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Specification of a Test Problem for HYDROCOIN Level 3 Case 2: Sensitivity Analysis for Deep Disposal in Partially Saturated, Fractured Tuff

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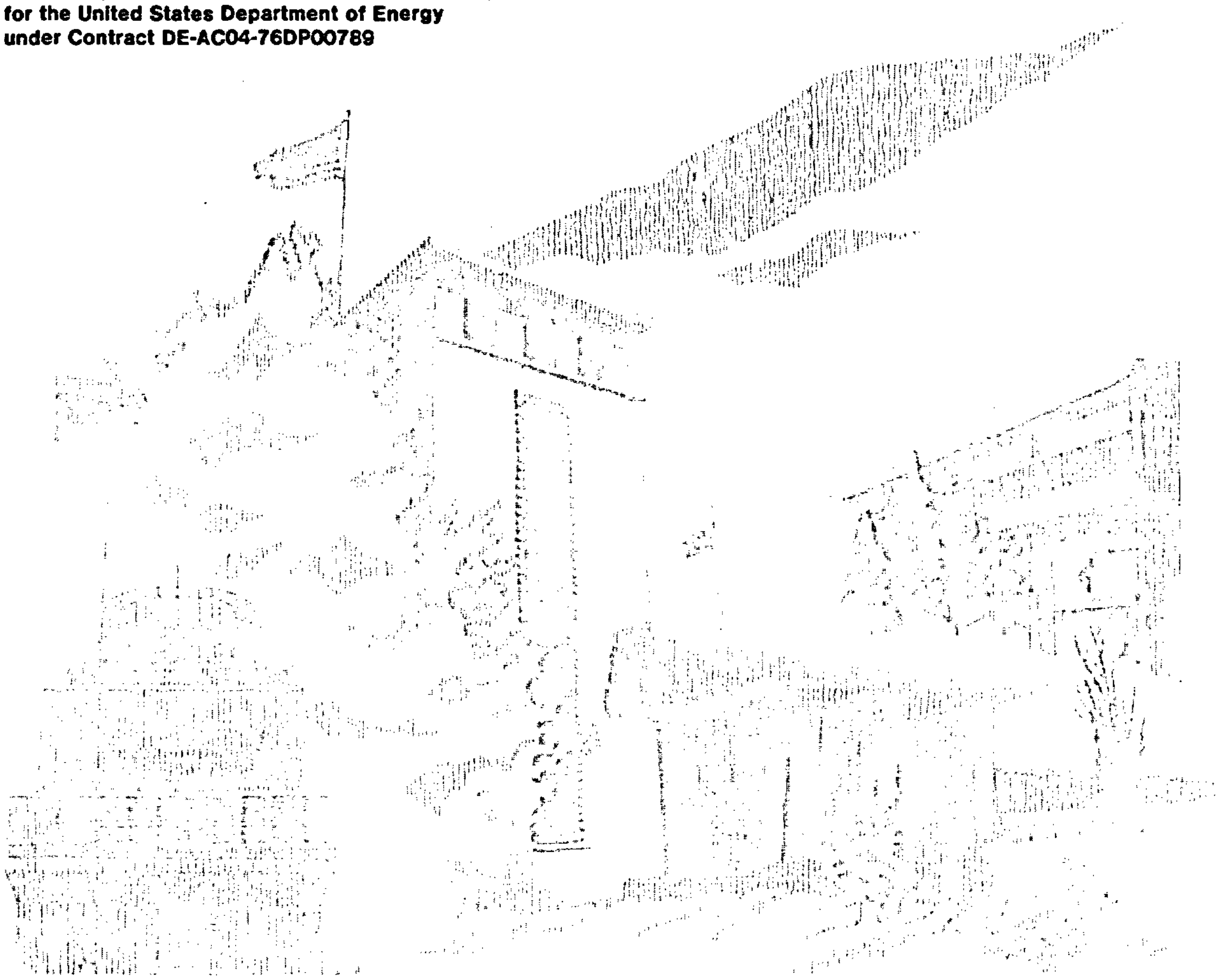

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Abstract

The international Hydrologic Code Intercomparison Project (HYDROCOIN) was formed to evaluate hydrogeologic models and computer codes and their use in performance assessment for high-level radioactive waste repositories. There are three principal activities in the HYDROCOIN Project: Level 1, verification and benchmarking of hydrologic codes; Level 2, validation of hydrologic models; and Level 3, sensitivity and uncertainty analyses of the models and codes. This report presents a test case defined for the HYDROCOIN Level 3 activity. The purposes of this test case are to explore the feasibility of applying various sensitivity-analysis methodologies to a highly nonlinear model of isothermal, partially saturated flow through fractured tuff, and to develop modeling approaches to implement the methodologies for sensitivity analysis. These analyses involve an idealized representation of a repository sited above the water table in a layered sequence of welded and nonwelded, fractured, volcanic tuffs. The analyses suggested here are divided into three groups with varying levels of complexity and computational difficulty: (1) one-dimensional, steady flow; (2) one-dimensional, nonsteady flow; and (3) two-dimensional, steady flow. Performance measures to be used to evaluate model sensitivities are also defined; the measures are related to regulatory criteria for containment of high-level radioactive waste.

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List of Symbols

K	hydraulic conductivity
$\overline{K}$	hydraulic conductivity tensor
n	porosity
$\overline{q}$	specific discharge
S	saturation
t	time
$\overline{v}$	velocity of water
z	elevation

Greek Symbols

α	curve-fitting parameter (primarily describes the pressure head at which desaturation begins)
α'_{bulk}	coefficient of consolidation
β	curve-fitting parameter (primarily describes the slope of the desaturation portion of the saturation curve)
β'_w	compressibility of water
∇	differential operator
λ	curve-fitting parameter $= \left(1 - \frac{1}{\beta}\right)$
σ'	stress in the rock mass
ρ	density of water
ψ	pressure head

Subscripts

f	fracture
m	matrix
f,b	bulk fracture values for a unit volume of fractured, porous media
r	residual
s	saturated

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Specification of a Test Problem for HYDROCOIN Level 3 Case 2: Sensitivity Analysis for Deep Disposal in Partially Saturated, Fractured Tuff

Introduction

Mathematical models have been developed to describe the processes that are expected to occur in geologic repositories for high-level radioactive waste. These models are generally embodied in complex computer codes that will be used to assess the long-term safety of the proposed repositories. We need to demonstrate that the models are appropriate and adequate and that the codes that embody them are numerically correct. We also need to understand the limits of applicability and the sensitivities and uncertainties of the models and codes for the ranges of hydrologic and radionuclide-transport parameters that are expected to be encountered at the proposed repository sites.

Of the models that are used to assess the performance of a total repository system, those that describe the movement of groundwater at a potential repository site are especially important. The international Hydrologic Code Intercomparison Project (HYDROCOIN) was formed to evaluate hydrogeologic models and codes and their use in performance assessment for high-level-radioactive-waste repositories.

Hodgkinson et al., 1985, described the purposes of the HYDROCOIN project:

> The primary aim of *Level 1* of HYDROCOIN is the *verification* of the numerical accuracy of groundwater flow codes by intercomparing their solutions to certain well-defined test problems and by comparison with analytical solutions.
>
> *Level 2* of HYDROCOIN is concerned with the *validation* of computer models in order to test their ability to describe the results of laboratory and field experiments.
>
> HYDROCOIN *Level 3* is concerned with the *application* of hydrogeological models in performance assessments, taking into account uncertainties in the models and data. In particular, Level 3 is concerned with the sensitivity of results to characteristics of the site which are poorly known or which could change with time, and the associated uncertainties in the model predictions. Its aims are to explore alternative methodologies and calculational techniques for carrying out sensitivity and uncertainty analyses, to derive some general results which apply to each of a number of different geological settings, and to act as a forum for exchanges of ideas and information.

This paper presents a problem specification for a HYDROCOIN Level 3 sensitivity analysis of models that could be used to describe partially saturated flow through fractured tuff. The proposed analyses involve a nonlinear mathematical model and materials with highly nonlinear hydrologic properties. These analyses may be of interest to groups whose performance-assessment analyses involve any of the following: nonlinear analyses, partially saturated flow, combined matrix and fracture flow, volcanic tuffs, or layered materials with sharp layer boundaries and large contrasts in material properties.

The problem defined in this paper is entirely conceptual in character and is put forth strictly for the purposes of the HYDROCOIN Project. It is specifically not intended that the problem, as defined, be taken as representative of the potential tuff repository site being evaluated by the U.S. Department of Energy. The physical constants, analytical methods, and numerical results are therefore not to be construed as U.S. Department of Energy perceptions of the proposed tuff site.

Purpose

The purposes of the analyses outlined in this report are

- To explore the feasibility of applying various sensitivity-analysis methods to a highly nonlinear model of isothermal, partially saturated flow through layered, fractured tuff
- To develop approaches for site modeling that will help when implementing the methods for sensitivity analysis
- To investigate, for a particular mathematical model of partially saturated flow at an idealized site, the sensitivity of the output of the model to variations in its input

Sensitivity will be evaluated by observing the changes in performance measures that are based on model output. Because this mathematical model is intended for use in performance-assessment analyses, the performance measures chosen for these sensitivity analyses are directly related to the long-term performance of the site as a potential repository for high-level radioactive waste. Knowledge of the sensitivities of the performance measures to various inputs can then be used to decide where the greatest effort should be spent to refine conceptual models, to quantify parameters in the mathematical model, and to decide which parameters may be safely deleted when developing simplified models. Inputs that will be varied include both the values assigned to the parameters in the mathematical model and the conceptual models that describe the hydrogeology and geologic structure of the idealized site.

Overview of Proposed Analyses

Six sets of analyses are described in this report to provide a range of physical and analytical complexity that will allow interested HYDROCOIN Project teams to take on as much or as little work as desired. The sensitivity analyses proposed here are unquestionably difficult, and, depending on which cases are undertaken, personnel and computing costs could be high. Because of the level of technical difficulty and the potentially high costs, it may not be possible to complete all of these analyses within the framework of the HYDROCOIN project.

