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The Appropriateness of One-Dimensional Yucca Mountain Hydrologic Calculations

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THE APPROPRIATENESS OF ONE-DIMENSIONAL YUCCA MOUNTAIN HYDROLOGIC CALCULATIONS

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Abstract

This report brings into focus the results of numerous studies that have addressed issues associated with the validity of assumptions which are used to justify reducing the dimensionality of numerical calculations of water flow through Yucca Mountain, NV. It is shown that, in many cases, one-dimensional modeling is more rigorous than previously assumed.

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1.0 INTRODUCTION

Yucca Mountain, located in southwestern Nevada, is the site for a potential high-level nuclear waste repository. Numerical simulations that accurately represent our knowledge of aqueous flow through the mountain are necessary to demonstrate whether or not the repository system can adequately retard release of radionuclides as defined by regulations.

The rock units that comprise Yucca mountain are predominately volcanic ash flow tuffs. Measurement of the physical and hydrologic properties of these rock sequences show extreme variability (Klavetter and Peters, 1986). The variability is greatest in the vertical direction as a result of differences in depositional, cooling, and alteration histories of the individual units. These same differences occur in a lateral sense, however, they generally do not vary as rapidly as in the vertical sense. In addition, the layered rock mass itself is cut by faults that cause offset of the layers and by fractures that introduce discontinuities. Therefore, stochastic simulations that can sample from a range of parameter values are required to reduce the uncertainty and variability of those values. Including the details of all these heterogeneities in numerical models of the mountain, results in computer calculations which are computationally intensive.

Because of these difficulties, one-dimensional numerical models are often used to make predictions of the water flow through the mountain. This is particularly true when reliable results cannot be obtained deterministically because of material property uncertainties. Consequently, computationally intensive multiple realizations are required to account statistically for these uncertainties. When the dimensionality of a problem is reduced for computational purposes, the applicability of the results obtained using the simplified model may be of questionable value.

This report outlines numerous issues which help define the regimes in which one-dimensional modeling is applicable. The two primary issues addressed are: (1) When is it appropriate to use effective material characteristics to aid in the inclusion of small scale geologic heterogeneities into large-scale modeling and (2) Can appropriate numerical boundary conditions, such as unit-gradient, be developed to make it computationally expedient to obtain lateral-flow estimates resulting from geologic down-dip using one-dimensional calculations?

The results of the studies imply that the use of one-dimensional modeling to analyze a multi-dimensional problem may be less restrictive than previously assumed. In most cases, the effect of small-scale, low-conductivity heterogeneities can be accounted for through the use of effective hydraulic conductivity. This occurs, in part, because of the highly nonlinear nature of unsaturated flows. It is also shown that when the media are assumed to be homogeneous along geologic units, a minor extension to one-dimensional calculations can be used to obtain reasonable estimates of multi-dimensional flow path lines without additional computational complexity. This two-dimensional effect can be beneficial when calculating solute transport because the geometry of the two-dimensional path lines can vary considerably from their one-dimensional counterpart.

2.0 EFFECT OF MATERIAL HETEROGENEITY

The simplest type of material heterogeneities are those of a perfectly layered system. For perfectly layered systems, one can analytically derive the effective conductivity of flow parallel and perpendicular to the layering (Freeze and Cherry, 1979). For materials which are not perfectly layered, approximating the effective material properties can be considerably more complex. One approach to reducing the number of dimensions required in numerical computations is to include the effect of small-scale material heterogeneities by lumping them into larger scale equivalent properties, such as effective hydraulic conductivity. Several studies have been made (Eaton and Dykhuizen, 1988; Martinez et al., 1992) which attempt to identify the flow regimes in which the effective material properties concept is appropriate. These studies are outlined below.

2.1 Effect of Low-Conductivity Obstructions on Effective Properties

A numerical investigation of the effect of material heterogeneities on two-dimensional deterministic calculations of water flow and particle travel times has been made by Eaton and Dykhuizen (1988). This section briefly summarizes that study. Upper and lower bounds on the infiltration rates for Dirichlet boundary conditions were defined as a function of the degree of material heterogeneity. The parallel/series concept for predicting flow limits was previously documented by Crane et al. (1977) for materials with constant-material properties. In this study, it was assumed that the materials with different conductivities were arranged in either a parallel or series configuration and that the materials were saturated. Because of the nonlinear nature of flow in partially saturated media, the techniques for determining the bounds for saturated flows were found not to apply. A new, less stringent set of limits was proposed.

2.1.1 Problem Definition

This study considered the flow through the Tiva Canyon unit of Yucca Mountain. For simplicity, it was assumed that this layer consists of a two-dimensional array of material units having small and large hydraulic conductivities (Figure 2.1). This arrangement is idealized as a uniform array of high- and low- conductivity materials (Figure 2.2). The flow through the 4-m by 12-m unit cell, outlined in Figure 2.2, was investigated. The conductivity for the highly permeable material is chosen to be that of Tiva Canyon (Klavetter and Peters, 1986) (Figure 2.3). The conductivity of the low-permeability obstruction into the unit cell is assumed to be zero, which is the limiting case.

