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Three-Dimensional Modeling of Unsaturated Flow in the Vicinity of Proposed Exploratory Shaft Facilities at Yucca Mountain, Nevada

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April 1992

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THREE-DIMENSIONAL MODELING OF UNSATURATED
FLOW IN THE VICINITY OF PROPOSED EXPLORATORY
SHAFT FACILITIES AT YUCCA MOUNTAIN, NEVADA

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ABSTRACT

This report describes the results of a study to investigate the influence of proposed exploratory shafts on the moisture distribution within unsaturated, fractured rock at Yucca Mountain, Nevada. The long-term effects of exploratory shafts at Yucca Mountain are important in the estimation of potential waste migration and fate, while short-term effects may be important in the planning and interpretation of tests performed at the site.

Numerical simulations, using a three-dimensional model, suggest that most episodic pulses of water from natural precipitation should not reach the proposed repository directly through fractures or through modified permeability zones around exploratory shafts, due to capillary imbibition into the rock matrix. The results of these simulations also suggest that the ambient moisture content and distribution in the vicinity of the shafts should not change significantly within a reasonable time frame for subsurface characterization work (20 years).

Relatively few data exist on the hydrologic properties of unsaturated, fractured rock at Yucca Mountain. The simulation results reported in this document are specific to the discretization schemes, boundary conditions, and hydrologic properties that were used. Therefore, these results simply represent approximations of the potential effects of exploratory shafts on unsaturated water flow at the site. Improved confidence and quantification of the uncertainty in this type of modeling study will be attained as more data become available.

EXECUTIVE SUMMARY

This report was prepared by Pacific Northwest Laboratory for the Office of Civilian Radioactive Waste Management of the U.S. Department of Energy. This study was undertaken to demonstrate the capability to estimate the moisture distribution within unsaturated fractured media in the vicinity of a hypothetical exploratory shaft facility (ESF) at the potential high-level nuclear waste repository site at Yucca Mountain, Nevada.

The ESF is an important part of the subsurface-based site characterization activities that are outlined in the Yucca Mountain Site Characterization Plan. During the construction and operation of the ESF, methods will be selected to minimize rock disturbances. However, some alterations in the properties of rocks close to the excavations are to be expected. The objective of this study is to investigate the influence of these altered rock zones on the distribution of moisture in the vicinity of the ESF.

This study is limited to investigation of extremely long-term (steady-state) and short-term (on the order of 20 years) impacts of the ESF on the moisture distribution in the unsaturated zone. The long-term effects are important in the estimation of waste migration and fate, while short-term effects may be important in the planning and interpretation of tests performed in the ESF.

The PORFLO-3 computer code was used for simulation of moisture flow through the geologic units adjacent to the ESF. Rather than represent fractures as discrete elements, an equivalent continuum was stipulated, in which the fractured units were assigned equivalent or composite hydrologic properties. Explicit treatment of fractures is not feasible because of the extremely large number of fractures contained in the site-scale problem and the difficulties in characterizing and modeling the fracture geometries.

A three-dimensional geometry was used for the simulations. The exploratory shafts and drifts and the altered property rock zones [called the modified permeability zones (MPZs) in the context of hydrology] associated with them are represented as one-dimensional line elements that are embedded in the

general three-dimensional elements. The Ghost Dance fault, one of the prominent structural and hydrologic features, is included in the calculation domain. This fault is represented using two-dimensional planar elements. The ability to incorporate one- and two-dimensional features within general three-dimensional elements is a unique feature in the PORFLO-3 formulation.

The results of these simulations suggest that the MPZs around the exploratory shafts may act as conduits for preferential flow of water in the welded tuff units when locally saturated conditions and fracture flow occur. However, given the moisture and flux conditions in these simulations, fracture flow with an equivalent continuum approximation is limited to the Tiva Canyon welded tuff unit. Also, with the initial moisture and flux conditions specified, the Topopah Springs welded tuff unit is sufficiently thick that most episodic pulses of water from natural precipitation should not reach the potential repository through fractures due to capillary imbibition into the rock matrix.

A potential for significant lateral flow above the interface between the Paintbrush nonwelded unit and the Topopah Springs welded unit is shown by the simulation results. Where laterally flowing water intersects preferential flow paths or structural features, such as fault zones, locally saturated or perched water-table conditions could develop, which could lead to fracture flow in the Topopah Springs welded unit (i.e., the repository horizon). The Ghost Dance fault was embedded within the model domain for these simulations, and was represented by using the hydraulic properties of a much more permeable material similar to gravel. These hydraulic properties are estimates because of the lack of site-specific data. The simulations suggest that there will be no appreciable change in the moisture-content distribution below the Tiva Canyon welded unit within 20 years after the construction of the ESF. Therefore, even though excavations associated with the ESF will alter the fracture densities and permeabilities of the tuff units, the ambient moisture content and distribution in the vicinity of the shafts should not change significantly within a reasonable time frame for subsurface characterization work.

A relatively coarse grid was used for the model simulations, with the shafts and fault embedded as one- and two-dimensional features within three-dimensional computational cells. Therefore, the results from these model simulations are not as accurate in proximity to the shafts and fault as they would be if these features were explicitly discretized in three dimensions. In addition, relatively few data exist on the hydrologic properties of the vadose zone at Yucca Mountain. Considering the comparatively large scale of this model, and the uncertainty of the hydrologic properties, the results presented should be reasonable. However, these results are specific to the discretization schemes, boundary conditions, and material properties used for these simulations, and simply represent approximations of potential effects of the exploratory shafts on unsaturated water flow at the Yucca Mountain site.

Postclosure thermal effects and vapor-phase transport of moisture caused by heat generated from the potential repository were not considered in this study. However, these factors may have a significant effect on repository performance. Therefore, postclosure modeling studies should consider nonisothermal flow and vapor-phase transport of moisture. The MPZs and shaft back-fill material may become more important for future, smaller scale simulations when coupled fluid flow, heat transfer, and mass transport are considered.

Future simulations with intermediate- and large-scale multidimensional models of the potential repository should include site topography and surface expressions of major fractures and faults to determine potential areas for preferential local recharge. Then, spatially nonuniform, time-varying recharge fluxes can be applied as surface boundary conditions to determine the importance of time and spatial variation of surface recharge to the flow fields in the natural system at depth.