The six analysis sets are described in terms of base cases that include one-dimensional (1-D) and two-dimensional (2-D) conceptual flow models, steady and nonsteady flow conditions, and both low and high initial fluxes to compare sensitivities during matrix-dominated and fracture-dominated flow. The base cases are

Case 1: 1-D, low flux, steady, matrix-dominated flow

Case 2: 1-D, high flux, steady, fracture-dominated flow

Case 3: 1-D, low flux, nonsteady, matrix-dominated flow

Case 4: 1-D, high flux, nonsteady, fracture-dominated flow

Case 5: 2-D, low flux, steady, matrix-dominated flow

Case 6: 2-D, high flux, steady, fracture-dominated flow

Cases 1 and 2 are the simplest but are sufficient to provide useful insights into the behavior of this unsaturated-flow system and into the process of modeling it. Because these cases involve 1-D, isothermal, steady-state flow, they can be analyzed using standard numerical solvers for ordinary differential equations. Such solvers are fast and efficient so a wide variety of methods for sensitivity analysis can readily be applied and compared. It should be noted that, in the analyses of 1-D, steady-state flow, the materials between the ground surface and the repository have no effect on flow conditions between the repository and the water table and can therefore be ignored.

Cases 3 through 6 are significantly more difficult than Cases 1 and 2, and they will require codes that use finite-element or finite-difference methods or some other technique such as dynamics of contours. These analyses can be expected to consume a large amount of computer time. Selected local sensitivity analyses should be within the reach of project teams using appropriate analytical tools. Global sensitivity analyses on Cases 3 through 6 are probably beyond the resources available within the HYDROCOIN Project.

We need to remember that the ultimate goal of this particular Level 3 exercise is to develop modeling approaches and sensitivity-analysis methods that will yield useful insights into the behavior of this complex hydrologic system. Even a simple comparison of changes in performance among the six base cases would be a valuable contribution. While it may not be possible to complete all of the suggested analyses during the HYDROCOIN Project, we still should be able to make significant progress toward this goal.

Site Description

The hydrogeologic system described here is shown schematically in Figure 1. The idealized site is made up of a sequence of ash-fall and ash-flow tuffs. The amount of welding, fracturing, and chemical alteration varies greatly from one layer to the next. Fracturing in all units is dominated by two sets of nearly vertical fractures and one set of horizontal fractures. Major fault zones cut through the entire vertical section.

The water table is relatively flat beneath most of the site. The repository horizon lies entirely within the partially saturated zone in Unit D. The principal hydrogeologic units that make up the unsaturated zone and will be considered in these analyses are briefly described in Table 1. Hydrologic characteristics vary greatly from one layer to another because of the differences in the degree of welding, fracturing, and chemical alteration.

Klavetter and Peters, 1986, have described three broad categories of hydrogeologic units in these tuffs:

1. Densely welded tuffs that are highly fractured. These units have low saturated matrix conductivities (10^{-11} m/s or less) and high saturated fracture conductivities. For a unit volume of rock, the total saturated conductivity of the fracture system is probably several orders of magnitude higher than the total saturated conductivity of the matrix. This group includes Units A, C, and D.
2. Nonwelded, vitric tuffs that have few fractures. These units have high saturated matrix conductivities (in the range of 10^{-6} to 10^{-8} m/s) and relatively low saturated fracture conductivities. This group includes Units B and Ev.
3. Nonwelded, zeolitized tuffs that have few fractures. These units have low saturated matrix conductivities (10^{-11} m/s or less) and low saturated fracture conductivities. The unit above the water table in this group is Unit Ez.

The contacts between these units generally tend to be sharp; thus, there can be extreme contrasts in hydraulic conductivities occurring over very short distances.

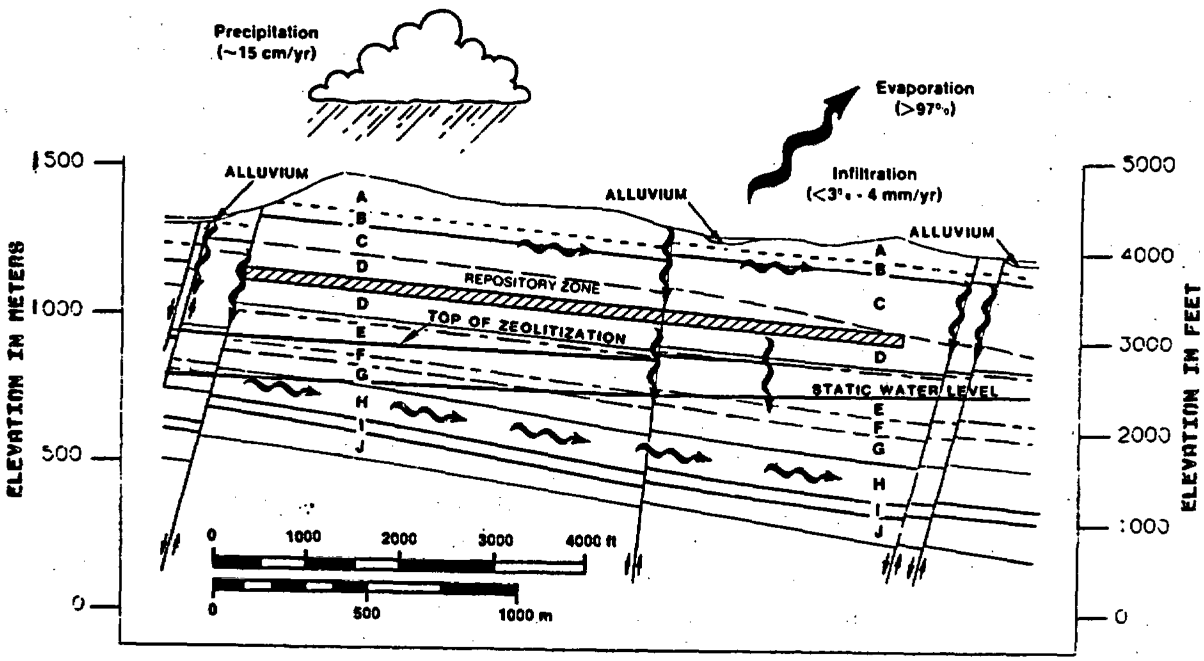

Figure 1. Generalized Hydrogeologic System

Table 1. Hydrogeologic Units in the Unsaturated Zone (after Ortiz et al., 1985)

Unit Name	Description
Unit A, welded	Moderately to densely welded, devitrified ash-flow tuff
Unit B, nonwelded	Partially welded to nowelded vitric tuffs
Unit C, welded, lithophysae-rich	Moderately to densely welded, devitrified ash-flow tuffs that locally contain more than approximately 10% by volume lithophysal cavities
Unit D, welded, lithophysae-poor	Moderately to densely welded, devitrified ash-flow tuffs that locally contain less than approximately 10% by volume lithophysal cavities
Unit E, nonwelded	Nonwelded ash-flows, bedded and reworked tuffs; includes both the vitric (Ev) and zeolitic (Ez) sections

Conceptual Models

Two conceptual models of flow that have been postulated for semi-arid and wetter climatic conditions have been characterized as:

1. One-dimensional, vertical, downward flow
2. Multidimensional flow, in particular with flow diverted laterally at layer contacts and from within the nonwelded units into the major structural features of the site

Both conceptual models appear reasonable, although for different ranges of flux as described below.

Under semi-arid climatic conditions, with estimates of average flux through the mountain on the order of 0.1 mm/yr or less, the flow of liquid water would be dominated by flow through the rock matrix and it may be possible to represent it as 1-D, vertical, downward flow. If the flow were in fact 1-D, then performance assessment analyses could be greatly simplified. In this conceptual model, as long as conditions are isothermal, all of the water that percolates past the zone where evapotranspiration occurs ultimately passes through the repository horizon and flows down to the water table.

The existence of sharp permeability contrasts and fault zones may cause flow to be diverted down-dip either below or above the repository horizon toward or into the fault zones. This may be especially true at higher fluxes (approximately 1.0 mm/yr or greater) where flow in fractures might be expected to predominate over flow through the rock matrix. Water diverted below the repository from the bulk rock into the fault zones would have passed through the repository and would be carrying leached radionuclides. This diverted water might reach the water table relatively quickly and have a detrimental effect on repository performance. If water is diverted above the repository horizon, the amount of water available to contact waste packages and leach radionuclides could be significantly less than the average recharge rates might indicate. Such a diversion of water could greatly benefit the performance of the waste packages. Also, a repository could be designed so that water diverted into the faults above the repository would never come into contact with any waste packages.

To do performance assessment analyses efficiently, it is necessary to distinguish the conditions that would or would not give rise to lateral diversion of flow. Then analysis methods that are appropriate for the chosen conceptual model may be applied.

Six base cases are defined below: four for the 1-D flow model and two for the 2-D flow model. Analyses of both steady and nonsteady flow are suggested for the 1-D cases. With currently available analytical techniques, it is expected to be very costly to perform analyses of nonsteady flow that start from a well-characterized steady-flow state, so only steady-flow analyses are suggested at this time for the 2-D cases.

Mathematical Model for Partially Saturated Flow in a Compressible, Fractured Tuff

The model for partially saturated flow in a compressible medium that is suggested for these analyses has been described in detail by Klavetter and Peters, 1986. This highly nonlinear model uses a composite continuum approach to describe the effective hydrologic properties of the fractured rock mass. The model is cast with pressure head, ψ, as the primary variable. Klavetter and Peters, 1986, list the following important assumptions used in the derivation of the flow equations presented here:

1. The continuity equation for the matrix grain mass

2. The three-dimensional bulk-rock-consolidation equation with only vertical displacement (Reeves and Duguid, 1975)
3. The assumption that a unit change in the quantity "total saturation times pressure head" at a point causes a unit change in the local stress field (McTigue, Wilson, and Nunziato, 1984)
4. Darcy's equation for flow
5. Identical pressure head in the fractures and the matrix in the direction perpendicular to flow
6. Total head defined as the sum of pressure head and the elevation above some reference surface

The equations and definitions of variables are given below. The same mathematical model is applicable to the conceptual models for both 1-D and 2-D flow. The derivation of this mathematical model is tailored specifically for the problem of partially saturated flow in layered, fractured tuffs. The complete derivation with discussion of the assumptions can be found in Klavetter and Peters, 1986.

