1	0.15	1	0.17	1	0.18
1	0.15	1	0.17	1	0.13	1	0.15	1	0.16
1	0.12	1	0.15	1	0.10	1	0.13	1	0.14
1	0.09	1	0.14	1	0.08	1	0.11	1	0.13
1	0.08	1	0.12	1	0.07	1	0.10	1	0.12
1	0.06	1	0.11	1	0.05	1	0.09	1	0.10
1	0.05	1	0.10	2	0.04	1	0.08	1	0.09
1	0.04	1	0.09	1	0.03	1	0.07	2	0.08
1	0.03	1	0.08	3	0.02	1	0.06	1	0.07
3	0.02	2	0.07	2	0.01	1	0.05	1	0.06
2	0.01	1	0.06	2		2	0.04	2	0.05
		2	0.05	3		3	0.03	3	0.04
		3	0.04	3		3	0.02	3	0.03
		5	0.03	4		4	0.01	5	0.02
		4	0.02					4	0.01
			0.01						
376	91.40	56	8.50	48	9.20	56	9.70	464	110.60

Simultaneous matrix and fracture flow model. Fifteen stratigraphic layers were used in this conceptual model. The layers and their hydrologic properties are shown in Table 3.1. Three cases were studied for this model. The first case, called the "large case" in this report, used the transfer factors that appear in Table 3.1. The second case, called the "medium case", used transfer factors that were 1/10 those presented in Table 3.1. The third case, called the "small case", used transfer factors that were 1/100 those presented in Table 3.1. The transfer factors were reduced to simulate features, such as fracture surface coatings, which may reduce water transfer between the fractures and the porous matrix. The grid spacing was the same as for the matrix-dominated flow model (Table 3.2).

The recharge into the top of the grid block was divided between the matrix and the fractures based on the unsaturated hydraulic conductivity of the matrix and the fractures. The amounts going into the matrix and the fractures are:

$$r_m = \frac{r K_m(h_m)}{K_m(h_m) + K_f(h_f)} \quad (3-14)$$

and

$$r_f = \frac{r K_f(h_f)}{K_m(h_m) + K_f(h_f)} \quad (3-15)$$

respectively, where r is the total recharge, r_f is the recharge into the fractures, r_m is the recharge into the matrix, K_f is the unsaturated hydraulic conductivity of the fractures, and K_m is the unsaturated hydraulic conductivity of the matrix. At the repository horizon, the infiltration into the matrix was much larger than that into the fractures. In fact, more than 99.99% of the recharge goes into the matrix because the matrix and fracture pressures at the repository are nearly the same and the relative hydraulic conductivity characteristic curves are much steeper for the fractures than for the matrix. Hence, at the repository horizon, the unsaturated hydraulic conductivity for the matrix is much higher than that for the fractures.

Alternative stratigraphic layering model. Four layers were used in the alternative stratigraphic layering model. In this model Layer 1 and Layer 2 were combined to form the first layer; Layer 3 through Layer 5 were combined to form the second layer; Layer 6 through Layer 14 were combined to form the third layer; and Layer 15 formed the fourth layer. The effective hydrologic properties of a given combined layer were estimated from the properties of the actual layers comprising the combined one. Arithmetic average properties were calculated after weighting the properties of the actual layers by their respective thickness. The grid spacing used for this model is presented in Table 3.4. The recharge into the matrix and fractures were determined from the unsaturated hydraulic conductivities of the matrix and the fractures as given by Equation 3-5 and Equation 3-6. The large transfer coefficient was used for this model.

Table 3.4. Grid Block Properties for Four-Layer Stratigraphy Flow Model

Layer Number	Number of Grid Blocks	Thickness of Grid Block (m)	Thickness of Layer (m)
1 and 2	40	2.2850000	91.4
3 thru 5	128	0.2140625	27.4
6 thru 14	112	0.9633929	107.9
15	4	0.6750000	2.7
Totals	284		229.4

3.1.2 Radionuclide Transport Analysis

NEFTRAN II (NEtwork Flow and TRANsport II) is a performance assessment code designed to conduct computationally efficient simulations of transport of multiple, n-membered (where $n \geq 1$) radionuclide chains through fractured, saturated and unsaturated media, across large distances, and over long simulation times.

The NEFTRAN II code uses the Distributed Velocity Method (DVM) (Campbell et al., 1981) to simulate convective-dispersive transport of radionuclides through a series of one-dimensional legs or stream tubes. For unsaturated zone transport, NEFTRAN II was designed so that the transport migration path, mean pore velocities for each leg along the path, and saturations for each leg along the path would each be determined from an external flow calculation. For saturated zone transport, NEFTRAN II can internally calculate a flow network based on prescribed pressure head data, and determine a transport migration path through the network. However, NEFTRAN II is intended to rely on sophisticated flow calculations external to the code to provide the necessary ground water flow information, and on assumptions about solute transport to justify the use of the NEFTRAN II mathematical model.

To simulate transport, the DVM partitions the radionuclides within each leg into discrete packets, and determines a distribution of packet velocities about the mean velocity, based on the mean retarded particle velocity and a dispersivity for each leg. Mean retarded particle velocity within a leg is the mean pore velocity divided by the particle retardation factor. Legs along the migration path can be designated as either single-porosity matrix, single-porosity fracture, or dual-porosity fracture. Included with the dual-porosity fracture legs is an immobile matrix volume, into and out of which matrix diffusion can be simulated. The equation governing exchange by matrix diffusion for any

given cell along the path is

$$C_m(t+\Delta t) = \frac{\beta \Delta t}{n_m R_m} [C_f(t) - C_m(t)] + C_m(t) \quad (3-16)$$

where

C = radionuclide concentration,

β = an exchange coefficient,

n = porosity,

t = time and,

R = retardation factor.

The subscripts m and f denote matrix and fracture. Matrix diffusion is important because, in theory, the matrix can essentially act as a storage volume and enhance retardation of the radionuclides (Bonano et al., 1989).