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1.0 INTRODUCTION

The geologic formations in the unsaturated zone underlying Yucca Mountain, Nevada, are being evaluated by the U.S. Department of Energy as the potential location for a high-level nuclear waste repository. Investigations are currently under way to evaluate the hydrologic conditions, processes, and properties of the unsaturated zone at this site.

Yucca Mountain consists of a series of north-trending fault-block ridges composed of volcanic ash-flow and ash-fall tuffs that generally have a regional dip of 5 to 7 degrees to the east (Scott and Bonk 1984). Some of the welded tuff units are highly fractured, which requires that the hydrologic properties of these units be evaluated before estimating the rate at which radionuclides could migrate to the accessible environment. Determining the significance of fracture flow at Yucca Mountain is important because the estimated continuum-saturated hydraulic conductivities of the welded tuff units are up to three orders of magnitude greater than the saturated hydraulic conductivities of the matrix in the welded tuffs (Peters and Klavetter 1988). Therefore, if fracture flow is significant, it could greatly reduce the travel time of water percolating downward through the potential repository horizon. The equivalent continuum approximation that was used to represent the hydraulic properties of the fractured, welded tuffs is described in Section 2.2. The potential repository area, depicted in Figure 1.1, is bounded by steeply dipping faults or by fault zones, and is transected by a few normal faults. Therefore, the effects of fault zones on unsaturated water flow and contaminant transport should be investigated.

The exploratory shaft facility (ESF) is an important part of the subsurface-based site characterization activities that are outlined in the Yucca Mountain site characterization plan (DOE 1988, 1989). The ESF will consist of surface facilities and underground excavations, as conceptualized in Figure 1.2. The underground excavations include two 4.4-m-diameter shafts (called ES-1 and ES-2) connected by drifts at the potential repository horizon. Descriptions of 34 test activities to be performed in the ESF are provided in the site characterization plan. While the construction and operation methods will be selected to minimize rock disturbances, some

FIGURE 1.1. Location Map of the Yucca Mountain Site, Nevada
(after Lin et al. 1986)

alterations in properties of the rocks close to the excavations are to be expected. Therefore, it is important to determine the potential effects of these altered-rock zones [also referred to as modified permeability zones (MPZs)] on the moisture distribution in the vicinity of the ESF.

FIGURE 1.2. Conceptual Exploratory Shaft Facility (from DOE 1988, 1989)

This study is limited to investigation of extremely long-term (steady-state) and short-term (on the order of 20 years) impacts of the ESF on the moisture distribution in the unsaturated zone. Long-term effects are important for estimating the migration and fate of wastes, while short-term

effects may be important in the planning and interpretation of the tests performed in the ESF. This study is focused primarily on short-term effects of the ESF on the unsaturated zone.

To study the spatial effects of the ESF, a three-dimensional geometry was used in the simulations of the unsaturated zone. The exploratory shafts and drifts, and MPZs associated with them, are represented as one-dimensional line elements that are embedded in the general three-dimensional elements. The Ghost Dance fault, one of the prominent structural and hydrologic features, is included in the calculation domain and is represented with two-dimensional planar elements. The ability to incorporate one- and two-dimensional subdomain features within the general three-dimensional elements is a unique feature of PORFLO-3 (Sagar and Runchal 1990). Results of both steady-state and transient simulations are presented.

This report is organized as follows. Section 2.0 describes the conceptual model, hydrologic properties, and initial and boundary conditions. Section 3.0 provides a brief description of the PORFLO-3 code and options used for model simulations. Section 4.0 describes the simulation results. Conclusions and recommendations for future work are provided in Section 5.0. Cited references are listed in Section 6.0.

This work was conducted by Pacific Northwest Laboratory^(a) for the U.S. Department of Energy, Office of Civilian Radioactive Waste Management.

(a) Pacific Northwest Laboratory is operated for the U.S. Department of Energy by Battelle Memorial Institute.

2.0 MODEL DESCRIPTION

2.1 GEOMETRY OF CALCULATION DOMAIN

For the purpose of these simulations, the lithologic units at Yucca Mountain have been grouped into five hydrologic units: 1) the Tiva Canyon welded unit (TCw); 2) the Paintbrush Tuff nonwelded unit (PTn); 3) the Topopah Springs welded unit 1 (TSw1); 4) the Topopah Springs welded units 2 and 3, which are treated as a single composite unit (TSw2-3); and 5) the Calico Hills nonwelded vitric unit (CHnv). The thicknesses of these units are 25, 40, 130, 205, and 130 m, respectively. These thicknesses are based on the stratigraphy of borehole USW-G4, which is located near the eastern edge of the potential repository boundary.

The decision to treat TSw2 and TSw3 as a single unit (TSw2-3) is based on the similarity of the hydrologic properties of the two units and the relatively small thickness of TSw3 (15 m) relative to that of TSw2 (190 m). The potential repository is to be located within unit TSw2-3 at a depth of approximately 310 m below the ground surface (with reference to borehole USW-G4).

Computations were performed in a three-dimensional cartesian grid system. The axes of this system are aligned with east-west (X-axis), north-south (Y-axis), and vertical (Z-axis). The dimensions of the calculation domain are 615, 300, and 530 m in the X-, Y-, and Z-directions, respectively. A total of 25,056 nodes (29, 16, and 54 in the X-, Y-, and Z-directions, respectively) were used to represent this domain for numerical calculations (Figure 2.1). The Ghost Dance fault, which is located near the west boundary, is represented with vertical planar elements (two dimensional), extending from the ground surface to the water table. The exploratory shafts (ES-1 and ES-2) are represented as vertical line elements (one dimensional), extending from the ground surface to a depth of approximately 310 m (i.e., in unit TSw2-3). The shaft elements are connected by offset horizontal line elements, representing connecting drifts, at the 310-m depth. The exploratory shafts and drifts have a 4.4-m diameter and are assumed to have zones of modified permeability around them, which extend 1 m beyond the edges of the

FIGURE 2.1. Yucca Mountain PORFLO-3 Computational Grid. TCw = Tiva Canyon welded unit; PTn = Paintbrush Tuff nonwelded unit; TSw1,2,3 = Topopah Springs welded units; CHnv = Calico Hills nonwelded, vitric unit.

shafts and drifts. Case and Kelsall (1987) report the value of 1 m as an upper bound estimate of the expected MPZ dimension for fractured, welded tuff.