Saturation

Saturation, S, is a nonlinear function of the pressure head, ψ. The functional form of the relationship suggested for these analyses is that developed by van Genuchten, 1978.

$$S = (S_s - S_r)\left\{\frac{1}{1+|\alpha\psi|^{\beta}}\right\}^{\lambda} + S_r \qquad \psi \le 0 \qquad (1)$$

$$S = S_s \simeq 1.0 \qquad \psi \ge 0$$

where $\lambda = 1 - 1/\beta$. In the equations that follow, the matrix saturation, S_m, and fracture saturation, S_f, are calculated using Equation 1.

Hydraulic Conductivity

Van Genuchten's relationship for saturation can be used with the method developed by Mualem, 1976, to develop an analytical expression for hydraulic conductivity, K, as a function of pressure head, ψ. This yields the following equation:

$$K(\psi) = K_s[1+|\alpha\psi|^{\beta}]^{-\frac{\lambda}{2}}\left\{1-\left[\frac{|\alpha\psi|^{\beta}}{1+|\alpha\psi|^{\beta}}\right]^{\lambda}\right\}^2 \qquad \psi \le 0 \qquad (2)$$

$$K(\psi) = K_s \qquad \psi \le 0$$

where $\lambda = 1 - 1/\beta$. In the equations that follow, the hydraulic conductivity tensors $\overline{K}_{m,b}$ and $\overline{K}_{f,b}$ (bulk conductivities for the matrix and fractures respectively) are calculated using Equation 2. When calculating bulk conductivities, K_s in Equation 2 assumes the value of the bulk saturated conductivity given later in Table 3.

Nonsteady-Flow Equation

The following nonlinear equation can be used to describe water flow under nonsteady conditions:

$$\begin{aligned}\rho\frac{\partial\psi}{\partial t}\Bigg\{ & n_m\frac{\partial S_m}{\partial\psi} + n_f\frac{\partial S_f}{\partial\psi} + \beta'_w(S_m n_m + S_f n_f) \\ & + \alpha'_{bulk}\left[\frac{S_m n_m + S_f n_f}{n_m + n_f}\right][S_m - n_f(S_m - S_f)] \\ & - \frac{\partial n_f}{\partial\sigma'}\left[\frac{S_m n_m + S_f n_f}{n_m + n_f}\right](S_m - S_f)\Bigg\} \\ & = \nabla \cdot \{\rho(\overline{K}_{m,b} + \overline{K}_{f,b}) \cdot \nabla(\psi + z)\} \end{aligned} \qquad (3)$$

This mathematical model for nonsteady, partially saturated flow includes the effects of the compressibilities of water and of the bulk rock mass. Including these effects makes the equation both more correct physically and, for some of the hydrogeologic units, more stable numerically. In this formulation of the mathematical model, compressibility effects are included as capacitance coefficients. Klavetter and Peters, 1986, defined five components in the capacitance term. These components are given in Equations 4 through 8. The five capacitance coefficients have been evaluated using base-case parameters and are shown graphically in Appendix A (Figures A1 through A6) for each of the hydrogeologic units.

$$\text{Matrix Sat.: } n_m\frac{\partial S_m}{\partial\psi} \qquad (4)$$

$$\text{Fracture Sat.: } n_f\frac{\partial S_f}{\partial\psi} \qquad (5)$$

$$\text{Water Comp.: } \beta'_w(S_m n_m + S_f n_f) \qquad (6)$$

Bulk Rock Comp.:

$$\alpha'_{bulk}\left[\frac{S_m n_m + S_f n_f}{n_m + n_f}\right][S_m - n_f(S_m - S_f)] \simeq \alpha'_{bulk}S_m^2 \qquad (7)$$

Fracture Comp.:

$$\frac{\partial n_f}{\partial\sigma'}\left\{\frac{S_m n_m + S_f n_f}{n_m + n_f}\right\}(S_m - S_f) \simeq \frac{\partial n_f}{\partial\sigma'}S_m(S_m - S_f) \qquad (8)$$

The capacitance coefficients shown above were derived from fundamental relationships among porosity, n, saturation, S, water density, ρ, pressure head, ψ, and effective stress, σ'. The effects of compressibility of water and the bulk rock mass could also be incorporated into the model by explicitly retaining the fundamental relationships among pressure head, effective stress, porosity, and saturation rather than by using the derived capacitance coefficients.

Steady-Flow Equation

The steady-state version of the flow equation is also taken from Klavetter and Peters, 1986:

$$-(\overline{K}_{m,b}+\overline{K}_{f,b}) \cdot \nabla(\psi+z) = \overline{q}_m + \overline{q}_f = \overline{q}_{total} \quad (9)$$

Flow Velocity of Water

The following formulation can be used to calculate the average linear flow velocities of water in the matrix, $\overline{v}_m$, and fractures, $\overline{v}_f$. The average water velocity is the Darcy flux, $\overline{q}$, divided by the area through which the water moves. It is assumed that the water present at residual saturation does not contribute to the effective flow area. This formulation is taken from Peters, Gauthier, and Dudley, 1986.

$$\begin{aligned}\overline{v}_m &= \frac{\overline{q}_m}{n_m(S_m-S_{m,r})} \\ &= -\overline{K}_{m,b} \cdot \nabla(\psi+z)\left\{\frac{1}{n_m(S_m-S_{m,r})}\right\} \quad (10)\end{aligned}$$

$$\begin{aligned}\overline{v}_f &= \frac{\overline{q}_f}{n_f(S_f-S_{f,r})} \\ &= -\overline{K}_{f,b} \cdot \nabla(\psi+z)\left\{\frac{1}{n_f(S_f-S_{f,r})}\right\} \quad (11)\end{aligned}$$

Numerical-Convergence Criteria

The combined nonlinearities of the mathematical model and of the hydrologic properties for unsaturated tuff make it difficult to achieve numerical results that are stable and accurate. In calculations similar to these (Bixler and Eaton, 1986, and Peters, Gauthier, and Dudley, 1986), it has been observed that predicted pressures are relatively insensitive measures of calculational error. Velocities, on the other hand, are relatively good measures of error for these analyses because they are very sensitive to small perturbations in the pressure field. This mathematical model is cast so that pressure head, ψ, is the primary variable. A very strict convergence criterion must be applied to ψ to ensure reasonable accuracy in calculated velocities, $\overline{v}$, and fluxes, $\overline{q}$ (see Bixler and Eaton, 1986, for an example).

Sensitivity Analyses for 1-D Flow

Description

In the conceptual model for 1-D flow, it is assumed that all moisture that infiltrates past the zone of evapotranspiration flows vertically downward to the water table. In this model, it is assumed that, at all fluxes being considered, the existence of the following conditions are not sufficient to cause water to be diverted laterally:

1. Anisotropic hydraulic conductivities
2. Conductivity contrasts at contacts between hydrogeologic units
3. Structural tilting of the hydrogeologic units
4. Distortions of the flow field caused by the presence of major structural features having hydraulic properties that are different from those of the surrounding rock mass

The vertical column for the 1-D base cases is shown in Figure 2. It is made up of five distinct, effectively horizontal, hydrogeologic units. The lowermost unit may be made up of either vitric or zeolitc materials (Ev or Ez). Assume that the repository is located in the welded tuffs of Unit D. Coordinates for the locations numbered in Figure 2 are listed in Table 2.

The overall height of the modeled column is 530.4 m. In the column being modeled, the water table, defined as the point at which ψ = 0.0 m, is located in Unit E. Since the purpose of these analyses is to test the sensitivity of model outputs (i.e., the performance measures) to variations in the parameters for the zone of partially saturated flow, the water table is taken as the lower boundary of the modeled region. The water table is also taken as the reference datum, z = 0.0 m. A known flux, $\overline{q}$, is applied at the upper boundary, z = 530.4 m. Temperature conditions are isothermal. It is assumed that the presence of the repository does not affect the hydrologic properties of Unit D, so the properties of Unit D are taken to be uniform from elevation z = 130.3 m to z = 335.4 m. In the base case, Unit E consists of all zeolitized material (Ez). Each unit is initially assumed to be homogeneous and isotropic.

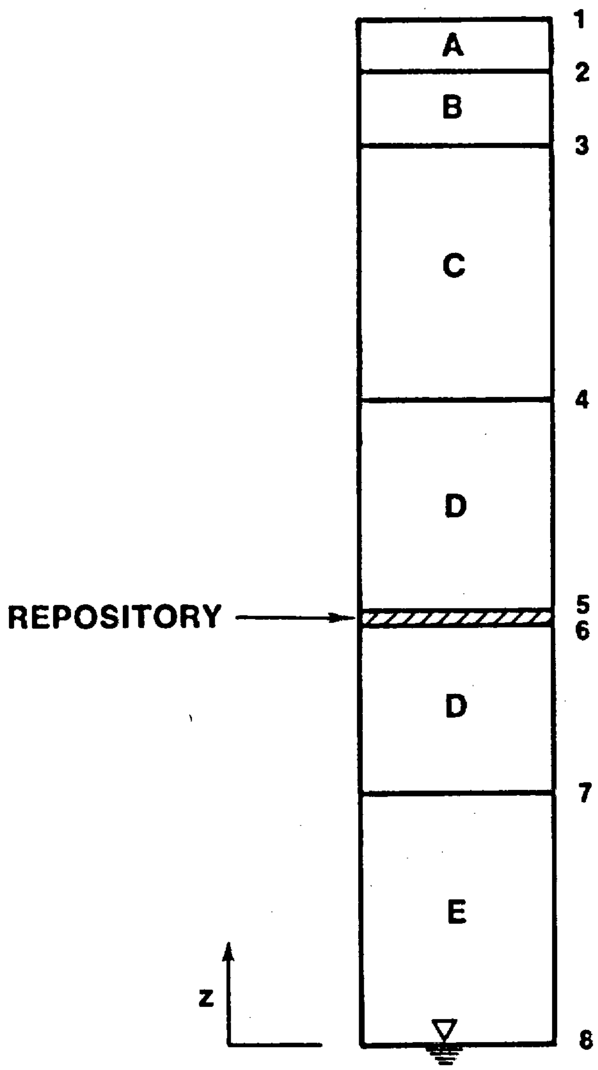

Figure 2. Stratigraphy for 1-D Base Cases (Cases 1 through 4)

Table 2. Coordinates of the Numbered Points for the 1-D Flow Analyses (see Figure 2)

Point	Elevation, z (m)
1	530.4
2	503.6
3	465.5
4	335.4
5	224.0
6	219.5
7	130.3
8	0.0

Performance Measures

Performance measures are defined for both the steady- and nonsteady-flow cases.