Because the spatial orientation of the transport legs in NEFTRAN II is neither specified by the user nor implied within the code, the orientation of the legs can be arbitrary. As a result, if a dominant, non-branching, migration path (or paths) can be defined in two or three dimensions by a flow calculation external to NEFTRAN II, the program can simulate quasi multi-dimensional transport through this path. The models in this study did not utilize this capability as they were all one-dimensional and vertical.

Additional discussion of the mathematical, and numerical models used in NEFTRAN II can be found in Longsine et al. (1987) and Olague et al. (1991).

Specifically, the transport analysis was based on the nominal system geometry described in Figure 2.2. The conceptualized system consisted of 15 hydrogeological units from the base of the proposed repository to the water table. The number and nature (i.e., fracture or matrix) of transport legs varied from model to model depending on the flow field. The transport migration path for NEFTRAN II was determined using a DCM3D post-processor (described in Section 3.2). A summary of the flow and transport conceptualized systems will be provided in Section 4.2.

As was mentioned in Section 2.3, three fission products (^{99}Tc , ^{129}I , ^{135}Cs) and one actinide (^{237}Np) were included in the transport simulations. The selection of these four radionuclides was made for several reasons. No short-lived nuclides (e.g., ^{90}Sr , ^{137}Cs) were considered because of the expected long travel times. The half-lives for the selected radionuclides range from 2.15×10^5 years (^{99}Tc) to 1.6×10^7 years (^{129}I). Radionuclides with solubility-limited (^{237}Np) and reaction-rate-limited (^{99}Tc , ^{129}I , and ^{135}Cs) dissolution mechanisms are included. Furthermore, ^{99}Tc , ^{129}I and ^{135}Cs have rapid-release fractions, as well as alteration-rate-controlled releases. Finally, these radionuclides represent a range of sorption properties, ranging from non-sorbing ^{129}I , to weakly sorbing ^{99}Tc and ^{237}Np , to strongly sorbing ^{135}Cs . These sorption properties are for matrix rock; because of uncertainty in fracture surface characteristics, all of the radionuclides were considered to be non-sorbing in the fractures.

The source term used was based on a continuous, 'wet-drip' waste-water contact process for mobilization of the radionuclides from the waste form (Apted et al., 1991). This mechanism considers the possibility that the flow field of water percolating through the tuff surrounding a waste container is such that the water is diverted into fractures which intersect the emplacement hole. Further, water must then drip from the rock to the container, eventually causing perforations, through which water can enter the container. After the bottom of the container has also been breached, release from the waste form begins. Release curves for the four isotopes considered are shown in Figure 3.1. ^{99}T , ^{129}I and ^{135}Cs all have essentially the same source term except with different amplitudes. This source term was used for all of the conceptual models.

3.2 Flow and Transport Coupling

The DCM3D and NEFTRAN II codes are not directly linked to one another. Therefore, some post-processing of the DCM3D-generated flow field is required to produce a useable transport migration path for NEFTRAN II. This is described below.

The post-processor is an enhanced particle-tracking routine that takes the Darcy flow velocities, moisture contents and material porosities produced or used by DCM3D and designates a single, nonbranching transport migration path for NEFTRAN II. As described above, attributes of the transport migration path include number of transport legs, transport leg lengths, mean degree of saturation for each transport leg, and mean pore velocity (Darcy velocity divided by moisture content) of each transport leg. For single-continuum, one-dimensional models, the particle tracker simply calculates the pore velocities along the flow path. However, NEFTRAN II can only handle transport in either a fracture or matrix continuum but not both simultaneously. For dual-continuum models the particle tracker must look at the velocities in both the fracture continuum and the matrix continuum and decide which is the dominant path. The particle tracker designates the one with the higher pore velocity to be the dominant transport path. As a result, the transport path does not allow for simultaneous fracture and matrix transport. An alternative approach to transport modeling would be to treat the fracture and matrix continua together as an equivalent porous medium (Erickson et al., 1986; Dudley et al., 1988). This was the approach taken in the fifth conceptual model, described in Section 2.3.

The particle tracker defines a new transport leg whenever a change in material properties occurs along the transport path. A change in either the hydrological or the geochemical properties warrants the definition of a new leg. A new leg is also defined whenever the dominant transport path changes from fracture to matrix or vice versa. A mean pore velocity and a mean degree of saturation are calculated based on the pore velocities and saturations in each of the grid blocks (from DCM3D) that make up that leg.

Figure 3.1. Source Term Release Rates for Isotopes Considered

3.3 CCDF Generation

The primary performance criterion chosen as a measure of comparison between the alternative conceptual models is total integrated release of radionuclides to the water table below the repository, expressed in terms of a CCDF. This performance measure is, in principle, consistent with the proposed EPA Containment Requirements, 40 CFR 191 (EPA, 1985). Simulating release of radionuclides beyond the water table to the accessible environment could result in a proportionately larger number of zero-release realizations for certain conceptual models. The larger number of zero-release realizations would likely make any type of uncertainty analysis and sensitivity analysis less meaningful.

To generate the CCDF, data and parameter uncertainty was treated primarily for the radionuclide transport parameters. The parameters that were assumed to have some uncertainty associated with them include matrix retardation factors, longitudinal dispersivity, path length, and mean pore velocity. The distributions and ranges for these are summarized in Table 3.5. The range given in Table 3.5 is the range of values by which the base values were multiplied. For example, for a leg length of 100 m, the base value for longitudinal dispersivity would be 10 m. Therefore, the range of dispersivities for that leg would be 2 m to 50 m. This range contains 99.8% of the normal probability density function and was chosen arbitrarily. The 'nominal' base retardation factors were

calculated using distribution coefficients (K_d) from Thomas (1987). These are presented in Table 3.6. The path lengths and mean pore velocities were determined using the DCM3D post-processor (see Section 3.2). Dispersivities were assumed to be 1/10 of the leg length, based on discussion by de Marsily (1986). Uncertainty was assumed for the fracture/matrix transfer coefficient in the fracture/matrix flow simulations; however, only the largest transfer coefficient run was used to provide a flow field for the transport simulations used to generate the CCDFs. A full uncertainty analysis for flow was not conducted because of computational and time constraints. However, treating uncertainty in only the transport parameters was considered sufficient for the purpose of this investigation, which is to qualitatively evaluate conceptual model uncertainty. Note that a sensitivity analysis based on parameter values is not presented as part of this investigation. Only the sensitivity of results to conceptual modeling assumptions was assessed.