The shafts and fault are positioned within the model domain with reference to borehole USW-G4 (Scott and Bonk 1984; Fernandez et al. 1988). The geometry of the computational grid was designed in consideration of the spatial position of the exploratory shafts relative to the Ghost Dance fault. The line of symmetry dividing the north and south halves of the model domain, indicated by the finer spaced grid, roughly corresponds with the position of

Coyote Wash, which is an east-west-trending watershed that drains off Yucca Ridge, located to the west. The intersection of Coyote Wash with the Ghost Dance Fault is a potential location for preferential local recharge. The finer grid spacing could be used to represent preferential recharge in future simulations.

2.2 HYDROLOGIC PROPERTIES

The welded tuff units (TCw, TSw1, and TSw2-3) are distinguished hydrologically from the nonwelded units (PTn and CHnv) by their matrix hydraulic conductivities and observed fracture density. Table 2.1 lists the fracture characteristics of the five tuff units.

Although there are no direct measurements of fracture properties, the hydrologic properties of the rock matrix and the fractures are expected to differ considerably, with respect to both saturated and unsaturated conditions. The saturated hydraulic conductivities for the bulk rock containing

TABLE 2.1. Fracture Characteristics of Hydrologic Units
(after Peters et al. 1986)

<u>Unit</u>	<u>Sample Code^(a)</u>	<u>Fracture Aperture (microns)</u>	<u>Fracture Density^(b) (no./m³)</u>	<u>Fracture Porosity^(c)</u>	<u>Fracture Conductivity (m/s)</u>
TCw	G4-2F	6.74	20	1.4E-4	3.8E-05
PTn	G4-3F	27.00	1	2.7E-5	6.1E-04
TSw1	G4-2F	5.13	8	4.1E-5	2.2E-05
TSw2-3	G4-2F	4.55	40	1.8E-4	1.7E-05
CHnv	G4-4F	15.50	3	4.6E-5	2.0E-04

- (a) Fracture properties were measured on a limited number of samples using confined fracture-testing methods described by Peters et al. (1984). The differences in the fracture properties of the three welded units (TCw, TSw1, TSw2-3) reflect different confining pressures representing overburden weight evaluated at the average unit depth in borehole USW-G4.
- (b) Based on a report by Scott et al. (1983).
- (c) Fractures are assumed to be planar; therefore, fracture porosity is calculated as fracture volume (aperture times 1 m²) times number of fractures per cubic meter.

fractures are expected to be several orders of magnitude higher than those of the matrix. Unsaturated hydraulic properties are specified as moisture-retention characteristics, which describe the relationship of saturation (or moisture content) with pressure head, and as unsaturated hydraulic conductivity, which describes the relationship of hydraulic conductivity with either pressure head or saturation. For application in numerical models, these relationships are described by analytical functions (van Genuchten 1978; Mualem 1976). The parameters of the water-retention and hydraulic-conductivity functions used to represent the rock matrix of the five hydrologic units are displayed in Table 2.2 (after Peters et al. 1986). The corresponding parameters for the fractures are estimated by Wang and Narasimhan (1986) to be $S_r = 0.0395$, $\alpha = 1.2851/\text{m}$, and $n = 4.23$. These fracture parameters were used to generate equivalent continuum approximations of hydrologic properties to represent the fractures in all three welded units.

The van Genuchten (1978) water-retention curve is defined by

$$S = (S_s - S_r) [1 + (\alpha\psi)^n]^{-m} + S_r$$

where S = saturation (dimensionless)
 S_r = residual saturation (dimensionless)
 S_s = total saturation (≈ 1)

TABLE 2.2. Parameters for Matrix Hydrologic Properties
(after Peters et al. 1986)

Unit	Sample Code	Grain Density (g/cm ³)	Total Porosity	Hydraulic Conductivity (m/s)	S_r	α (1/m)	n
TCw	G4-1	2.49	0.08	9.7E-12	0.002	8.21E-3	1.558
PTn	GU3-7	2.35	0.40	3.9E-07	0.100	1.50E-2	6.872
TSw1	G4-6	2.58	0.11	1.9E-11	0.080	5.67E-3	1.798
TSw2-3	G4-6	2.58	0.11	1.9E-11	0.080	5.67E-3	1.798
CHnv	GU3-14	2.37	0.46	2.7E-07	0.041	1.60E-0	3.872

ψ = capillary pressure head (L)

n, m = empirical parameters (dimensionless)

α = inverse air-entry pressure head (L^{-1}).

The effective porosity, ϕ_e , of each unit is calculated as

$$\phi_e = \phi_b(1 - S_r) \quad (2.2)$$

where ϕ_b is the total or bulk porosity listed in Table 2.2.

In this analysis, rather than represent the fractures as discrete elements, an equivalent continuum is stipulated, in which the fractured units are assigned equivalent or composite properties (Peters and Klavetter 1988). Explicit treatment of the fractures is not feasible because of the extremely large number of fractures contained in the site-scale problem and the difficulties in characterizing and modeling the fracture geometries.

In the equivalent continuum approximation (Peters and Klavetter 1988), the fracture porosity, ϕ_f , can be defined as the ratio of the fracture volume to the total bulk rock volume. The matrix porosity, ϕ_m , can be defined as the ratio of the volume of the voids in the matrix (excluding fracture void space) to the volume of the matrix. A bulk, equivalent porosity, ϕ_b , can then be defined after Nitao (1988) as

$$\phi_b = \phi_f + (1 - \phi_f)\phi_m \quad (2.3)$$

Given the saturation of the fractures, S_f , and matrix, S_m , the equivalent bulk saturation, S_b , can be defined as

$$S_b = \frac{S_f\phi_f + S_m(1 - \phi_f)\phi_m}{\phi_f + (1 - \phi_f)\phi_m} \quad (2.4)$$

The weighting procedure of Klavetter and Peters (1986) is used to obtain the equivalent bulk hydraulic conductivity

$$K_C = K_m(1 - \phi_f) + K_f\phi_f \quad (2.5)$$

where K_c , K_m , and K_f are the composite, matrix, and fracture conductivities, respectively.

Because the two nonwelded units have relatively few fractures, their composite properties are approximately equivalent to those of the rock matrix. Thus, for PTn and CHnv, the properties listed in Table 2.2 are used directly in the van Genuchten (1978) and Mualem (1976) equations. Graphic representations of the properties of these two units are shown in Figures 2.2 and 2.3. In Figures 2.2a and 2.3a, hydraulic conductivity is plotted as a function of pressure head. In Figures 2.2b and 2.3b, relative hydraulic conductivity and pressure head are shown as functions of saturation.