Steady Flow

The performance measure for the 1-D steady-flow calculations is the shortest water travel time between the base of the repository and the water table. We note that for most HYDROCOIN participants, the flux of water is of more importance to performance assessments than the water travel time. However, since the flow is 1-D, isothermal, and steady-state, the flux throughout the entire column is prescribed by the flux applied at the upper boundary. The volumetric rate of flow through the repository horizon is thus determined by the problem specification. Therefore, volumetric rate of water flow through the repository, though it is a good indicator of calculational stability and accuracy, is not a meaningful measure of sensitivity for the 1-D, steady-flow cases.

In steady-state analyses, water travel time is a function of the flux and of the effective volume of water along the flow path. The effective water volume is in turn a nonlinear function of pressure head, ψ. Thus, the travel time is a nonlinear function of all of the parameters that affect the distribution of moisture and pressure head in the column, Equations 1, 2, and 9, and can be used as a performance measure to test the sensitivity of the mathematical model to these parameters.

Nonsteady Flow

The first performance measure for the 1-D, nonsteady-flow cases is again taken to be the shortest water travel time between the base of the repository and the water table. In these analyses, it is assumed that the change in infiltration rate at the upper boundary occurs when radionuclides are first released from the repository. The flux pulse will then overrun water that has already passed through the repository under the influence of the initial steady-state flux conditions. Therefore, travel time from the repository should be calculated starting at the time the upper boundary condition is changed to the new infiltration rate.

The second and third performance measures are, respectively, the time-dependent normalized volume of flow passing the base of the repository, z = 219.5 m, and the normalized volume of flow passing the water table, z = 0.0 m. The flow volume at any time, t, is to be calculated for a 1.0-m^2 flow area and is to be normalized by the initial flow volume, $\bar{q}(t)/\bar{q}(t_o)$.

Criterion for Nonnegligible Flow Volume

The calculation of the minimum water travel time from the repository to the water table will be based on the greater of the velocity of flow in the fractures, $\bar{v}_f$, or in the rock matrix $\bar{v}_m$. The volume of water flowing at the higher velocity must be a significant portion of the total volume of flow; otherwise the travel time would not be a meaningful performance measure. It is expected that, under some conditions, the calculated velocity of water flowing in the fractures will be much higher than the velocity in the rock matrix, while the volume of water flowing through the fractures will be negligible by comparison with the volume flowing through the matrix. To ensure that small volumes of water flowing at relatively high velocity in the fractures do not inappropriately dominate the calculation of minimum travel times, the following cut-off criterion should be applied: if $\bar{v}_f$ is greater than $\bar{v}_m$, use $\bar{v}_f$ to calculate the minimum travel time only if $\bar{q}_f/\bar{q}_{total} \geq 10^{-3}$.

Base-Case Parameters

For local sensitivity analyses, a base-case analysis determines the point in parameter space at which model sensitivities are tested. Because of the extremely nonlinear nature of this problem, sensitivities are expected to be dependent on the flux chosen for the base cases. For this reason, two base cases each are proposed for steady and nonsteady analyses. For steady-flow conditions, the base-case fluxes are

Case 1: $\bar{q}$ = 0.1 mm/yr for matrix-dominated flow

Case 2: $\bar{q}$ = 1.0 mm/yr for conditions near the transition from matrix-dominated to fracture-dominated flow

For the nonsteady-flow cases, it is assumed that steady-flow conditions prevail under the initial flux and then a step change in flux is applied. Nonsteady flow is then observed until a new steady-flow condition is reached. For nonsteady-flow conditions, the base-case fluxes are

Case 3: $\bar{q}$ changes from 0.1 mm/yr to 0.2 mm/yr for nonsteady, matrix-dominated flow

Case 4: $\bar{q}$ changes from 0.5 mm/yr for nonsteady flow in the transition from matrix-dominated to combined matrix and fracture flow

Base-case values for the hydrologic properties are given in Table 3 for each of the hydrogeologic units. The base-case value for each parameter is given first and then, for those parameters to be varied, a suggested range of values to use for sensitivity analyses is given below it in parentheses. Base-case capacitance coefficients calculated from Equations 4 through 8 are displayed graphically in Appendix A, Figures A1 through A6, for each of the hydrogeologic units included in these analyses. The base-case hydraulic conductivities for each unit are plotted in Appendix A, Figures A7 through A12. Calculations using parameters similar to these have been reported by Peters, Gauthier, and Dudley, 1986, and Dudley et al., in preparation.

Table 3. Base-Case Values and Ranges of Properties for the Hydrologic Units in the Unsaturated Zone of the Tuff Site

Compressibility Factors

The compressibility of water, β'_w, is 9.8E−7/m.

Unit	A	B	C	D	Ev	Ez
Coefficient of Consolidation [a] α'_{bulk} (1.E−7/m)	6.2 (0.1–50)	82. (10–250)	12. (0.1–50)	5.8 (0.1–50)	39. (1–150)	26. (1–150)

Matrix Properties [b]

Unit	Grain Density (g/cm³)	Porosity n_m	Saturated Hydraulic Conductivity, $K_{m,b}$ (m/s) [c]	Residual Saturation, S_r	Alpha α (1/m)	Beta β
A	2.49	0.08 (0.05–0.15)	9.7×10^{-12} $1.0\times10^{-13}-5.0\times10^{-10}$	0.002 (0.00–0.18)	0.00821 (0.003–0.024)	1.558 (1.3– 2.4)
B	2.35	0.40 (0.20–0.70)	3.9×10^{-07} $1.0\times1^{-09}-5.0\times10^{-05}$	0.100 (0.00–0.15)	0.01500 (0.001–0.031)	6.872 (1.2–15.0)
C	2.58	0.11 (0.05–0.20)	1.9×10^{-11} $1.0\times10^{-13}-5.0\times10^{-10}$	0.080 (0.00–0.23)	0.00567 (0.001–0.020)	1.798 (1.2– 2.5)
D	2.58	0.11 (0.05–0.20)	1.9×10^{-11} $1.0\times10^{-13}-1.0\times10^{-09}$	0.080 (0.00–0.32)	0.00567 (0.001–0.020)	1.798 (1.2– 2.5)
Ev	2.37	0.46 (0.30–0.55)	2.7×10^{-07} $1.0\times10^{-13}-5.0\times10^{-06}$	0.041 (0.00–0.25)	0.01600 (0.005–0.060)	3.872 (1.3– 7.0)
Ez	2.23	0.28 (0.20–0.45)	2.0×10^{-11} $1.0\times10^{-14}-5.0\times10^{-10}$	0.110 (0.00–0.30)	0.00308 (0.001–0.030)	1.602 (1.2– 3.5)

Notes: a) Based on Nimick, *et al.*, 1984.
b) All base-case matrix data in this section are from Peters *et al.*, 1984.
c) The matrix saturated conductivity and the bulk matrix saturated conductivity ($K_{m,b}$) are essentially the same because the factor that converts the matrix value to the bulk matrix value, $(1-n_f)$, is nearly equal to one.

(continued)

Table 3. concluded

Fracture Properties [d]

Unit	Horizontal Stress [e] (bars)	Fracture Aperture (microns)	Saturated Fracture Hydraulic Conductivity (m/s)	Fracture Density [f] (no./m^3)	Fracture Porosity [g] n_f
A	1.1	6.74	3.8×10^{-5} $5.0\times10^{-7}-5.0\times10^{-3}$	20	1.4×10^{-4} $1.0\times10^{-5}-1.0\times10^{-3}$
B	3.3	27.0	6.1×10^{-4} $5.0\times10^{-6}-5.0\times10^{-2}$	1	2.7×10^{-5} $2.0\times10^{-6}-2.0\times10^{-4}$
C	9.5	5.13	2.2×10^{-5} $5.0\times10^{-7}-1.0\times10^{-3}$	8	4.1×10^{-5} $2.0\times10^{-6}-1.0\times10^{-3}$
D	21.9	4.55	1.7×10^{-5} $1.0\times10^{-7}-1.0\times10^{-3}$	40	1.8×10^{-4} $1.0\times10^{-5}-5.0\times10^{-3}$
Ev	34.3	15.5	2.0×10^{-4} $2.0\times10^{-6}-2.0\times10^{-2}$	3	4.6×10^{-5} $5.0\times10^{-6}-5.0\times10^{-4}$
Ez	34.3	15.5	2.0×10^{-4} $2.0\times10^{-6}-2.0\times10^{-2}$	3	4.6×10^{-5} $5.0\times10^{-6}-5.0\times10^{-4}$

Unit	Fracture Compressibility (1/m)	Bulk Fracture Saturated Hydraulic Conductivity [h] $K_{f,b}$ (m/s)	Residual Saturation, S_r	Alpha α (1/m)	Beta β
A	1.3×10^{-6} $1.0\times10^{-7}-1.0\times10^{-5}$	5.3×10^{-9} $5.0\times10^{-12}-5.0\times10^{-6}$	0.0395 (0.00–0.15)	1.2851 (0.2–6.0)	4.23 (1.2–7.0)
B	1.9×10^{-7} $2.0\times10^{-8}-2.0\times10^{-6}$	1.6×10^{-8} $1.0\times10^{-11}-1.0\times10^{-5}$	0.0395 (0.00–0.15)	1.2851 (0.2–6.0)	4.23 (1.2–7.0)
C	5.6×10^{-8} $6.0\times10^{-9}-6.0\times10^{-7}$	0.9×10^{-9} $1.0\times10^{-12}-1.0\times10^{-6}$	0.0395 (0.00–0.15)	1.2851 (0.2–6.0)	4.23 (1.2–7.0)
D	1.2×10^{-7} $1.0\times10^{-8}-1.0\times10^{-6}$	3.1×10^{-9} $1.0\times10^{-12}-5.0\times10^{-6}$	0.0395 (0.00–0.15)	1.2851 (0.2–6.0)	4.23 (1.2–7.0)
Ev	2.8×10^{-8} $3.0\times10^{-9}-3.0\times10^{-7}$	9.2×10^{-9} $1.0\times10^{-11}-1.0\times10^{-5}$	0.0395 (0.00–0.15)	1.2851 (0.2–6.0)	4.23 (1.2–7.0)
Ez	2.8×10^{-8} $3.0\times10^{-9}-3.0\times10^{-7}$	9.2×10^{-9} $1.0\times10^{-11}-1.0\times10^{-5}$	0.0395 (0.00–0.15)	1.2851 (0.2–6.0)	4.23 (1.2–7.0)

Notes: d) Unless otherwise noted, base-case fracture information is based on Peters *et al.*, 1984.
e) Horizontal stress is assumed to be one-third of the overburden weight, evaluated at the average unit depth.
f) Based on Scott *et al.*, 1983.
g) Calculated as fracture volume (aperture times 1 m^2) times the number of fractures per cubic meter.
h) This value of $K_{f,b}$ was obtained by multiplying the fracture conductivity by the fracture porosity.