Table 3.5. Parameters Varied in Transport Analysis

PARAMETER VARIED	RANGE	DISTRIBUTION	BASE VALUES
Matrix Retardation Factor	0 - 1	Normal	Nominal
Longitudinal Dispersivity	0.2 - 5	Normal	0.1*Path Length
Path Length	0.5 - 2	Normal	Nominal
Mean Pore Velocity	0.2 - 5	Normal	DCM3D Results

Uncertainty in these parameters reflect the inaccuracies known to exist in the base values used. For example, the reports from which the retardation factor data were retrieved have incomplete data sets, and the values they present are thought to be imprecise based on current laboratory techniques. The dispersivities used are only a rule of thumb and are based on saturated flow, yet are thought to be a reliable prediction. Furthermore, the actual path length that a solute particle is going to travel from the proposed repository to the water table is not going to exactly equal the distance of 230 m, but rather, due to rise in a rise in the water table or macroscopic diversion, some value approximately this distance. Finally, varying the pore velocity is fully justified as this is a calculated parameter based on several uncertain parameters and models.

Random sampling of parameter values was carried out using the Latin Hypercube Sampling (LHS) technique (Iman and Shortenearr, 1984). LHS is a stratified

Table 3.6. Retardation Factors Used in Transport Analyses

Leg #	⁹⁹ Tc	¹²⁹ I	¹³⁵ Cs	²³⁷ Np
1	18.7	1.0	17,660	884
2	18.7	1.0	17,660	884
3	24.4	1.0	23,360	1,169
4	71.4	1.0	140,700	705
5	1.0	1.0	1.0	1.0
6	1.0	1.0	1.0	1.0
7	1.0	1.0	7.2×10^{12}	7.5×10^9
8	1.0	1.0	36,780	38
9	1.0	1.0	101,700	103
10	1.0	1.0	35,890	37
11	1.0	1.0	101,700	103
12	1.0	1.0	35,840	37
13	1.0	1.0	101,600	103
14	1.0	1.0	35,730	37
15	1.0	1.0	1.9×10^{14}	1.9×10^{11}

sampling technique in which the range of values for each variable is divided into intervals of equal probability so that a value is sampled from each interval. Sampling in such a way ensures that values for each parameter are obtained covering the entire range of values. The base parameter values, listed in Table 3.5, were multiplied by the LHS samples, which were from the ranges given. Using this set of parameter values, the release to the water table was calculated using NEFTTRAN II. Fifty samples required to distinguish between certain groups of alternative conceptual model. For example, differences between the all fracture and fracture with matrix diffusion models, and the models with matrix transport, were quite apparent with only 50 realizations. On the other hand, 500 samples were used to clarify some of the differences among the models containing matrix transport.

3.4 Comparison Criteria

As mentioned in Section 3.3, the CCDF of total radionuclide release to the water table is the regulatory-related performance measure used to compare conceptual models with each other in this investigation. However, intermediate calculations, such as saturation profiles, pressure profiles, and mean isotope travel times, can provide a great deal of insight as to the effect fundamental assumptions can have on results. These intermediate steps were taken in calculating the CCDFs and the results will be presented in Section 4.

Because the CCDF, in general, incorporates all sources of uncertainty (including conceptual, mathematical, and numerical model uncertainty, data and parameter uncertainty, and uncertainty about future states of the system), it can be difficult to discern which source(s) of uncertainty contributes most to changes in the CCDF. For this study, however, the same mathematical and numerical models and data and parameter values were used for each of the conceptual models. Also, uncertainty about the future state of the system was not included in the modeling. Consequently, relative changes in the CCDF could be attributed primarily to differences in the fundamental assumptions used in developing the conceptual models.

The CCDF's generated for each of the alternative conceptual models will be qualitatively and graphically compared to one another using a sensitivity analysis type approach. That is, the comparison should assist in identifying those fundamental assumptions, if any, that have the greatest impact on the performance measure.

4.0 RESULTS

The calculations carried out by DCM3D and NEFTRAN II, and outlined in Section 3, eventually resulted in integrated releases for each isotope and realization. The multiple realizations for each conceptual model were then summed and plotted as a CCDF curve. The results of these calculations are described below.

4.1 Ground Water Flow Simulations

Results from the DCM3D simulation consisted of pressure heads, moisture contents, and Darcy velocities for both the matrix and fractures. Degrees of saturation were calculated from the moisture contents and the porosities for each geologic unit. The total heads were calculated from the elevation of a grid block center and the corresponding pressure head at that grid block center.

4.1.1 Matrix-Dominated Flow Model

In general, the matrix pressure head is always negative and has an average negative gradient between the water table and the repository bottom (Figure 4.1). However, in Layer 1, the matrix pressure head has a positive gradient. This may be due to this layer

Figure 4.1. All Matrix Flow Model - Pressure Head

having a steeper characteristic curve than many of the other layers. The positive gradient in this layer indicates a downward movement of water due to suction. Between 841 m and 868 m, in the combined layer, the pressure gradient is almost -1.0 which counteracts the gravitational component of flow so that the total head gradient in this layer is almost zero (see Figure 4.2). This unit was assigned a saturated hydraulic conductivity several orders of magnitude larger than the recharge rate, which accounts for this phenomenon. Throughout the remainder of the column, the pressure gradient is negative.

The total head gradient is positive everywhere in the column (see Figure 4.2). This indicates a downward flux of water from the repository to the water table. Between 841 m and 868 m, the gradient is extremely flat but it is still positive. The matrix saturated hydraulic conductivity in this layer is very large and only a small gradient is required to let water flow through it.

The moisture contents are quite variable below 841 m (Figure 4.3). In this region the layers have alternating hydrologic properties and the moisture contents reflect this. The moisture contents vary rapidly between 0.36 and 0.23. However, in the layers with similar hydrologic properties, the moisture contents decrease slightly with increasing elevation. This indicates a general downward movement of water.