Figure 2.4a shows the composite hydraulic conductivity curve for the TCw unit. A large jump in the value of the composite hydraulic conductivity

FIGURE 2.2. (a) Matrix Hydraulic Conductivity Curve and (b) Relative Hydraulic Conductivity and Saturation Curves for Unit PTn

FIGURE 2.3. (a) Matrix Hydraulic Conductivity Curve and (b) Relative Hydraulic Conductivity and Saturation Curves for Unit Chnv

at a certain value of pressure head (≈ -1 m in Figure 2.4a) is a distinguishing characteristic of the composite curve. In physical terms, the discontinuity indicates that at a pressure head of ~ 1 m (or the corresponding value of moisture content) flow switches from the matrix-dominated to the fracture-dominated flow and vice versa. This abrupt change in the hydraulic conductivity introduces extreme nonlinearity in the problem, which can lead to numerical instabilities. Figure 2.4b shows the composite relative conductivity and pressure head as functions of saturation for the TCw unit. Figures 2.5 and 2.6 show the composite hydrologic properties of the TSw1 and TSw2-3 units. In the numerical model, the discontinuous continuum curves cannot be easily represented by the analytical expression. Therefore, the hydrologic properties of the TCw, TSw1, and TSw2-3 units are introduced in tabular form rather than the analytic van Genuchten relation.

FIGURE 2.4. (a) Composite Hydraulic Conductivity Curve and (b) Relative Hydraulic Conductivity and Saturation Curves for Unit TCw

Calculations, based on the continuum properties, are valid assuming that there are enough fractures of varied orientation to ensure continuum behavior. According to Pruess et al. (1990), the continuum approach will generally break down for processes involving rapid transitions and for conditions of a very tight rock matrix or large fracture spacing. These calculations are also based on the assumption that each hydrogeologic unit is homogeneous, except where hydrologic properties have been modified for the shafts, drifts, MPZs, and Ghost Dance fault. Isothermal conditions also are assumed, although the PORFLO-3 code will solve nonisothermal flow and transport problems as well.

The air-entry pressure heads ($1/\alpha$ in the van Genuchten model) for the MPZs associated with the shafts and drifts in each unit are assumed to be half as great as the air-entry heads of the rock matrix in each unit. This

FIGURE 2.5. (a) Composite Hydraulic Conductivity Curve and (b) Relative Hydraulic Conductivity and Saturation Curves for Unit TSw1

modification is somewhat arbitrary because data are not available, but reflects the assumption that the excavation process will change the pore-size distribution in the MPZs such that the MPZs will effectively behave as a coarser porous medium than the undisturbed rock matrix. The van Genuchten model "n" parameter, used to represent the MPZs, was the same as that used to represent the undisturbed rock matrix. The saturated hydraulic conductivities of the MPZs are assumed to be 40 and 80 times greater than those of the undisturbed matrix in units TSw1 and TSw2-3, respectively. These multiplying factors are based on the upper bound estimates reported by Case and Kelsall (1987), as shown in Table 2.3. The saturated hydraulic conductivity of the MPZs in unit TCw was assumed also to be 80 times greater than the matrix hydraulic conductivity of this unit. This assumption was based on the similarity of fracture densities and porosities between the TCw and TSw2-3 units, as shown in Table 2.1. For the nonwelded units (PTn and CHnv), the saturated hydraulic conductivities of the MPZs were assumed to be 20 times

FIGURE 2.6. (a) Composite Hydraulic Conductivity Curve and (b) Relative Hydraulic Conductivity and Saturation Curves for Unit TSw2-3

higher than the hydraulic conductivities of the matrix of each unit. The nonwelded units have a much higher porosity and lower fracture density than the welded units. Therefore, it was assumed that permeability modifications, resulting from shaft construction in these units, would be less extensive than for the welded units. All other properties of the MPZs in each unit are assumed to be equal to the properties of the undisturbed rock matrix in the units.

The hydraulic properties of the shafts and drifts are represented with parameters that describe the properties of a coarse material such as gravel. The van Genuchten (1978) model retention curve parameters used to represent the shafts and drifts are: $S_r = 0.0$, $\alpha = 1.0$, and $n = 6.2$. Figure 2.7 shows these curves graphically. These water-retention characteristics were selected to create a capillary barrier, effectively restricting flow into the shafts and drifts until the surrounding MPZs are close to saturation. Each section of the shafts and drifts was assigned a saturated hydraulic

TABLE 2.3. Saturated Hydraulic Conductivity Multiplying Factors for the Modified Permeability Zone^(a) (after Case and Kelsall 1987).

Depth (m)	Stress Redistribution Without Blast Damage		Expected ^(b) Case	Upper Bound ^(c) Case
	Elastic	Elastoplastic		
100	15	20	20	40
310	15	40	20	80

- (a) Equivalent permeability is averaged over an annulus one radius wide around the 4.4-m-diameter exploratory shaft.
 (b) This is based on an elastic analysis with expected strength, in situ stress, sensitivity of permeability to stress, and a 0.5-m-wide blast-damage zone.
 (c) This is based on an elastoplastic analysis with lower bound strength, upper bound stress, greatest sensitivity of permeability to stress, and a 1.0-m-wide blast-damage zone.

FIGURE 2.7. (a) Hydraulic Conductivity Curve Representing Shafts and Drifts and (b) Relative Hydraulic Conductivity and Saturation Curves Representing Shafts and Drifts in Unit TSw2-3

conductivity value 1000 times greater than the saturated hydraulic conductivity of the MPZ adjacent to it. Thus, the rate at which water flows through the shaft and drift elements is governed by the hydraulic conductivity of the adjacent MPZs.

No data are available regarding the hydrologic properties of the rubblized shear zone around the Ghost Dance fault. Therefore, the fault MPZ was arbitrarily modeled as 0.5 m wide, with an air-entry pressure head half as great as the air-entry pressure head of the rock matrix. Saturated hydraulic conductivities were taken to be 40 times greater than the undisturbed matrix saturated hydraulic conductivities of each unit. The van Genuchten (1978) "n" parameters that were used to represent the fault were the same as those used to represent the matrix in each unit adjacent to the fault.