Variations

To make good decisions about the amount and quality of data required to properly support the use of a particular mathematical model, it is necessary to test the sensitivity of that model to the parameters involved to determine which parameters are most important. The following paragraphs suggest variations for parameters for which sensitivities of the 1-D model for partially saturated flow in fractured tuff should be investigated.

Estimates of the flux under semiarid climatic conditions and possible fluxes that could result from a change to a wetter climate vary widely. For the steady-flow analyses, two ranges of flux should be considered:

1. 0.01 mm/yr $\leq \bar{q} \leq$ 0.5 mm/yr for base case 1 with $\bar{q}$ = 0.1 mm/yr
2. 0.50 mm/yr $\leq \bar{q} \leq$ 4.0 mm/yr for base case 2 with $\bar{q}$ = 1.0 mm/yr

Saturated hydraulic conductivities for both matrix and fractures have significant natural variability within each hydrogeologic unit. The low measured conductivities are also subject to experimental errors. Possible ranges for the saturated conductivities for each unit are listed in Table 3. Uncertainty in these values is not expected to be correlated between units.

A further uncertainty in the hydraulic conductivity values is introduced by the model being used to relate pressure head, degree of saturation, and conductivity for conditions of partial saturation and by the experimental techniques used to estimate the parameters for that model. Neither the model nor the experimental techniques have been validated for welded or nowelded, fractured tuffs. Possible ranges for residual saturation, S_r, and the modeling parameters α and β are suggested in Table 3.

Matrix and fracture porosities are known to be highly variable. The distributions of matrix porosities are moderately well known, but the distributions of fracture porosities are poorly known. Currently available data suggest that there is no direct correlation between porosity and hydraulic conductivity. Possible ranges of porosity for sensitivity analyses are listed in Table 3.

Water travel time from the repository to the water table is nonlinearly related to the location of the water table because of the dependence of the moisture distribution on the lower boundary condition. A climate change could raise the level of the water table and shorten the water travel time from the repository to the accessible environment. For these analyses, the water table could be considered to rise anywhere from 0.0 m to 20.0 m above its current elevation.

Portions of Unit E in the unsaturated zone have been thermally and chemically altered from their original vitric form (Ev) to a zeolitized form (Ez). The relative thicknesses of vitric and zeolitic materials vary across the repository site. Any given column could contain all vitric material, all zeolitic material, or any combination in between these two extremes. Whenever both forms are present, the vitric materials (Ev) always overlie the zeolitic materials (Ez). Because saturated hydraulic conductivities of the matrix material in the zeolitic form (Ez) are several orders of magnitude lower than in the vitric form (Ev), water travel time could be very sensitive to the thickness of each material in the geologic column.

Sensitivity Analyses for 2-D Flow

Description

Montazer and Wilson, 1984, suggested that both the bedding within nonwelded units and the sharp contrast in hydraulic conductivities at contacts between welded and nonwelded units could give rise to a significant amount of lateral flow. In the proposed 2-D analyses, all of the factors that could cause lateral flow are allowed to act. As in the conceptual model for 1-D flow, it is assumed that the flux entering the top of the column has already migrated past the zone of evapotranspiration.

The hydrogeologic units involved in the conceptual model for 2-D flow are those previously described in Table 1. Figure 3 shows the geologic section for these analyses. The earlier 1-D column has simply been expanded to a 2-D section and the units have been tilted to an average dip of 6°. The dip of the units ranges from 5° to 8°. The modeled region is bounded on the right by a fault zone, and it is assumed that the repository extends across the fault zone. The overall height of the modeled section is 635.5 m; the width is 1000.0 m. Coordinates for the locations numbered in Figure 3 are listed in Table 4.

Each unit is taken to be homogeneous and isotropic. A known vertical flux, $\bar{q}$, is applied along the upper boundary. The left boundary, x = 0.0 m, is a no-flow boundary; the fault zone along the right boundary, x = 1000.0 to 1000.5 m, is also initially taken to be represented by a no-flow boundary at x = 1000.0 m. The water table, ψ = 0.0 m at z = 0.0 m, is again taken as the lower boundary of the modeled region; it is located within Unit E and is assumed to be horizontal. Temperature conditions are isothermal.

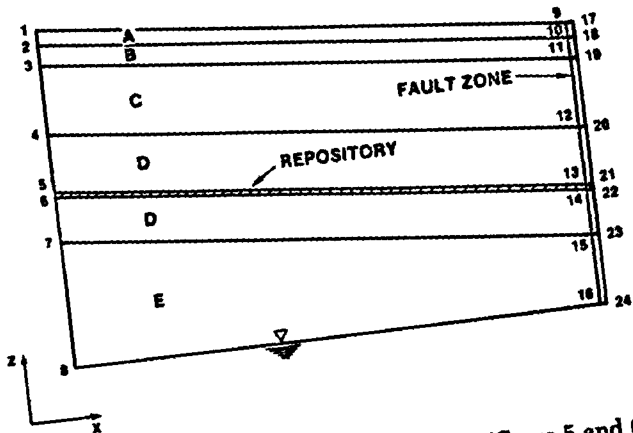

Figure 3. Stratigraphy for 2-D Base Cases (Cases 5 and 6)

Table 4. Coordinates of the Numbered Points for the 2-D Flow Analyses (see Figures 3 and 4)

Point	Coordinates (m) x	z
1	0.0	635.5
2	0.0	608.7
3	0.0	570.6
4	0.0	440.5
5	0.0	329.1
6	0.0	324.6
7	0.0	235.4
8	0.0	0.0
9	1000.0	530.4
10	1000.0	503.6
11	1000.0	465.5
12	1000.0	335.4
13	1000.0	224.0
14	1000.0	219.5
15	1000.0	130.3
16	1000.0	0.0
17	1000.5	530.4
18	1000.5	503.6
19	1000.5	465.5
20	1000.5	335.4
21	1000.5	224.0
22	1000.5	219.5
23	1000.5	130.3
24	1000.5	0.0

Simplified 2-D Analyses

Because of the computational requirements involved in attempting to analyze the entire five-layer, two-dimensional section, some HYDROCOIN teams may prefer to attempt a simplified section consisting either of the upper three layers (Units A, B, and C) or of the lower three layers (Units C, D, and E). All of the phenomena of interest can be observed in these layers. The stratigraphies for these simplified sections should be as shown in Figure 4. Coordinates of the numbered locations are the same as those listed in Table 4.

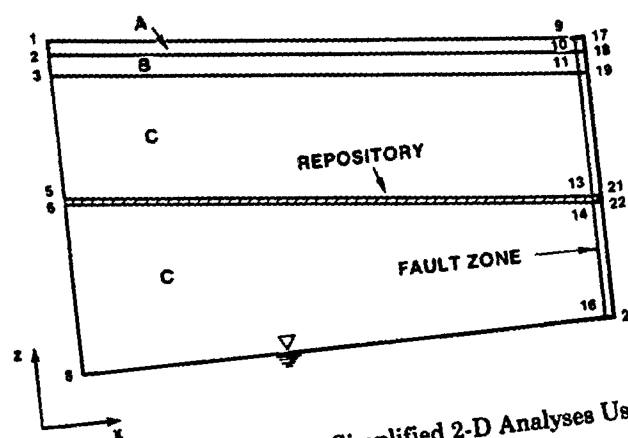

Figure 4a. Stratigraphy for Simplified 2-D Analyses Using Units A, B, and C

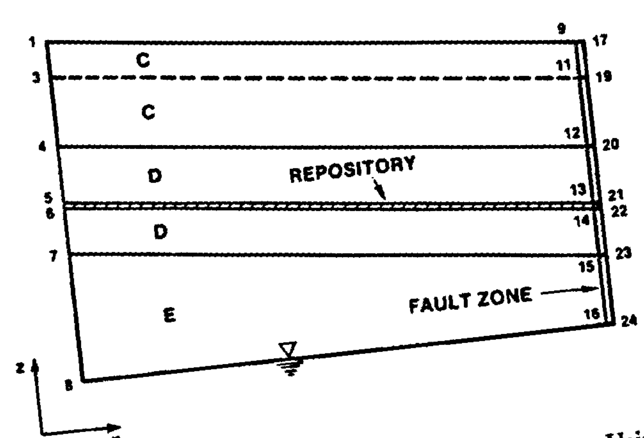

Figure 4b. Stratigraphy for Simplified 2-D Analyses Using Units C, D, and E

If the upper three layers are analyzed, Unit C should be extended downward to the water table, Figure 4a. Naturally, if this section is chosen, no conclusions can be drawn regarding the flow conditions below the repository, and the representation of the conditions between the top of Unit D and the repository are only approximate.

If the lower three layers are analyzed, the infiltration boundary condition can be applied at the top of Unit C, dashed line in Figure 4b, or Unit C could be extended upward to the original infiltration surface, solid lines in Figure 4b. In either case, no conclusions can be drawn regarding the flow conditions above the top of Unit C. Also, any conclusions about flow through Units C, D, and E are conditioned by the fact that any lateral diversion of flow caused by Units A and B is ignored.

It may be possible to construct a global sensitivity analysis from separate "global" analyses of the two simplified sections. Construct input parameter vectors as if the entire five-layer section were to be analyzed. Use the same vectors for analyses of both the upper and lower sections; parameters for Unit C will be common to vectors used in both sets of analyses. When performing the analyses of the lower simplified section, take the pressure head and flux conditions at the top of Unit C from corresponding analyses of the upper three layers and apply them as boundary conditions at the top of Unit C. Then, by matching cases with the same input parameter vectors, recouple the separate analyses to draw conclusions regarding the global sensitivity of the entire five-layer system. Check the validity of this approach by analyzing a few cases with the full five-layer section.