Numerical calculations were carried out using the finite-element code NORIA (Bixler, 1985). Steady-state results for a wide range of obstruction sizes and water-flow rates were obtained. The equation solved by the code is Richards' equation (1931).

2.1.2 Initial and Boundary Conditions and the Numerical Mesh

A bottom pore-pressure condition of -100 m was specified for all cases. Three different flow rate regimes were investigated by fixing the top pressure at -17.86 m to give flow rates of ~ 0.2 mm/yr, Case A; -1.225 m to give ~ 1.0 mm/yr, Case B; and -0.6 m to give ~ 64 mm/yr, Case C. The variation in the conductivity range is shown in Figure 2.3.

Figure 2.1 Nonhomogeneous Material Concept (Eaton and Dykhuizen, 1988).

Figure 2.2 Assumed Idealized Symmetric Array of Low and High-Permeability Materials (Eaton and Dykhuizen, 1988).

Figure 2.3 Material Hydraulic Conductivity (Eaton and Dykhuizen, 1988).

Case A spans a relatively constant portion of the conductivity curve, while Cases B and C span the nonconstant portion of the conductivity curve. This conductivity function is a result of the composite treatment of the matrix and fractures. The mesh shown in Figure 2.4 was used for the two-dimensional calculations. The size of the flow obstruction was varied by altering the mesh horizontally.

Figure 2.4 Two-Dimensional Mesh With Three Obstruction Sizes: (a) $x_0/W = 0.95$, (b) $x_0/W = 0.5$, and (c) $x_0/W = 0.25$ (Eaton and Dykhuizen, 1988).

2.1.3 Results and Discussion of Low-Conductivity Obstructions

Solutions were obtained for the three different pressure boundary conditions for reduced-flow areas (x_0/W) varying from 0.0125m to 0.95 m. Additionally, a $x_0/W = 0.0$ solution was computed for each case. The average nondimensional flux, as a function of reduced flow area, is given for all three cases in Figure 2.5. This figure also shows the flow rates that result when the low- and high-permeability materials in the region are arranged in parallel and series configurations. For Case A, the flux through the region gradually decreases as the obstruction size is increased and it is always bounded

by the parallel and series cases. Intuitively, this is reasonable because the material conductivity in the resulting pressure range is relatively constant. However it still changes by an order of magnitude. Some of the water undergoes a more tortuous path around the obstruction, thus increasing the total resistance to flow.

Case B is more interesting in that the average flux through the region is nearly independent of the obstruction size. The flow is independent of the obstruction size because of the highly nonlinear nature of the unsaturated material conductivity in this pressure range. This is a pronounced departure from the parallel limit for fixed-conductivity material.

For the high-flux condition, Case C, the calculated flux rate is less sensitive to obstruction size than in Case A, but more sensitive than in Case B. The level of sensitivity is a function of material nonlinearities and the zone of influence of the obstruction on pressure gradients. A detailed explanation of these results is given by Eaton and Dykhuizen (1988).

The effect of the geometry change, resulting from the nonhomogeneous properties, on particle-travel times was investigated for Case B. Particle travel times across the region decreased by a factor

Figure 2.5 Nondimensional Fluxes for Three Geometric Configurations (Eaton and Dykhuizen, 1988).

of three and dispersion increased. The ratio of fastest to slowest travel times varied from one to four as the obstruction size increased. These results are not necessarily intuitive in that one might think that an obstruction would decrease the flow rate and, consequently, increase travel times. This is not the case. As the obstruction increases in size, saturation increases and water previously flowing through the matrix now experiences less resistance to flow in the fractures. The result is an increase in fracture flow and a decrease in particle-travel time because of the small-fracture porosity.

2.1.4 Conclusions Regarding Low-Conductivity Obstructions

In the Eaton and Dykhuizen (1988) paper, only the case of a discontinuous low-conductivity material intruding into a relatively high-conductivity, continuous material was considered. This combination yields some insights into multidimensional, heterogeneous unsaturated flow. The effect of obstruction size on average flux rate through the heterogeneous-flow region is a strong function of nonlinearities in the material characteristic curves. When flow is such that the highly nonlinear portion of the conductivity curve is not involved, the average flux rate through the region decreases monotonically with obstruction size and the flow rates are bounded by the parallel and series equivalents. When the flow is such that the flow involves the highly nonlinear portion of the curves (corresponding to the onset of fracture flow), the average flux rate is a weaker function of the obstruction size and flow rates are not bounded by the parallel and series equivalents.

2.2 Effects of Unsaturated Fractures on Effective Properties

The influence of horizontal fractures on the steady seepage of moisture in variably saturated porous media was analyzed by analytical and numerical means (Martinez et al., 1992). In their work, the fractures were assumed to contain many open (dry) regions and assumed to be distributed periodically in two dimensions.