2.3 INITIAL CONDITIONS

Two steady-state simulations were performed. In the first, or Case 1, the initial conditions were prescribed as uniform saturation in each unit. The saturation percentages used were determined from core samples from various units at Yucca Mountain, reported by Montazer and Wilson (1984). From these reported average saturation values, pressure heads were calculated for input as initial conditions to Case 1 simulations, using the matrix water-retention curve parameters listed in Table 2.2. These average saturation values and initial pressure heads for the various hydrologic units are listed in Table 2.4. The shafts, drifts, and MPZ subdomain elements were excluded from the Case 1 simulation. The Case 1 simulation was performed to establish the initial conditions for Case 2.

The steady-state vertical pressure distribution from the approximate center of the model domain in the Case 1 simulation was used as the initial pressure distribution everywhere in the domain for the Case 2 simulation to ensure that the specified boundary conditions were consistent with the internal solution. In the Case 2 simulation, the shafts, drifts, and MPZ subdomain elements were included in the model domain. The steady-state

TABLE 2.4. Initial Conditions for the Case 1 Steady-State Simulation
(saturation values from Montazer and Wilson 1984)

<u>Unit</u>	<u>Average Saturation</u>	<u>Initial ψ(-m)</u>
TCw	0.67 (0.23)	194
PTn	0.61 (0.15)	64
TSw1	0.65 (0.19)	232
TSw2-3	0.65 (0.19)	232
CHnv	0.90 (n/a) ^(a)	38

(a) No value given by Montazer and Wilson (1984).

pressure distribution from the center of the model domain in the Case 1 simulation was used also as the initial pressure distribution for the transient simulation.

2.4 BOUNDARY CONDITIONS

The surface boundary condition for the simulations was specified as a flux boundary, with fluxes representing recharge rates of 0 or 4.0 mm/yr. The 4.0-mm/yr recharge rate is comparable to the 4.5-mm/yr recharge estimate cited by Montazer and Wilson (1984). This estimate assumes that after evaporative losses, 3% of the average annual precipitation (≈ 150 mm/yr) at Yucca Mountain percolates back into the groundwater flow system. A surface boundary flux equivalent to 4.0 mm/yr was applied over a 4-month simulation period, and alternated with a zero-flux surface boundary condition for an 8-month simulation period for the transient simulation to approximate the seasonal distribution of precipitation. The lower boundary was specified as a fixed pressure (atmospheric) boundary, representing the water table.

The regional dip of the units in the vicinity of the ESF at Yucca Mountain is approximately 6 degrees to the east (Scott and Bonk 1984). Under certain conditions, this may create a driving force in the lateral (down-dip) direction, which is approximately 10% of gravity. The regional dip was not explicitly accounted for in the model simulations. However, the lateral boundaries of the model domain were specified such that a lateral flow component was created that approximated the effects of the regional dip.

The left, or west, boundary of the model domain was specified as a zero-flux or "no-flow" boundary so that water could not move "up dip" across the Ghost Dance fault. The north, south, and east boundaries of the model domain were specified as fixed-pressure boundaries, with pressures corresponding to the initial conditions described in the previous section. The east boundary was specified as a fixed-pressure rather than a zero-flux boundary to create a lateral flow component, approximating the effects of the regional dip of the stratigraphy. The combination of the specified boundary conditions creates a preferential recharge area corresponding to the locations of Coyote Wash and the Ghost Dance fault, which is consistent with our conceptual model. Future simulations will utilize a modified version of PORFLO-3, which incorporates a gravity tensor so that the effects of the lateral driving force created by tilted beds are directly accounted for.

3.0 COMPUTER CODE DESCRIPTION

The flow simulations were performed with the PORFLO-3 computer code (Runchal and Sagar 1989; Sagar and Runchal 1990). This code is designed to simulate fluid flow, heat transfer, and mass transport in variably saturated porous and fractured media. Up to three-dimensional simulations in either steady or transient mode can be performed. The steady-state solution can either be obtained directly by putting the time-dependent term to zero in the governing equation or by solving a transient problem until the solution becomes steady. The first option is very efficient and was used for the steady-state simulations reported here.

Fractures, faults, shafts, and drifts can be discretized as fully three-dimensional features or embedded as one- and two-dimensional features. The basic assumption for including one- and two-dimensional features in three-dimensional calculational domains is that the pressure values at grid nodes represent both the subdomain features within calculational cells (i.e., shafts or faults) and the calculational cells (i.e., adjoining rock). Thus there is no transfer of fluid between the cells and the subdomains within the cells, as transfer occurs only across cell boundaries. As a result, calculated pressure values are not as accurate close to the subdomain features as they would be if the features were discretized as fully three-dimensional features. Embedding one- and two-dimensional features within a three-dimensional domain is much more efficient, however, because it requires fewer nodes and, therefore, less computational time. Because of the large calculational domain used for the simulations reported here, the shafts, drifts, and Ghost Dance fault were included as one- and two-dimensional features rather than being discretized as full three-dimensional features.

The options available in the code for describing hydraulic properties of porous media are the Brooks and Corey (1966) or the van Genuchten (1978) water-retention models, with hydraulic conductivities determined by either the Mualem (1976) or the Burdine (1953) formulae. An additional option is to provide the water-retention and relative hydraulic conductivity data in tabular form. This last option is useful for specifying the characteristic curves of a fractured medium that is represented as an equivalent (continuum)

porous medium. If tabular values are input for the hydraulic properties, the code linearly interpolates between the values as needed while solving the unsaturated flow equation.

The PORFLO-3 code uses the pressure-based formulation of the flow equation that is discretized using an integrated finite-difference approach. Alternate methods of solution are provided to solve the set of algebraic equations. An iterative conjugate gradient solution method (Kincaid et al. 1982) is employed for the results reported here.

4.0 RESULTS AND DISCUSSION

The following results represent quasi-steady-state and transient simulations with upper-bound MPZ properties (see Table 2.3) at a recharge rate of 4.0 mm/yr. Other net infiltration estimates for Yucca Mountain range from 0.1 to 0.5 mm/yr (Peters et al. 1986). Therefore, the results of these simulations should be considered as conservative estimates of the effects of the exploratory shafts on the hydrology of the Yucca Mountain site.