Below 841 m, the layers with the lower moisture contents have a higher degree of

Figure 4.2. All Matrix Flow Model - Total Head

Figure 4.3. All Matrix Flow Model - Moisture Content

saturation (Figure 4.4). This is a reflection of the properties of the characteristic curves; the layers with the higher porosities tend to have steeper characteristic curves. At elevations between 841 m and 868 m, the saturation decreases relatively rapidly. This phenomenon occurs in the combined layer with the very high saturated hydraulic conductivity.

4.1.2 Fracture-Dominated Flow Model

The pressure head gradients in each of the five layers of the fracture-dominated flow model are 0.0 except at the bottom of the layers, where they become steep (Figure 4.5). Because the van Genuchten parameters are the same for each layer, the pressure heads between layers change solely to differences in the fracture saturated hydraulic conductivity of the layers. In general, layers with the higher fracture saturated hydraulic conductivities have the lower pressure heads and vice versa. The rapid change in the pressure heads at the bottom of the layers is due to the steep fracture characteristic curves. Small changes in the pressure heads can cause rapid changes in the relative hydraulic conductivities.

The zero pressure head gradient behavior indicates that flow is mostly dominated by gravity everywhere except at the bottom of the layers. At 730 m and 841 m, the gravity

Figure 4.4. All Matrix Flow Model - Saturation

Figure 4.5. All Fracture Flow Model - Pressure Head

effects and suction effects almost counteract each other so that the total head gradient is almost 0.0. At 868 m, the pressure head and total head gradients counteract each other somewhat. The total head gradient there is 0.33. At 851 m and 860 m, the pressure head and total head gradients are both positive, resulting in strong positive total head gradients at these locations.

The total head gradient averages 1.0 throughout the column (Figure 4.6). This gradient indicates that gravity dominates the downward flow of the water. The scale of this figure is too large to show the total head gradient at the layer bottoms. However, the total head gradients are nearly zero at the layer bottoms at 730 m and 841 m. The gradients are positive at 851 m, 860 m, and 868 m.

Throughout the column the saturations do not change within a layer except rapid saturation changes at the bottom of the layers (Figure 4.7). The saturations reflect the pressure heads, which do not change within at the bottom. The saturations are higher than the residual saturations everywhere throughout the column.

In addition, the moisture contents do not change within a layer except at the bottom of the layer (see Figure 4.8). The moisture contents change rapidly at the bottom of each layer which reflects the porosity and saturation changes between the layers.

Figure 4.6. All Fracture Flow Model - Total Head

Figure 4.7. All Fracture Flow Model - Saturation

Figure 4.8. All Fracture Flow Model - Moisture Content

4.1.3 Simultaneous Fracture and Matrix Flow Model

Large transfer coefficient case. The pressure head for the large transfer coefficient case shows an average negative gradient throughout the column (see Figure 4.9). However, in some layers the gradient is positive and in others it is negative. The matrix and fracture pressure heads are equal everywhere except at the water table (730 m), 843 m, and 850 m (see Figure 4.10). A positive difference indicates transfer of water into the fractures from the matrix. A negative difference indicates transfer into the matrix from the fractures. Thus, at the water table and 850 m, water is transferred into the fractures, and at 843 m water is transferred into the matrix. The water transfers at 843 m and 850 m both occur in Layer 5.

Between 840 m and 868 m, the pressure head changes rapidly (see Figure 4.9). In Layer 3, between 860 m and 868 m, there is a positive pressure head gradient. Because the matrix saturated hydraulic conductivity of this layer is less than the recharge rate, the gradient must be greater than 0.0 in order for the recharge to flow through it. After flowing through Layer 3, the water must flow through Layer 4 between 851 m and 860 m. Layer 4 has an extremely high matrix saturated hydraulic conductivity. As a result, the total head gradient in this unit is very small (see Figure 4.11) and the pressure head gradient approaches -1.0. At the top of the underlying unit, Layer 5, water starts to transfer into the fractures. This is caused by the small matrix saturated hydraulic conductivity (less than the recharge rate) of Layer 5, between 841 m and 851 m. Except

Figure 4.9. Matrix/Fracture Flow Model (Large Transfer Coefficient) - Pressure Head

Figure 4.10. Matrix Fracture Flow Model (Large Transfer Coefficient) - Head Difference

Figure 4.11. Matrix/Fracture Flow Model (Large Transfer Coefficient) - Total Head

at the bottom, flow through Layer 5 is driven by gravity in both the matrix and the fractures. This is indicated by the flat pressure head gradient in this unit. 78.7% of the water flow through Layer 5 occurs in the fractures (see Figure 4.12). Near the bottom of Layer 5, a transfer of water from the fractures into the matrix begins. At the very bottom of Layer 5 and underneath the region of water transfer from the fractures into the matrix, a very steep pressure head gradient forms. Because almost all the water has transferred back into the matrix, a steep gradient must form in order for water to move through this low matrix saturated hydraulic conductivity unit. The underlying unit, Layer 6, has such shallow characteristic curves (resulting from small alpha values) that even large pressure head changes affect the matrix unsaturated hydraulic conductivity only slightly. As a result, in the thin Layer 6, between 840 m and 841 m, the pressure head changes only slightly. From 840 m to the water table, the pressure head gradually increases toward a totally saturated condition in both the matrix and the fractures.

Near the water table there is another transfer of water from the matrix to the fractures. At this point the fractures are nearly saturated as a result of being close to the water table. Because the fractures have both a large saturated hydraulic conductivity and a relative hydraulic conductivity near 1.0 from being closer to the water table, the fractures provide a less resistant conduit for flow than the matrix. Therefore, water is transferred from the matrix into the fractures. At the water table, the flow in the fractures nearly equals the recharge rate (see Figure 4.12).