Performance Measures

Performance measures for the 2-D flow cases are intended to assess the magnitude of lateral diversion of flow and its effect on the performance of the repository. The first measure is the spatial distribution of the volumetric flow rate of water passing through the repository horizon. There are two complementary flow rates that are of interest:

1. The flow rate of water moving through the bulk rock mass at the level of the repository
2. The flow rate of water diverted above the repository into the fault zone

All flow rates should be calculated for a 1.0-m thickness of the vertical section. This performance measure is applicable to analyses of the full five-layer section and to analyses of only the upper three layers.

The spatial distribution of water travel times from the base of the repository to the water table is the second performance measure. It will be interesting to observe what portion of the water flowing through the bulk rock mass at the level of the repository is diverted below the repository toward or into the fault zone and what effect this has on the distribution of water travel times. The criterion for nonnegligible flow volume that was described for the 1-D analyses also applies here. This performance measure is applicable to analyses of the full five-layer section and to analyses of only the lower three layers.

Base-Case Parameters

For the same reasons described previously for the 1-D flow analyses, two base-case fluxes are proposed for the 2-D, steady-flow analyses:

Case 5: $\bar{q}$ = 0.1 mm/yr for matrix-dominated flow

Case 6: $\bar{q}$ = 1.0 mm/yr for conditions near the transition from matrix-dominated to fracture-dominated flow

Base-case values for the hydrologic properties for each of the hydrogeologic units are those given in Table 3. No base-case values are given for hydrologic properties of the fault zone because the right boundary is being treated as a no-flow boundary in the base cases.

Variations

All of the variations suggested for the 1-D flow analyses also apply to the 2-D cases: changes in applied flux; saturated conductivities and parameters for conductivities for partially saturated flow; porosities; location of the water table; and relative proportions of vitric (Ev) and zeolitic (Ez) materials in Unit E. The two-dimensionality of these analyses introduces additional sources of uncertainty. Some of these are discussed below.

Little is known about the conditions at lateral boundaries or even what might be an appropriate boundary for site-scale analyses. In the base cases, the fault zone along the right boundary is treated as a no-flow boundary at x = 1000.0 m. It could also be modeled as a seepage face or as a column of fractured or unfractured, porous material between x = 1000.0 m and x = 1000.5 m. The right boundary of the column of porous material representing the fault can be taken as a no-flow boundary. The porous materials in the fault zone could have hydraulic conductivities that are

1. Slightly lower than those of the adjacent material from which they were derived
2. Comparable to those in the adjacent rock mass
3. Several orders of magnitude greater than those in the adjacent rock

In these variations, the saturated conductivities and parameters for partially saturated conductivities in the fault zone should be taken to be correlated with the properties of the parent rock. For simplicity, porosities in the fault zone will be taken to be identical to those of the adjacent rock mass.

It has been suggested that, when the nonwelded materials of Unit E are sheared at high confining stress, the hydrologic properties of the sheared material may be very similar to those of the intact rock. The result is that the fault zone may be hydraulically discontinuous through Unit E and may not act as an effective conduit for flow from the ground surface to the water table. To observe the effect this might have on the performance measures, allow the hydrologic properties of the fault zone through Units A, B, C, and D to vary as described in the previous paragraph while keeping the properties of the fault zone through Unit E the same as those of Unit E.

The effective width of materials in the fault zone having altered hydraulic properties is not known. For analyses with the fault modeled as a porous material, the width is initially taken to be 0.5 m and should be varied over a range of 0.1 to 3.0 m (0.0 to 3.0 m in Unit E).

Hydraulic conductivities were assumed to be isotropic in the 2-D base-case analyses. There is weak evidence that the effective, bulk, saturated conductivities of the various tuff units are anisotropic. The correlation between measured anisotropy in saturated conductivities and in conductivities for partially saturated flow is very poorly known. The magnitudes of the relative contributions to anisotropy from matrix and fractures are also uncertain. Ratios of horizontal to vertical conductivity could range from 0.1 to 1000. Here "horizontal" is taken to mean parallel to the dip of the hydrogeologic units and "vertical" is taken to mean perpendicular to dip. Anisotropy can be varied unit by unit, or the relative degree of anisotropy can be randomly selected for each unit.

Unit B, though primarily nonwelded, is assumed to contain numerous horizontal lenses of less-permeable welded materials. This heterogeneous unit could be modeled as a homogeneous unit with effectively anisotropic hydraulic conductivity. Because Unit B could intercept and divert water above the repository horizon, it may be particularly interesting to investigate the sensitivity of the performance measures to anisotropy in this unit.

If there is a significant volume of water diverted above the repository from the rock mass into the fault zone, the volume of water contacting the waste could be reduced by not storing waste close to the fault. Consider truncating the repository 0.0 to 50.0 m to the left of the fault zone to observe the effect of the distance between the repository and the fault zone on the volumetric rate of water flow through the repository.

Mesh Design Considerations

Experience from analyses similar to those proposed in this paper indicates that results can be very sensitive to mesh design. Attention to mesh design is especially important in those parts of the problem domain having very steep hydraulic gradients.

Fine mesh zoning is needed where steep hydraulic gradients occur. If the mesh is too coarse, the steeper parts of the gradient may not be observed, and incorrect conclusions could be drawn about the flow conditions. For example, it has been observed in 1-D calculations that coarse gridding near layer boundaries, where there is a large contrast in hydraulic conductivity across the boundary, can lead to the appearance of perched water above the boundary. When the grid is further refined, the steepness of the hydraulic gradient is properly resolved, and water moves across the boundary without appearing to become perched.

Steep hydraulic gradients are typically observed at the boundaries between adjacent hydrologic units when there is a large contrast in hydraulic conductivity across the boundary. Also, in nonsteady analyses, saturation fronts moving through the problem domain create a moving zone with a steep gradient in the hydraulic conductivity because of large differences in saturation ahead of and behind the front. It is expected that steep conductivity gradients may also occur along the right boundary in the 2-D analyses. For an example of the steepness of the hydraulic gradients that can occur, see the analyses described by Peters, Gauthier, and Dudley, 1986.

Because of the wide range of values assigned to the hydrologic properties for these sensitivity analyses, it is not possible to state, in advance, where the steepest gradients will occur, since their location could change with each iteration. However, as previously mentioned, an ordinary differential equation (ODE) solver can be used to efficiently analyze 1-D, isothermal, steady-state flow. When setting up any of the above analyses for finite-element or finite-difference codes, use of the ODE solver can help guide mesh design by identifying regions where very steep hydraulic gradients are likely to occur. An ODE solver can also be used to obtain reasonable estimates of initial conditions for steady-flow analyses.