4.1 STEADY-STATE SIMULATIONS

Direct steady-state solutions did not converge at a recharge flux of 4 mm/yr without modifying the hydrologic properties of unit TCw. The primary cause of the divergence is the abrupt change in composite hydraulic conductivity of unit TCw, as shown in Figure 2.4a. With high recharge fluxes, pressures develop that indicate the beginning of fracture flow (i.e., saturation becomes close to one). However, the recharge is not large enough to sustain this fracture flow. The result is that the solution alternates from matrix to fracture flow between iterations and will not converge. Scaling up the composite saturated hydraulic conductivity of unit TCw by a factor of 25 for the Case 1 simulation was sufficient for successful convergence of the direct steady-state solution.

By scaling up the saturated hydraulic conductivity of unit TCw for the Case 1 simulation, higher recharge fluxes could pass through unit TCw and into the underlying PTn unit without jumping from fracture to matrix flow between iterations. It is not clear if the solution obtained with this modification is realistic because fracture flow in unit TCw was effectively eliminated. However, the Case 1 simulation was only used to establish initial and boundary conditions consistent with the internal solution at a recharge rate of 4 mm/yr for the Case 2 simulation, so the absence of pulse infiltration resulting from fracture flow was considered to be relatively insignificant.

The saturated hydraulic conductivities measured on core samples of unit TCw range over four orders of magnitude (Peters et al. 1984). In addition to

this variability, the hydrologic properties of the fractures reported by Peters et al. (1986) are estimated rather than measured directly (Wang and Narasimhan 1985). Therefore, scaling up the composite hydraulic conductivities of unit TCw by a factor of 25 should still yield hydraulic conductivities within the range of uncertainty of the equivalent continuum approximations. Without this hydraulic conductivity modification, steady-state solutions could not be obtained using the direct solution method. An alternative would be to run a transient problem until steady state is reached. Numerical stability could then be achieved by reducing the size of the time steps. However, this alternative is much more expensive computationally and, therefore, was not used.

A saturation profile through the center of the model domain from the Case 1 simulation is shown in Figure 4.1a. The reference elevation for this and all subsequent figures is the ground surface, located at a depth of 0 m. The shafts, drifts, MPZs, and Ghost Dance fault were excluded from this simulation. If one could assume that the initial conditions specified for the Case 1 simulation represent a quasi-steady state for the system (in the absence of the ESF), and that the hydrologic properties are reasonable, then the higher saturation obtained in this solution suggest that the long-term infiltration rate at Yucca Mountain is considerably lower than the 4 mm/yr assumed here. The pressure distribution corresponding to the saturation profile of Figure 4.1a is shown in Figure 4.1b. This pressure distribution was used for the initial and fixed-pressure boundary conditions specified in the Case 2 simulation.

As with the Case 1 simulation, the direct steady-state solution for the Case 2 simulation did not converge at a recharge flux of 4.0 mm/yr without modifying the composite saturated hydraulic conductivity of unit TCw. Scaling up the composite saturated hydraulic conductivity of unit TCw by a factor of 15 was sufficient for successful convergence in the Case 2 simulation. A smaller hydraulic conductivity scaling factor could be used for the Case 2 simulation because the initial and boundary conditions for this simulation were more consistent with the internal solution than the uniform average saturations in each unit that were imposed as boundary conditions in the Case 1 simulation.

FIGURE 4.1. (a) Saturation Profile and (b) Pressure Distribution from the Center of the Model Domain for the Case 1 Simulation (initial conditions specified for Case 2 simulation)

A saturation profile through the center of the model domain for the Case 2 simulation is shown in Figure 4.2a. The shafts, drifts, MPZs, and Ghost Dance fault were included in the Case 2 simulation. Comparison of Figures 4.2a and 4.1a indicates slightly higher saturation in the welded units for the Case 2 simulation with very little change in the saturations of the nonwelded units relative to the Case 1 simulation. The differences in the saturation profiles shown in Figures 4.1a and 4.2a show the influence of the imposed boundary conditions on the internal solution.

The pressure distribution through the center of the model domain for the Case 2 simulation is shown in Figure 4.2b. This pressure distribution corresponds to the saturation profile depicted in Figure 4.2a.

FIGURE 4.2. (a) Saturation Profile and (b) Pressure Distribution from the Center of the Model Domain for the Case 2 Simulation

Also, this figure is provided for comparison with Figure 4.1b, which shows the pressure distribution from the Case 1 simulation at the same location.

Figure 4.2 indicates near unit-gradient conditions between the 100- and 350-m depths. If this was a strictly one-dimensional problem, with vertical downward flow, at steady state one would expect saturations to be nearly constant between the 100- and 350-m depths. Therefore, Figures 4.1 and 4.2 suggest that a steady-state, one-dimensional flow field has not been obtained. However, the solutions are consistent with the specified boundary conditions.

Saturation and pressure distributions through the line elements, representing ES-1 for the Case 2 simulation, are shown in Figures 4.3a and 4.3b, respectively. The slight pressure/saturation discontinuity at the interface

FIGURE 4.3. (a) Saturation Profile and (b) Pressure Distribution Through the Line Element Representing ES-1 for the Case 2 Simulation

between units TSw1 and TSw2-3 reflects slight differences in the properties of these units. The maximum saturations obtained from the Case 2 simulation for units TSw1 and TSw2-3 are 0.957 and 0.936, respectively. The hydraulic conductivity curves shown in Figures 2.7a and 2.7b indicate that water in the fractures is essentially immobile at saturations of less than about 0.984. Therefore, the results of this simulation suggest that fracture flow, as represented with this equivalent continuum approximation, will not occur in these welded tuff units.

In one-dimensional simulations of vertical flow through the unsaturated zone at Yucca Mountain using the TOSPAC code, Dudley et al. (1988) used a 2303-node model extending from the water table (0.0 m) to the surface of Yucca Mountain (530.4 m). Results of these one-dimensional steady-state simulations show the TSw unit to be saturated or near saturated, and thus

amenable to fracture flow at recharge rates greater than 1.0 mm/yr. This is contrary to the results of the three-dimensional PORFLO-3 simulations reported here. This difference is attributed to the nature of the problem and the boundary conditions specified for the three-dimensional simulations, which allow laterally flowing water to exit the model domain. Any lateral diversion of vertical fluxes above the potential repository horizon decreases the likelihood of that horizon reaching saturated or near-saturated conditions, unless the laterally diverted water encounters a preferential flow path such as an MPZ around a shaft or a fault zone.