Figure 4.12. Matrix/Fracture Flow Model (Large Transfer Coefficient) - Darcy Velocity

The matrix saturations indicate a gradual drying as distance up the column increases (see Figure 4.13). The matrix saturations are near 1.0 between the water table and 930 m, indicating nearly saturated conditions. Above 930 m the matrix saturation drops rapidly to 0.88. The fracture saturations hover near the fracture residual saturation (0.04) throughout most of the column except at two places. At the water table, the fracture saturation approaches 1.0 due to the water table boundary condition. Between 841 m and 851 m, the fracture saturation approaches 0.08. This higher fracture saturation occurs in the low matrix hydraulic conductivity unit where there is a significant amount of flow in the fractures (Layer 5).

The moisture contents reflect the saturations and the porosities in the various layers (see Figure 4.14). The thin layers below 841 m are easily visible here. Even though those layers have high matrix saturations, their porosities cause a wide variation in the moisture contents.

The matrix Darcy fluxes equal the recharge rate everywhere except in Layer 5 and near the water table (see Figure 4.12). As a result, the fracture Darcy fluxes are negligible everywhere except in Layer 5 and near the water table. In Layer 5 the matrix Darcy flux reduces to 21.3% of the recharge rate and the fracture Darcy flux is 78.7% of the recharge rate. At the water table, the matrix Darcy flux decreases to 1.5% of the recharge rate. 98.5 % of the recharge at the water table flows in the fractures as indicated by the fracture Darcy flux approaching the recharge rate.

Figure 4.13. Matrix/Fracture Flow Model (Large Transfer Coefficient) - Saturation

Figure 4.14. Matrix/Fracture Flow Model (Large Transfer Coefficient) - Moisture Content

Medium transfer coefficient case. The medium transfer coefficient case produces results that are very similar to those for the large transfer case. However, there are some minor differences. These differences are caused mainly by the reduced transfer coefficient. Most of the statements made for the large transfer coefficient apply to this case also.

The matrix and fracture pressure and total heads for the medium transfer coefficient case (Figure 4.15 and Figure 4.16) are very similar to those for the large transfer coefficient case (see Figure 4.9 and Figure 4.11, respectively). The major contrast occurs in the pressure head differences (see Figure 4.17). Both the positive and negative pressure differences for the medium transfer coefficient case are larger than for the large transfer coefficient case (see Figure 4.10) by almost an order of magnitude. Since the transfer coefficient for the medium case is smaller than for the large case, a large pressure difference is required in order to transfer water to and from the fractures.

The saturations and moisture contents are relatively unaffected by this larger pressure difference (Figure 4.18 and Figure 4.19). However, at the bottom of Layer 4, there is a sharp peak in the fracture saturation. This is due to the large difference in the matrix saturated hydraulic conductivities between Layer 4 and Layer 5.

Except at the water table, Darcy fluxes in the matrix and the fractures for the medium transfer coefficient case are the same those for the large transfer coefficient case (see

Figure 4.15. Matrix/Fracture Flow Model (Medium Transfer Coefficient) - Pressure Head

Figure 4.16. Matrix/Fracture Flow Model (Medium Transfer Coefficient) - Total Head

Figure 4.17. Matrix/Fracture Flow Model (Medium Transfer Coefficient) - Head Difference

Figure 4.18. Matrix/Fracture Flow Model (Medium Transfer Coefficient) - Saturation

Figure 4.19. Matrix/Fracture Flow Model (Medium Transfer Coefficient) - Moisture Content

Figure 4.20). Flow in the matrix and fractures at the water table is significantly different. At the water table, the flux in the matrix increases to 21.1% of the recharge rate and the flux in the fractures decreases to 78.9%.

Small transfer coefficient case. The small transfer coefficient case produces similar behavior as the large transfer coefficient case. However, there are some differences worth noting.

The matrix pressure head for the small transfer coefficient case (see Figure 4.21) is similar to the matrix pressure head for the large and medium cases. The fracture pressure heads are similar everywhere except at 843 m in Layer 5. Here there is a large difference in the matrix and fracture heads (see Figure 4.22), which is due to the smaller transfer coefficient. In fact, the fracture pressure actually goes positive. This indicates that the fractures saturate at this elevation. Apparently the pressure head difference becomes so strong due to small transfer coefficient that the fractures must saturate in order for water to flow through this unit. The total head for the matrix and fractures reflects the head difference at 843 m; otherwise, the total head is the same as for the large and medium cases (see Figure 4.23).

The saturations and moisture contents are relatively unaffected by the small transfer coefficient except at two points (see Figure 4.24 and Figure 4.25). At the bottom of

Figure 4.20. Matrix/Fracture Flow Model (Medium Transfer Coefficient) - Darcy Velocity

Figure 4.21. Matrix/Fracture Flow Model (Small Transfer Coefficient) - Pressure Head

Figure 4.22. Matrix/Fracture Flow Model (Small Transfer Coefficient) - Head Difference

Figure 4.23. Matrix/Fracture Flow Model (Small Transfer Coefficient) - Total Head

Figure 4.24. Matrix/Fracture Flow Model (Small Transfer Coefficient) - Saturation

Figure 4.25. Matrix/Fracture Flow Model (Small Transfer Coefficient) - Moisture Content

Layer 4, there is a sharp peak in the fracture saturation. This is due to the large difference in the matrix saturated hydraulic conductivities between Layer 4 and Layer 5. Near the bottom of Layer 5, the fracture saturation becomes 1.0, which reflects the positive fracture pressure head at that point.

Flow in the matrix and the fractures for the small transfer coefficient case are the same as in the large case (see Figure 4.26) except in Layer 5 and at the water table. Matrix flux in Layer 5 increases slightly to 23.3% of total recharge and fracture flux reduces slightly to 76.7%. At the water table fluxes in the matrix and fractures are significantly different. The flux in the matrix increases to 54.1% of the recharge rate and the flux in the fractures decreases to 45.9%.

4.1.4 Alternative Stratigraphic Layering Flow Model

Matrix and fracture pressure heads are equal and the pressure head gradient is negative throughout the entire column (see Figure 4.27). The pressure gradient in the region between the water table and 841 m averages -0.45. The region between 841 m and 868 m shows a pressure head gradient of -1.0. The pressure head gradient in this region is almost identical to the negative of the gravitational gradient because the matrix saturated hydraulic conductivity is very large compared to the recharge rate. Thus, only an extremely small gradient is necessary to cause water to flow through this region.