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APPENDIX A

Plots of Capacitance Coefficients and Hydraulic Conductivities

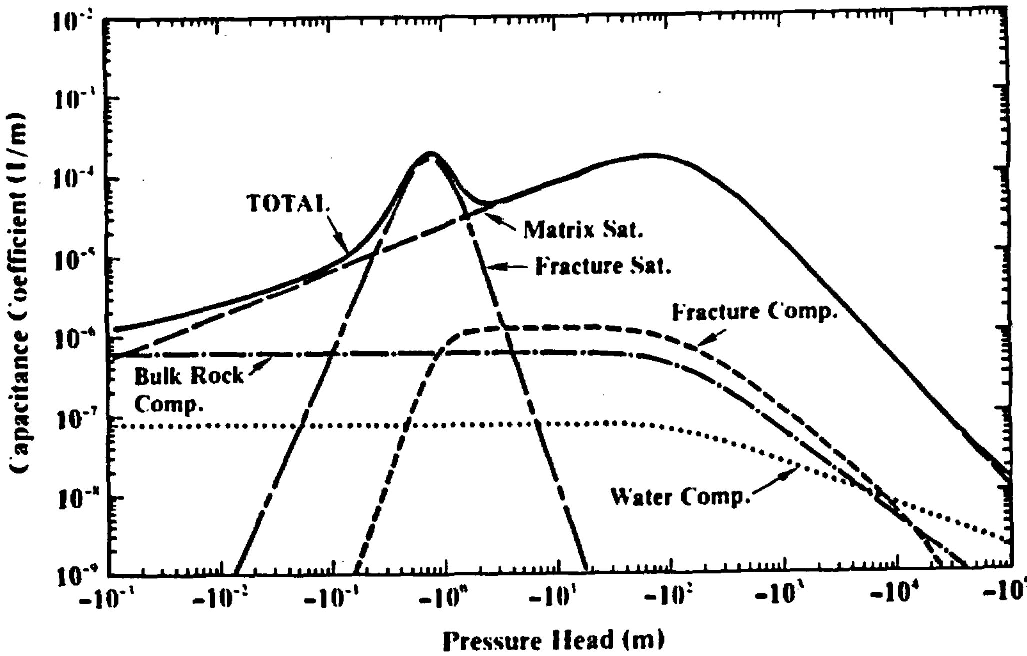

Figure A1. Capacitance Coefficients for Unit A

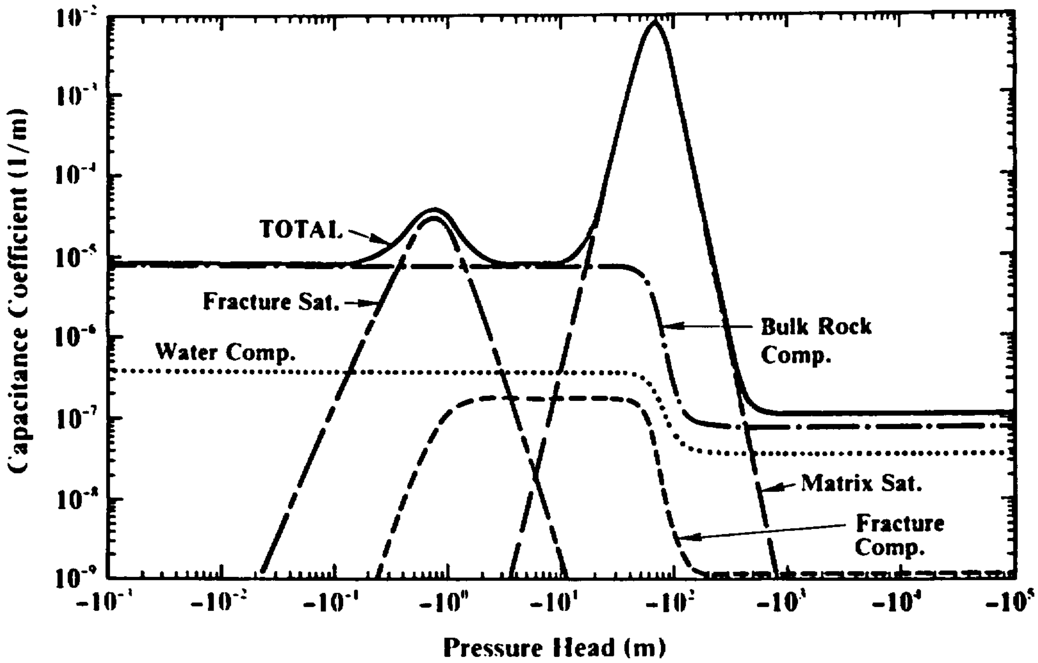

Figure A2. Capacitance Coefficients for Unit B

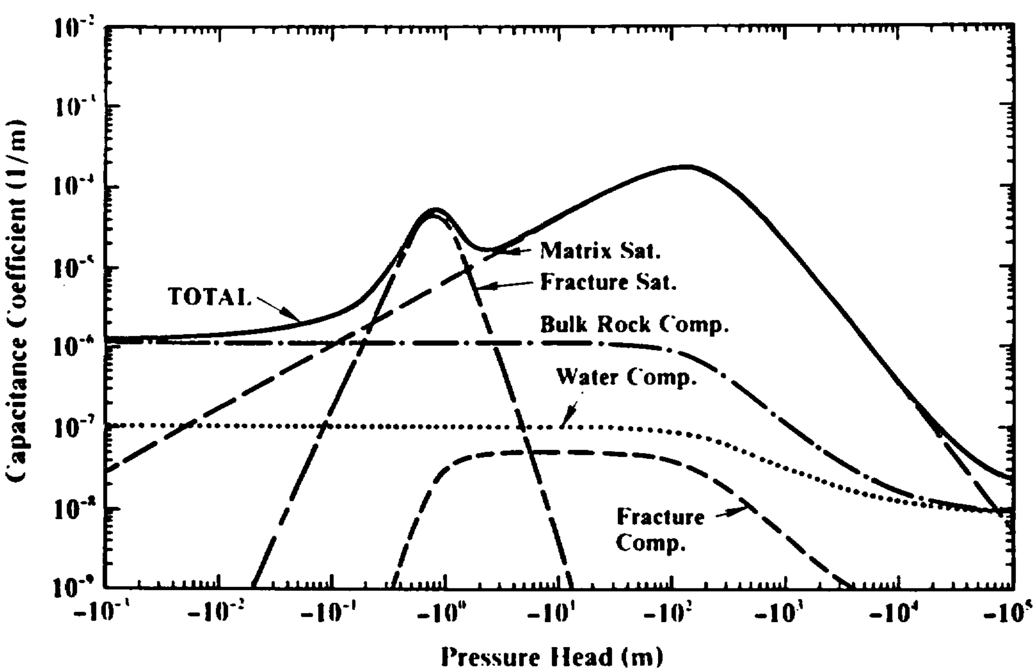

Figure A3. Capacitance Coefficients for Unit C

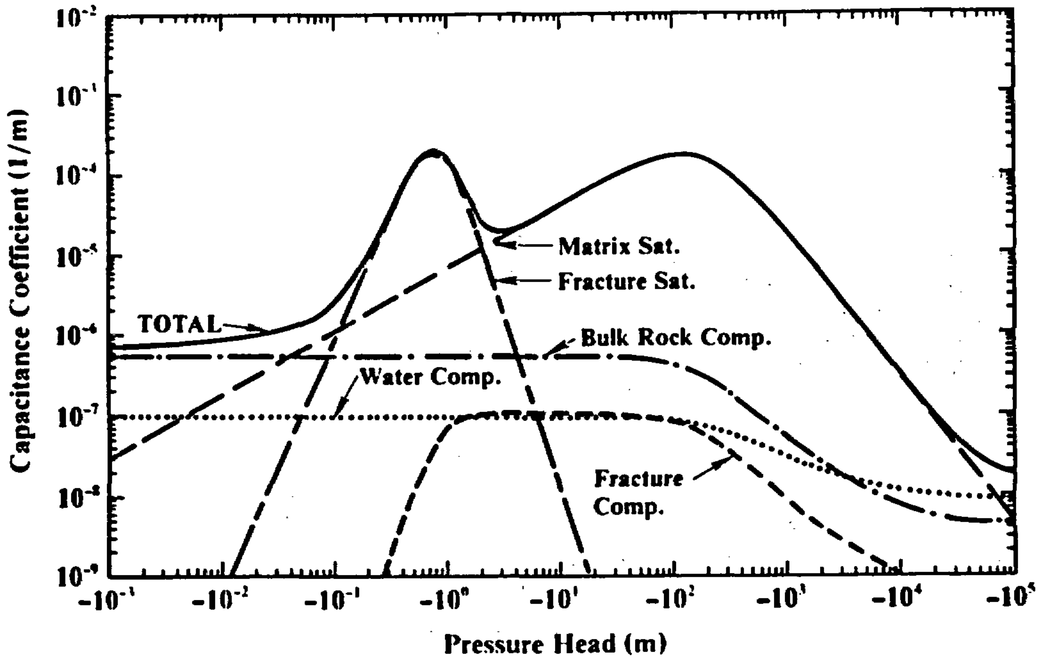

Figure A4. Capacitance Coefficients for Unit D

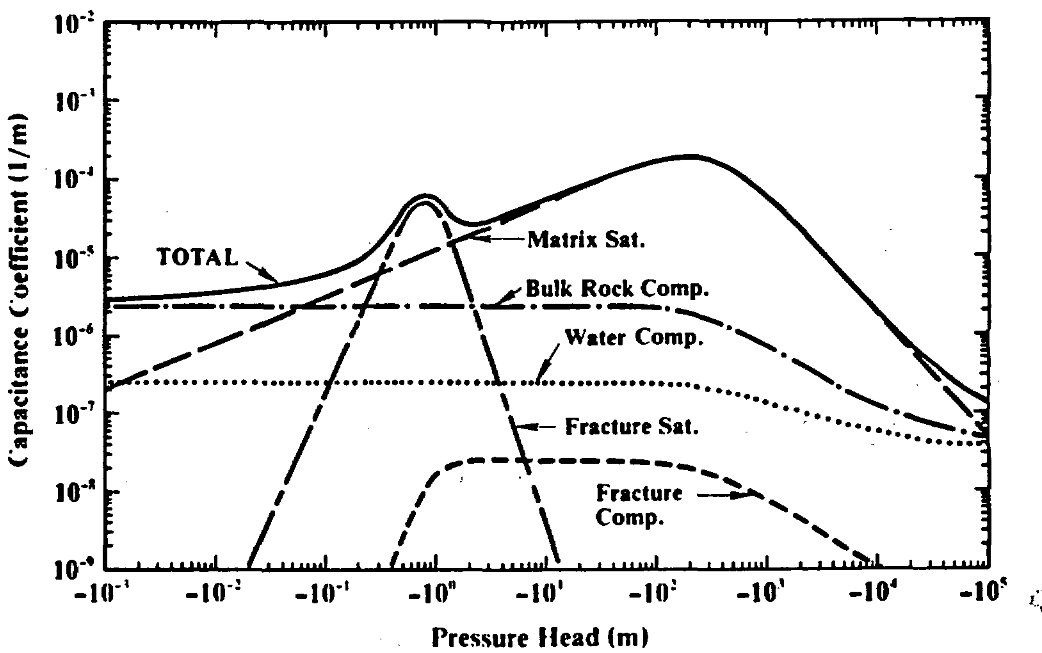

Figure A5. Capacitance Coefficients for Zeolitic Unit Ez

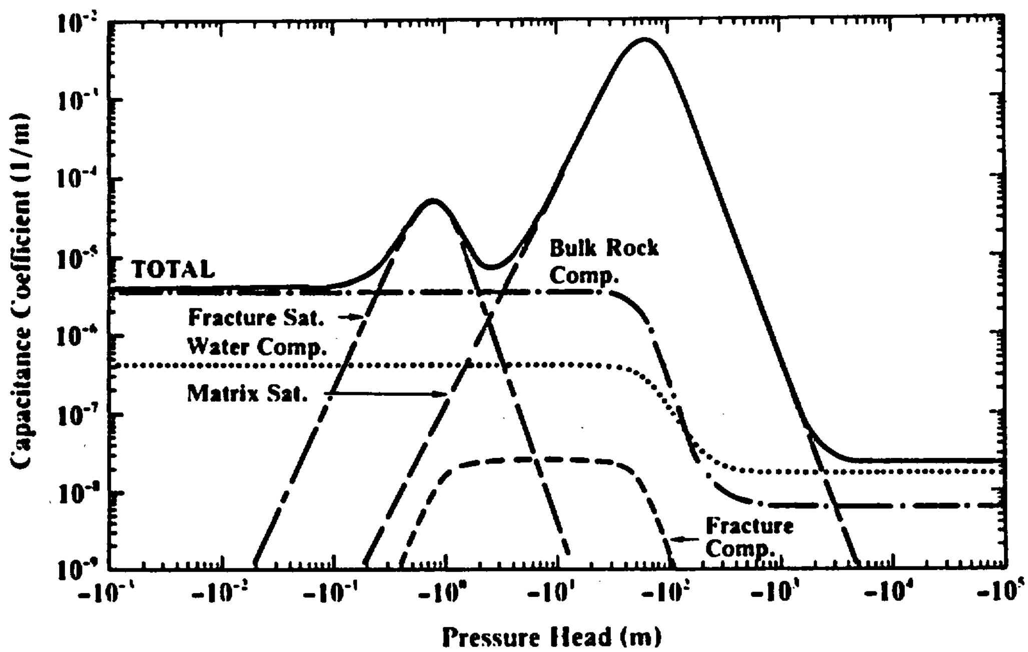

Figure A6. Capacitance Coefficients for Vitric Unit Ev

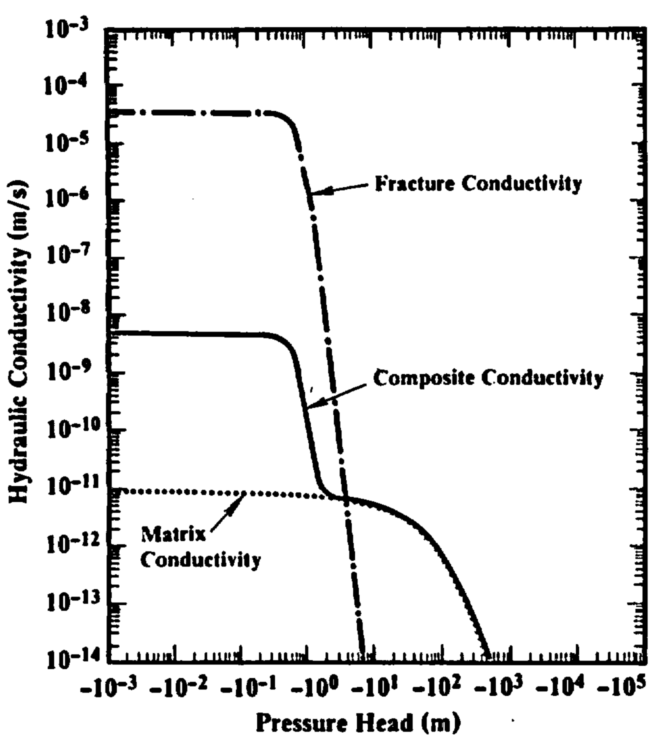

Figure A7. Hydraulic Conductivity Versus Pressure Head for Unit A

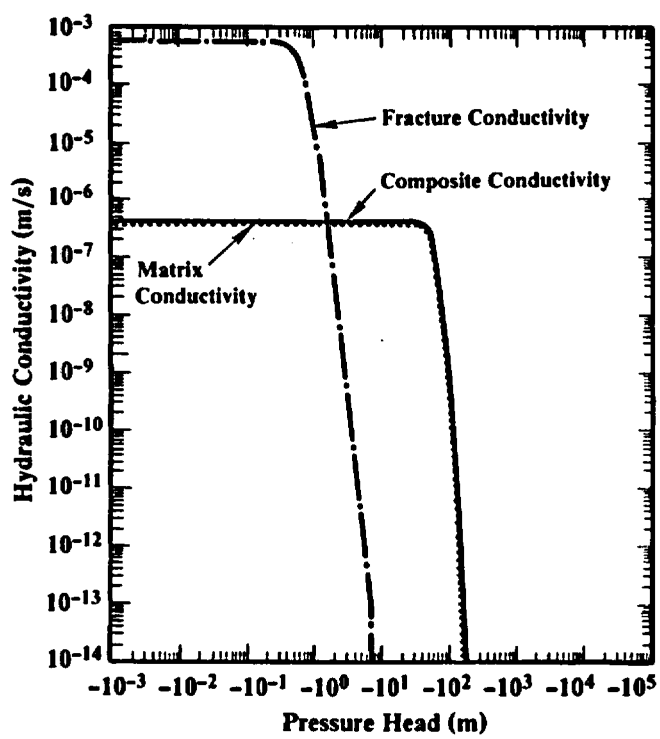

Figure A8. Hydraulic Conductivity Versus Pressure Head for Unit B

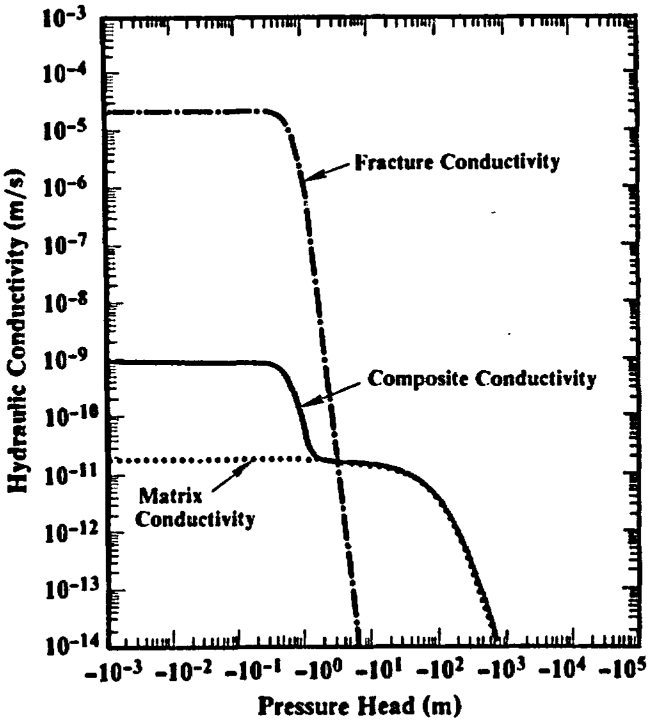