A vertical cross section of Darcy velocity vectors through the plane that intersects ES-1 for the Case 2 simulation is shown in Figure 4.4. Slight perturbations in the flow field caused by ES-1 and the MPZ around it are evident at the interface between units TSw1 and TSw2-3 and just above the drifts connecting the shafts in the potential repository horizon at a depth of approximately 275 m. A potential for significant lateral flow above the interface between units PTn and TSw1 is indicated also in Figure 4.4. This

FIGURE 4.4. Vertical Cross Section of Darcy Velocity Vectors Through Plane Intersecting ES-1 for the Case 2 Simulation

lateral flow is consistent with the results of Rulon et al. (1986) and Wang and Narasimhan (1988), who also show a potential for significant lateral flow above the potential repository horizon using two-dimensional cross-sectional flow models.

A horizontal cross section of Darcy velocity vectors from the Case 1 simulation, through the lower part of unit TCw, just above the interface with unit PTn, is shown in Figure 4.5. A horizontal cross section of the same plane depicted in Figure 4.5 is shown in Figure 4.6 for the Case 2 simulation. The effects of the exploratory shafts are clearly evident from the perturbations in the flow field shown in Figure 4.6 relative to Figure 4.5.

The pressure distribution, corresponding to the horizontal flow field depicted in Figure 4.6 for the Case 2 simulation, is shown in Figure 4.7. These pressure contours also indicate slight perturbations in the flow field, resulting from the presence of the exploratory shafts. The saturations, corresponding to the pressure distribution shown in Figure 4.7, are shown in Figure 4.8.

A horizontal cross section of Darcy velocity vectors from the Case 1 simulation, through the upper part of unit TSw2-3, just below the interface with unit TSw1, is shown in Figure 4.9. A horizontal cross section of the same plane depicted in Figure 4.9 is shown in Figure 4.10 for the Case 2 simulation. Again, the effects of the exploratory shafts are clearly evident from the perturbations in the flow field shown in Figure 4.10 relative to Figure 4.9.

The pressure distribution corresponding to the horizontal flow field depicted in Figure 4.10 for the Case 2 simulation is shown in Figure 4.11. Again, as shown in Figure 4.7, these pressure contours also indicate slight perturbations in the flow field, resulting from the presence of the exploratory shafts. The saturations, corresponding to the pressure distribution shown in Figure 4.11, are shown in Figure 4.12. The boundary conditions, fault placement, and symmetry of this model create a preferential recharge area on the left (or west) side of the model domain, which corresponds to the area where Coyote Wash crosses the Ghost Dance fault.

FIGURE 4.5. Horizontal Cross Section of Darcy Velocity Vectors Through the Lower Part of Unit TCw for the Case 1 Simulation

FIGURE 4.6. Horizontal Cross Section of Darcy Velocity Vectors Through the Lower Part of Unit TCw for the Case 2 Simulation

FIGURE 4.7. Pressure Distribution in Horizontal Cross Section Through Lower Part of Unit TCw for the Case 2 Simulation

A horizontal cross section of Darcy velocity vectors through the potential repository horizon, at the 310-m depth in unit TSw2-3 for the Case 1 simulation, is shown in Figure 4.13. A horizontal cross section of the same plane depicted in Figure 4.13 is shown in Figure 4.14 for the Case 2 simulation. The effects of the exploratory shafts are not as evident at this depth as they are near the interface between units TSw1 and TSw2-3 and in unit TCw.

The pressure distribution, corresponding to the horizontal flow field depicted in Figure 4.14, is shown in Figure 4.15. The saturations, corresponding to the pressure distribution shown in Figure 4.15, are shown in Figure 4.16. As shown by the flow fields in the previous figures, this pressure distribution also indicates that the effects of the exploratory shafts are less significant at the depth of the potential repository than at shallower depths.

FIGURE 4.8. Saturations in Horizontal Cross Section Through Lower Part of Unit TCw for the Case 2 Simulation

Simulations by Wang and Narasimhan (1986), using different constant and pulse infiltration rates applied to fractures in unit TCw, indicate that most pulse effects are effectively damped out by units TCw and PTn before water infiltrates down into unit TSw1. Calculations by Travis et al. (1984) indicate that the penetration distance of pulses of water into fractures contained in densely welded tuffs similar to unit TCw is on the order of 10 m or less if the fracture apertures are 100 μm or less. Therefore, although water flow in fractures may be significant in unit TCw, these simulations suggest that episodic pulses of water from natural precipitation should not propagate via fractures into the underlying units due to capillary imbibition of water into the rock matrix.

FIGURE 4.9. Horizontal Cross Section of Darcy Velocity Vectors Through the Upper Part of Unit TSw2-3 for the Case 1 Simulation

FIGURE 4.10. Horizontal Cross Section of Darcy Velocity Vectors Through the Upper Part of Unit TSw2-3 for the Case 2 Simulation

FIGURE 4.11. Pressure Distribution in Horizontal Cross Section Through Upper Part of Unit TSw2-3 for the Case 2 Simulation

4.2 TRANSIENT SIMULATIONS

An objective of this study was to determine the potential effects of the ESF on the moisture distribution at Yucca Mountain, with emphasis on short-term characterization work. Therefore, a transient simulation also was performed, using a time-varying recharge rate. The surface boundary flux for this transient simulation was represented with a step function, so that a recharge rate equivalent to 4 mm/yr in 4 months (the rainy season) alternated with no recharge for 8 months. This seasonal recharge was maintained for a 20-year simulation period. This was considered to be an adequate time frame in which to conduct subsurface characterization work at Yucca Mountain. The pressure solution from the center of the model domain in the Case 1 simulation was used as the initial condition for the transient simulation.

FIGURE 4.12. Saturations in Horizontal Cross Section Through Upper Part of Unit TS_w2-3 for the Case 2 Simulation

No modifications to the saturated hydraulic conductivity of unit TC_w were necessary for the transient simulation because the size of the time steps was reduced to achieve numerical stability.

During this simulation period there were no appreciable changes in the saturations of any of the units other than unit TC_w. The saturation profile for unit TC_w from the center of the model domain for the transient simulation is shown in Figure 4.17. The saturation profile for unit TC_w, along the plane representing the Ghost Dance fault for the transient simulation, is shown in Figure 4.18. The saturation profile for unit TC_w, at the location of ES-1 for the transient simulation, is shown in Figure 4.19. The plot of time zero in Figures 4.17, 4.18, and 4.19 represents the initial steady-state solution condition from the center of the model domain in the Case 1 simulation.