Figure 4.26. Matrix/Fracture Flow Model (Small Transfer Coefficient) - Darcy Velocity

Figure 4.27. Four-Layer Stratigraphy Flow Model - Pressure Head

Above 868 m, the pressure gradient averages -0.17, which reflects a higher matrix hydraulic conductivity being assigned to this region than to the lowest region (731 m to 841 m).

Matrix and fracture total heads are equal also (see Figure 4.28). The total head gradient is positive everywhere and reflects the downward movement of water. In the region between 841 m and 868 m, the pressure gradient is almost 0.0. The matrix saturated hydraulic conductivity is very large compared to the recharge rate; therefore, only a small hydraulic gradient is necessary for flow to occur.

For the region between 841 m and 868 m, in the simultaneous matrix and fracture flow conceptual models, the pressure and total heads were quite variable. The averaging of the hydrologic parameters in the alternative stratigraphy model removes this variability and smooths the heads in this region.

The matrix saturations are nearly 1.0 between the water table and 868 m (see Figure 4.29). Above this elevation the matrix saturations drop to 0.83. The fracture saturations hover near the fracture residual saturation of 0.04 except near the water table. At the water table the fractures saturate as a result of the water table boundary condition. The moisture contents reflect the saturations and porosities of the various regions above the water table.

Figure 4.28. Four-Layer Stratigraphy Flow Model - Total Head

Figure 4.29. Four-Layer Stratigraphy Flow Model - Saturation

The changes in moisture content are due almost entirely to porosity changes between the water table and 868 m (see Figure 4.30). Above 868 m the matrix moisture contents are determined mostly by the matrix saturation because it is lower in this region than in the region below 868 m.

Throughout the entire column, except near the water table, recharge is carried entirely by the matrix (see Figure 4.31). This indicates that there is no exchange between the matrix and the fracture anywhere except at the water table. Near the water table the fractures begin to saturate and provide an easier conduit for flow than the matrix. Because the fractures have a much higher hydraulic conductivity than the matrix, they are capable of maintaining more flow than the matrix. At the water table the fractures carry 98.5% of the recharge and the matrix carries 1.5%.

4.2 Radionuclide Transport Simulations

A summary of the alternative conceptual models is given in Table 4.1. In terms of comparative results, it is obvious, and expected, that the all-fracture model resulted in shortest travel time, and that the all-matrix model resulted in the longest travel time. The travel time for the fracture-with-matrix-diffusion model is the same as the all fracture model because the travel times are based on the mean pore velocity of an

Figure 4.30. Four-Layer Stratigraphy Flow Model - Moisture Content

Figure 4.31. Four-Layer Stratigraphy Flow Model - Darcy Velocity

isotope that is not retarded. The contrast in pore velocities is clearly demonstrated in Figure 4.32. Shown in this figure are the mean pore velocities for the all-fracture, all-matrix, and fracture/matrix (i.e., dual-continuum) models as calculated by the DCM3D post-processor. Note that the curves are not smooth because the mean pore velocity in each leg in the transport path has been assumed to be constant across the entire leg. Large jumps in the velocity curve from relatively low velocities to relatively high velocities for the fracture/matrix model are indicative of a switch from matrix to fracture flow.

The remaining information provided in Table 4.1 is either prescribed data or is data that are calculated by the DCM3D post-processor and are needed for the transport simulations. Although the first five conceptual models contained 15 hydrogeologic units except for the all-matrix model which contained 13, none but the all-matrix case contained the same number of transport legs as hydrogeologic units. As discussed in Section 3.2, the number of fracture legs and matrix legs is a function of the material properties and whether the dominant transport path switches from fracture to matrix or vice versa. For the all-fracture models (No. 2 and No. 3), several groups of adjacent hydrogeologic units had the same material properties and could therefore be grouped into a fewer number of equivalent legs. In the dual-continuum models, however, the dominant transport path switched, within certain hydrogeologic units, from matrix to fracture and from fracture to matrix; therefore, the number of transport legs exceeded

Table 4.1. Summary of Conceptual Model Properties

		1) All Matrix	2) All Fracture	3) Fracture w/ Diff	4) Dual Continuum	5) Equiv. Porous	6) 4 Layer Stratig.
Transport	Fracture Legs	-	6	6	4	15	2
	Matrix Legs	13	-	-	15	15	4
	Simulation Time (yrs)	10^5	10^4	10^4	10^5	10^5	10^5
	Exchange Coeff.	-	-	0.0001	-	-	-
Flow	Continuum	single	single	single	dual	dual	dual
	Coupling Term	-	-	-	1	1	1
	Travel Time (yrs)	1.3×10^6	14	14	5.0×10^5	4.8×10^5	5.4×10^5

Figure 4.32. Pore Velocities for All-Fracture, All-Matrix and Fracture/Matrix Conceptual Models.

the number of hydrogeologic units.

The fracture/matrix coupling term used in the flow calculations (which were in turn used to generate transport migration paths) was the largest of the three. The transport fracture/matrix mass exchange coefficient was relatively high compared to the values used in the study by Bonano et al. (1989); however, they were using values for a saturated system. Appropriate values for the transfer or coupling terms (for both flow and transport), and what those values imply has yet to be properly addressed and, therefore, is still not clear.