Figure A9. Hydraulic Conductivity Versus Pressure Head for Unit C

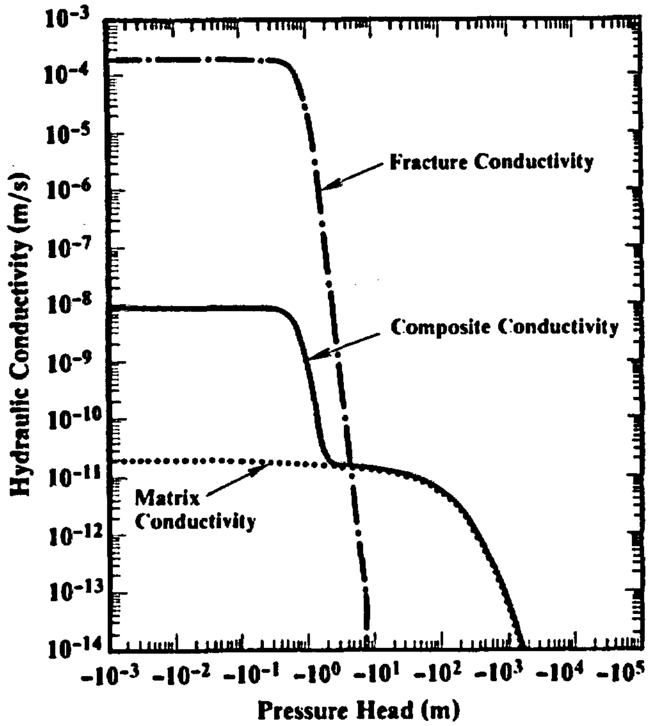

Figure A11. Hydraulic Conductivity Versus Pressure Head for Zeolitic Unit Ez

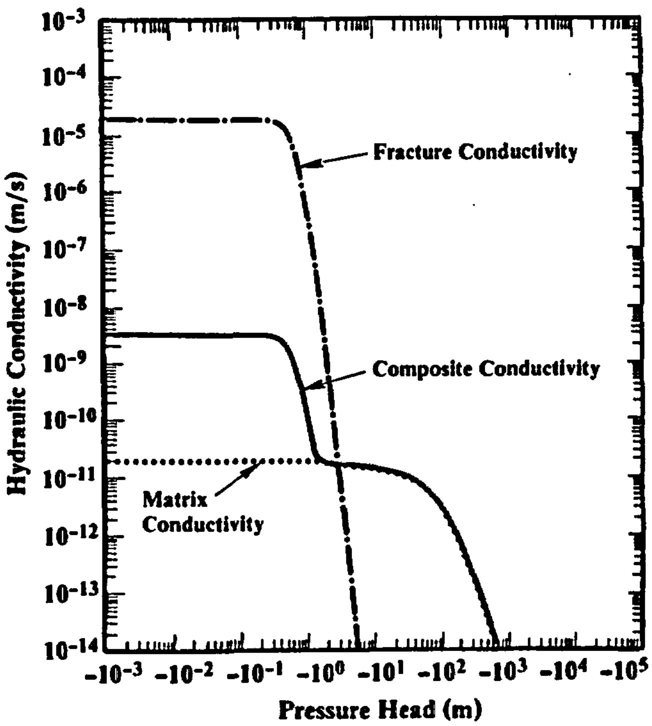

Figure A10. Hydraulic Conductivity Versus Pressure Head for Unit D

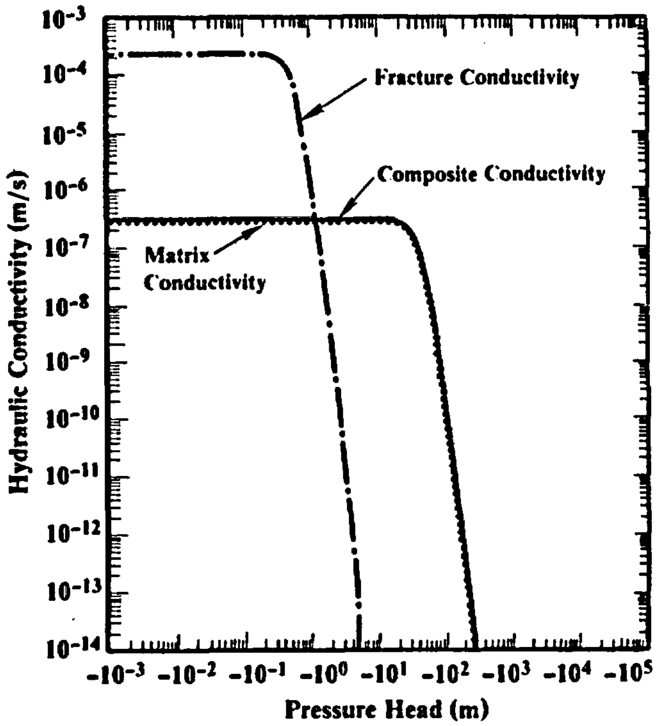

Figure A12. Hydraulic Conductivity Versus Pressure Head for Vitric Unit Ev

APPENDIX B

NNWSI Data Base Information

The analyses outlined in this paper are generic in nature and do not represent the proposed nuclear-waste-repository site at Yucca Mountain, Nevada. Therefore, requirements for conformance to the Nevada Nuclear Waste Storage Investigations (NNWSI) Project Reference Information Base do not apply. Also, no data are reported here that are appropriate for inclusion in the NNWSI Project Site and Engineering Properties Data Base.

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