FIGURE 4.13. Horizontal Cross Section of Darcy Velocity Vectors Through the Potential Repository Horizon in Unit TSw2-3 for the Case 1 Simulation

FIGURE 4.14. Horizontal Cross Section of Darcy Velocity Vectors Through the Potential Repository Horizon in Unit TSw2-3 for the Case 2 Simulation

FIGURE 4.15. Pressure Distribution in Horizontal Cross Section Through the Potential Repository Horizon in Unit TSW2-3 for the Case 2 Simulation

Comparisons of Figures 4.17, 4.18, and 4.19 indicate that, with the material properties used for these simulations, the MPZs around the exploratory shafts create a preferential flow path for water percolating down from the surface. The Ghost Dance fault also acts as a preferential flow path, but its effects are not as significant with the particular properties chosen to represent it relative to the MPZs and exploratory shafts. At the saturations shown in these figures, fracture flow, as represented with an equivalent continuum approximation, does occur in unit TCw.

The transient simulations presented in this report suggest that there will be no appreciable change in the moisture content distribution below unit TCw within 20 years after the construction of the ESF. These simulations, however, did not account for possible changes in moisture content that result from additions of drilling fluid into the system during the excavation

FIGURE 4.16. Saturation in Horizontal Cross Section Through the Potential Repository Horizon in Unit TSw2-3 for the Case 2 Simulation

FIGURE 4.17. Saturation Profiles for Unit TCw from the Center of the Model Domain for the Transient Simulations

FIGURE 4.18. Saturation Profiles for Unit TCw Along the Plane Representing the Ghost Dance Fault for the Transient Simulations

FIGURE 4.19. Saturation Profiles Through the Line Element Representing ES-1 in Unit TCw for the Transient Simulations

process. Work by Buscheck and Nitao (1987), however, suggests that imbibition of the drilling fluid used during the drill-muck-mining excavation process will be minimal. Therefore, even though shaft construction will alter the fracture densities and permeabilities of the tuff units, these simulations suggest that the moisture contents and distributions in the vicinity of the exploratory shafts below TCw will not change significantly within 20 years, which is a reasonable time frame for subsurface characterization work.

The MPZs around the exploratory shafts in unit TCw appear to create a preferential flow path for water when fracture flow occurs in this unit. This fracture flow appears to be damped with depth, however, so that no fracture flow occurs in the underlying units. However, it must be emphasized that these conclusions are specific to the initial and boundary conditions, discretization, and material properties used for these simulations, and do not preclude the possibility of lateral flow intersecting preferential flow paths that result in locally saturated conditions and fracture flow in the lower units.

5.0 CONCLUSIONS AND RECOMMENDATIONS

In this model, the exploratory shafts, drifts, and Ghost Dance fault are embedded as one- and two-dimensional features within three-dimensional calculational elements. These features are assumed to have their own distinct properties, but the results obtained from this model are not as accurate in close proximity to these features as they would be if the features were discretized as three-dimensional elements. Considering the lack of data regarding properties of the Ghost Dance fault and MPZs and the comparatively large calculational domain of the model, the results presented here are reasonable as best estimates of worst-case conditions that might exist. The size of the calculational domain used in this analysis is considered necessary to include the Ghost Dance fault and the exploratory shafts, while attempting to minimize boundary effects. If a more accurate representation of specific small-scale features is desired, the model domain should be reduced to a smaller scale and computational cell sizes reduced accordingly. Larger scale approximate solutions, such as those presented here, can readily be used as input to more finely discretized smaller scale models within the domain of the larger model. On a sufficiently smaller scale, the shafts may be included as three-dimensional features.

Several important conclusions may be drawn from these simulation results. The simulations suggest that fracture flow, as approximated by the equivalent continuum model (i.e., when hydrologic properties are represented as shown in Figures 2.5 to 2.7), does not occur at the level of the potential repository at recharge rates up to 4 mm/yr. Discrete fractures or faults were not simulated, however. Therefore, these results do not preclude the possibility of preferential flow reaching the potential repository horizon through regions of major structural features. The Ghost Dance fault is included in this model, but the hydraulic properties used to describe the fault zone were estimated because of a lack of data. These simulations also suggest that there will be no appreciable change in the moisture-content distribution below the TCw unit within 20 years after the construction of the ESF. This 20-year time frame was considered to be adequate for subsurface characterization work.

Previous one-dimensional simulations have indicated that the potential repository horizon will be saturated or nearly saturated and thus amenable to fracture flow at recharge rates of 1.0 mm/yr (Dudley et al. 1988). This is contrary to the results of the three-dimensional simulations reported here. This difference can be attributed primarily to the dimensionality of the problem and the nature of the three-dimensional flow field used in this study, such that water can exit from the model domain through lateral boundaries. The results of these three-dimensional simulations support previous two-dimensional modeling studies that show a potential for significant lateral flow above the potential repository horizon. Lateral diversion of vertical fluxes above the potential repository horizon decreases the likelihood of that horizon reaching saturated or near-saturated conditions unless the laterally diverted water encounters a preferential flow path or structural feature, such as a fault zone.

Postclosure thermal effects and vapor-phase transport of moisture caused by heat generated from the potential repository were not considered in this study. However, these factors may have a significant effect on repository performance. Therefore, postclosure modeling studies should consider nonisothermal flow and vapor-phase transport of moisture. The MPZs and shaft backfill material may become more important for future smaller scale model simulations when coupled fluid flow, heat transfer, and mass transport are considered.

It will be impossible to characterize all of the heterogeneities in the properties of the tuff units at Yucca Mountain in sufficient detail to predict all possible outcomes associated with a particular characterization activity or repository performance after waste emplacement. However, at a minimum, future simulations with intermediate- and large-scale multidimensional models of the potential repository at Yucca Mountain should include the topography of the site and surface expressions of major fractures and faults to determine areas for preferential local recharge. Then, spatially nonuniform, time-varying recharge fluxes can be applied as surface boundary conditions to determine the importance of time and spatial variation of surface recharge to the flow fields in the natural system at depth. In addition, it may be possible to use multidimensional stochastic modeling

approaches to evaluate the effects of the variability and uncertainty of the hydrologic properties of the tuff units on calculations of repository performance objective criteria, such as groundwater travel time.

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