Because the desired transport result is total integrated release, expressed in terms of a CCDF, the radionuclide transport simulations were conducted in a manner such that multiple data sets were accessed and run without user intervention between runs. The multiple data sets were the result of the random sampling described in Section 3.3. Because of the nature of this procedure, intermediate results from individual runs, such as isotope-specific cumulative release and release rates, were not reported. In spite of this, one set of sampled data was used to illustrate the impact of different conceptual models on intermediate results. An example of cumulative releases over the simulation time for the individual radionuclide species transported is shown in Table 4.2. These

Table 4.2. Cumulative Isotope Release to Water Table using NEFTRAN II

Conceptual Model	Cumulative Release to Water Table (Ci)			
	⁹⁹ Tc	¹²⁹ I	¹³⁵ Cs	²³⁷ Np
1) All Matrix *	197	7.15	0.0	0.0
2) All Fracture **	6.26x10 ⁵	1510	1.68x10 ⁴	0.043
3) Fracture w/ Matrix Diffusion **	5.8x10 ⁻⁴	8.5x10 ⁻⁷	4.5x10 ⁻¹²	4.3x10 ⁻¹⁵
4) Dual Continuum *	5.29x10 ⁴	515	0.0	0.0
5) Equivalent Porous Medium *	5.52x10 ⁴	416	0.0	0.0
6) Four-Layer Stratigraphy *	3.41x10 ⁴	535	0.0	0.0

* 10⁵ year simulation

** 10⁴ year simulation

values were generated using the random sample that resulted in the largest EPA sum. The EPA sum is the sum of the individual isotope's cumulative release normalized by the original inventory and the EPA containment requirements for that isotope. Again, note that the simulation times for the all-fracture and fracture-with-matrix-diffusion models were 10⁴ years while that for the other models is 10⁵ years. Also note that the

cumulative releases given in Table 4.2 have not been normalized by the quantity of waste and the EPA release limits provided in 40 CFR Part 191 (Appendix A, Table 1; EPA, 1985), as they would be when generating the CCDF.

The cumulative release to the water table for the all-fracture conceptual model and for all the radionuclides is, for all practical purposes, equal to the cumulative release from the source. This is because of the relatively short travel time for this case, which results from the relatively high fracture velocities and lack of radionuclide retardation in the fracture continuum. Also, because of the very short travel time, a negligible amount of the inventory is lost to radioactive decay. Obvious from Table 4.1 is that adding any matrix transport and/or matrix retardation significantly decreases the cumulative release. In fact, for ^{135}Cs and ^{237}Np , any of the models that contain matrix transport result in zero release to the water table, primarily because of the high matrix retardation factors for these two isotopes. Note that, even for the long simulation times, little of the initial inventory is lost as a result radioactive decay, because of the long half-lives of the radionuclides. For example, over 10^5 years, 28% of ^{99}Tc to 0.4% of ^{129}I is lost to decay.

Similar information about transport calculations is conveyed in Figure 4.33, where the release rate as a function of time is plotted for ^{129}I . These are the release rate curves that were used to calculate the cumulative releases for ^{129}I in Table 4.2. The four conceptual models that include matrix transport have breakthrough times for release greater than 10^4 years; therefore, to produce comparative results, a 10^5 year simulation

Figure 4.33. Release Rates to Water Table for ^{129}I

time was needed for these models. Note that the release rate for the all-fracture model, on the other hand, is virtually identical to the release rate from source (see Figure 3.1), both in breakthrough time and magnitude of release. The delay of 14 years (mean travel time for the all-fracture model) is not discernible in Figure 4.33. The inclusion of matrix diffusion significantly delayed the time of release although this model had the same mean travel time as the all-fracture model.

4.3 Assessment of Alternative Conceptual Models

The CCDFs for the four alternative conceptual models that include any matrix transport are shown in Figure 4.34. The simulation time for each of these conceptual models was 10^5 years. The EPA Containment Requirement (§ 191.13) is shown in the figure only to illustrate where the regulation lies on the plot. The containment requirement is in no way included to assess the site's ability to show compliance. Fifty realizations were used to generate each of the CCDFs shown in the figure. For the most part, the results are not surprising, except for possibly the all-matrix case (No. 1). Only a few parameter combinations for the all-matrix conceptual model resulted in realizations with summed normalized release greater than 10^{-2} , and no combinations resulted in realizations with release greater than 1. The other three matrix-transport conceptual models (No. 4, No. 5, and No. 6), on the other hand, had several realizations with summed normalized release greater than 10^{-2} and a few realizations with release greater than 1. Although

Figure 4.34. CCDF Curves for Conceptual Models That Consider Matrix Flow and Transport

it is not shown in the figure, all of the models had a number of **zero-release** realizations. Because the probability of release being greater than the summed normalized release (y-axis value) must be 1 when the summed normalized release (x-axis value) is zero, there may be a large jump in the CCDF y-value at this point. One would expect that because the majority of the flow and therefore, the transport, would occur in the matrix continuum, the four models would be quite similar. However, remember that the latter three conceptual models, because they were not restricted to matrix flow only, contained some fracture legs in the *transport* migration path. These fracture legs can, by the way the conceptual models are defined, act as bypasses to their matrix counterparts in the matrix-only model. Because the pore velocities in the matrix legs are so much lower than in the fracture legs, the transport in the matrix legs dominates the total release curve. Therefore, having only a few matrix legs that would otherwise be fracture legs, can decrease the release of radionuclides significantly. This seems to be the case with the conceptual models shown.

Of the three fifteen-layer conceptual models containing matrix transport, the equivalent-porous-medium transport model (No. 5), conceptually, should result in the greatest release because it includes transport in both fracture and matrix simultaneously. This is not very obvious from Figure 4.34, however. In fact, for the high-probability, low-consequence realizations, the equivalent-porous-medium model consistently resulted in a greater number of lower releases than the fracture/matrix model (No. 4). This is a consequence of the manner in which the transport pore velocities and retardation factors were varied. In the fracture/matrix model, the pore velocities and the retardation factors were varied independently (i.e., they were uncorrelated). Therefore, for a given pore velocity, both high and low retardation factors may be realized, resulting in a variety of effective transport velocities. In the equivalent-porous-medium model, on the other hand, an equivalent velocity was defined in terms of the velocities and retardation factors in the fracture and in the matrix. Only this equivalent velocity was varied (over the same range as the pore velocity for the fracture/matrix model), and the retardation factors were constant. In a sense, the velocity and retardation are completely correlated. Therefore, retardation factors were not allowed to affect the effective transport velocity as they were in the fracture/matrix model. As a result, the equivalent-porous-medium model results in a greater number of low releases, and also a greater number of high releases than the fracture/matrix model. If the velocities and the retardation factors were varied in the same way in each model, the equivalent-porous-medium model would consistently have fewer low-release realizations and more high-release realizations.

The CCDFs representing the conceptual models for fracture-dominated flow and transport are shown in Figure 4.35. Although these CCDFs are also based on fifty realizations, the simulation time is only 10^4 years. From Figures 4.34 and 4.35, it is obvious that given the assumptions of the conceptual models in this investigation, the assumption of identifying matrix or fracture as the dominant flow regime has the greatest impact on the performance measure. Although not shown in these figures, whenever a matrix block or leg is included in series with fracture legs, the release is reduced significantly to the point of zero release within the 10^4 -year regulatory time frame. The

Figure 4.35. CCDF Curves for Fracture Dominated Flow and Transport Conceptual Models

vertical CCDF curve for the all-fracture case indicates that the entire inventory of radionuclides is released to the water table for all realizations. This is not very surprising in that fracture retardation factors were assumed constant and equal to 1 for all radionuclides, and that the fracture velocities were relatively high. Matrix diffusion obviously has a significant impact on integrated release. This is not only because the matrix acts as an immobile storage volume, but also because the radionuclides that diffuse into the matrix are assumed to be able to adsorb to the matrix surface. Given the assumptions of these conceptual models, matrix diffusion can result in decrease in summed normalized releases over several orders of magnitude.

Also of particular interest in this investigation was the number of samples or realizations that were used to generate the CCDFs. The CCDFs of the four models which include matrix transport were presented in Figure 4.34. These were generated using 50 random samples, giving each realization of the summed normalized release a probability of 1/50 of occurring. In Figure 4.36, however, 500 samples were used to generate the CCDFs, giving each realization a probability of 1/500 of occurring. This result of a larger number of samples is characterized by a greater number of extreme results. That is, with a larger sample size, and therefore more parameter combinations, one would expect a larger number of high releases, as well as a larger number of low releases. In actuality, there is a larger number of realizations at all levels, but with more samples higher and lower releases will be realized. This is quite evident in the figures. Most

Figure 4.36. CCDF Curves for Conceptual Models That Contain Matrix Flow and Transport (Sample Size = 500)

significantly impacted is the all-matrix case. After a certain point, increasing the number of realizations will not result in any higher releases (i.e., convergence will be achieved). If one is comparing with the EPA Containment Requirements, which requires less than one chance in 1000 of exceeding a given value, then it would be logical to require at least 1000 simulations. A greater number of samples also assists in clarifying information about the behavior in the CCDF curves.

Some trends in the behavior of the CCDF curves for the different conceptual models are evident in Figure 4.36. In this figure, the CCDF for the four-layer stratigraphy model crosses over the CCDFs for the two fifteen-layer stratigraphy models. The trend is not as obvious in Figure 4.34 because there are few realizations beyond the cross-over point. The cross over occurs because there is less variability in the results of the four-layer stratigraphy. That is, the four-layer stratigraphy model results in fewer low-release realizations and fewer high-release realizations. Conceptually, this results because the release or (breakthrough) curves for the four layer case have, in general, a broader distribution than the fifteen-layer case. The broader distribution in the four-layer case is the result of effectively greater dispersion. Dispersivity values were assumed to be one-tenth of the leg length, and for the four-layer case, in NEFTTRAN, these were propagated for longer distances. An explanation of this impact on the CCDF follows.

For very short travel times, all solutes would be released, and for very long travel times,

none of the solute would be released, regardless of the spread in the release curve; however, for intermediate travel times, only a portion of the solutes are released. The amount that is released for these intermediate travel times is a function of the spread in the release curve. For example, for an intermediate, but somewhat long travel time, a broader breakthrough curve may have a small release corresponding to the leading tail of the curve, whereas a narrower breakthrough curve will have less release. The converse is true for intermediate, short travel times; the narrower breakthrough curve will result in a greater release than the broader breakthrough curve because the solutes representing the trailing tail of the broad curve are not released. The impact of this behavior on the CCDF is that the narrower breakthrough curves will tend to have more "all-or-nothing" release realizations than the broader breakthrough curves. This is exhibited as more variability in the CCDF for the narrower breakthrough curves.

Similar crossover behavior is evident between the equivalent-porous-medium model and the fracture/matrix model, but for the reasons described earlier (differences in the way velocities and retardation factors were sampled).

5.0 SUMMARY AND CONCLUSIONS

Some important qualifications have been recognized for the analysis presented. These qualifications are presented in Section 1.3 of this report and were due mainly to the limited scope of this investigation, and also to the numerical and mathematical constraints on the calculational tools applied. These limitations notwithstanding, the comparison between CCDFs has been used to assess the importance of fundamental assumptions on a hypothetical HLW repository site's performance, under a given set of assumptions. This investigation, therefore, directly addresses the issue of conceptual model uncertainty. This is considered to be a critical issue for performance assessment of HLW disposal sites.

Because the CCDF, in general, incorporates all sources of uncertainty (including conceptual, mathematical, and numerical model uncertainty, data and parameter uncertainty, and uncertainty about future states of the system) it can be difficult to discern which source(s) of uncertainty contribute most to changes in the CCDF. For this study, however, the same mathematical and numerical models and data and parameter values were used for each of the conceptual models. Also, uncertainty about the future state of the system was not included in the modeling. Consequently, relative changes in the CCDF could be attributed primarily to differences in the fundamental assumptions used in developing the conceptual models.

This investigation does not necessarily suggest that the conceptual models applied here are correct representations of an HLW disposal site in unsaturated, fractured tuff. However, this study has shown that fundamental assumptions used in the development of a conceptual model can have a significant impact on a regulatory measure for the performance of a site. In addition, analysis of intermediate results can provide insight as to the reasons why different conceptual models yield different results. It is important to realize that an analysis, such as the performance assessment of an HLW disposal site, must be cognizant of all the modeling assumptions, both explicit and implicit, and the potential impact of the uncertainty in those assumptions, in order to be meaningful.

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