A schematic of the periodic global fracture/matrix system is given in Figure 2.6. A unit cell of the region and boundary conditions is shown in Figure 2.7. The dry region of the fracture forms a barrier to moisture flow through the geologic medium. An idealized two-dimensional model that maximizes the effect of the fractures was analyzed. The results of the analysis quantified the effect of the dry regions of the fractures on global-water flow through the fractured medium. An apparent conductivity is determined such that the fractured system can be replaced by a homogeneous medium for describing steady-unsaturated flow. An asymptotic analysis yields an analytic expression for the apparent hydraulic conductivity through such a system in the limit of a small sorptive number (fracture spacing divided by a characteristic capillary suction) for the intact matrix material. The apparent hydraulic conductivity for arbitrary spacing and the sorptive number is determined by numerical means. The numerical model accounts for variable hydraulic conductivity as a function of the local pressure head, whereas the asymptotic solution represents the limit of constant conductivity. The numerical results confirm the analytical solution as a lower bound on the apparent hydraulic conductivity.

Figure 2.6 Schematic of the Periodic Global Fracture/Matrix System (Martinez et al., 1992).

Figure 2.7 Representative Unit Cell of the Periodic Fracture Model (Martinez et al., 1992).

2.2.1 Conclusions Regarding Unsaturated Fractures

It was concluded that the flow is relatively unimpeded by the fracture system except for the cases where the blockage ratio of the unit cell (b/w) approaches one (Figure 2.7). This was demonstrated using asymptotic analysis and numerical solutions of the full-nonlinear problem for an array of geometric combinations and conductivity nonlinearities. A lower bound on the apparent hydraulic conductivity was established from the analytical solution. The numerical calculations illustrated the variation of apparent conductivity with cell length and material characteristics. It was concluded that an analytical expression derived from the approximate analytical solution could be used to model the unsaturated flow through the fractured medium for moderately nonlinear systems. For highly nonlinear systems, the numerical results can be used to replace the analytical solution.

2.3 Effective Conductivities for Random Material Mixtures

A conceptual understanding of the effect of these material heterogeneities on the flow of water through hard rock was obtained by Dykhuizen and Eaton (1991) through the use of multiple realizations of the Richards' equation for materials randomly located within a meter-scale region. The material property values were taken from the PACE-90 study (Barnard and Dockery, 1991). The value given in the PACE-90 study for saturated hydraulic conductivity, $K_s = 2 \times 10^{-11}$ m/s, was assigned to the high-conductivity material.

Typical geometric mixes of conductivity are given in Figure 2.8. This figure also shows the calculated flow path line results for these three geometric mixes of high- and low-permeability materials. The results of these material variations on flow resistance, mechanical dispersion, and channeling were addressed using multiple realizations of random geometric conductivity mixes. Many equations have been proposed to find average arithmetic and harmonic averaging. Kirkpatrick's equation provides a power averaging for random geometric mixtures of materials that fall between the arithmetic and

harmonic extremes (Kirkpatrick [1973]). Kirkpatrick's solution and those obtained from the numerical results were in good agreement. The poorest agreement occurred for material mixes in the 50% range. The 50% mix also tends to result in noticeable flow channeling and the largest mechanical dispersion based on maximum and minimum particle path line travel times. The variation of path line travel times for the 50% mix was as high as a ratio of 8.

2.3.1 Conclusions Regarding Random Mixtures

For the types of geometries and material mixes considered in this study, two-dimensional flow can be reasonably approximated using one-dimensional calculations and the effective conductivity obtained from Kirkpatrick's theory.

(a) 25%

(b) 50%

(c) 75%

Figure 2.8 Flow Path Lines for Material Mixes: (a) 25%, (b) 50%, and (c) 75% (Dykhuizen and Eaton, 1991).

3.0 EFFECT OF BOUNDARY CONDITIONS

Sections 1.0 and 2.0 of this report deal with small-scale heterogeneities on the order of 0.1 to 10 meters. We shall now consider the difficulties associated with global-scale modeling. This scale has not received as much attention as smaller scales because it is computationally intensive. The results of numerical calculations are often strongly influenced by the flow conditions applied at the boundaries. In a comprehensive study by Prindle and Hopkins (1990), they give the results of a set of numerical calculations of water infiltration through a two-dimensional model of Yucca Mountain (Figure 3.1). These results were obtained using NORIA (Bixler, 1985). Up to 5000 eight-node biquadratic elements were used.

Computational parameters which were varied included: the rate of infiltration (0.01mm/yr to 3.0 mm/yr), the width of the fault (0.5 m to 5.0 m), anisotropy conductivity ratios (1v:1h to 1v:500h), and material characteristics. However, no variation was done on the applied-boundary conditions. All calculations were made using fixed pressure along the bottom (water table) and no flow on both vertical boundaries. A study of the Prindle and Hopkins (1990) results indicated that the application of this no-flow condition has a strong influence on the overall flow patterns. Simply by the nature of the no-flow condition, all flow approaching the fault at the down-dip boundary of the region is forced to flow vertically down through the flow domain. All of the extensive variation of fault width and fault material properties affected the exact width of the region with considerable downflow. However, the results for each case were essentially the same. The water was forced to flow down through a small region in the vicinity of the applied no-flow boundary condition.

Figure 3.1 Two-Dimensional Base Case Stratigraphy (Prindle and Hopkins, 1990).

The unit-gradient boundary condition shows promise for relaxing this unrealistic no-flow boundary restraint. The application of this condition assumes that the component of flow exiting the boundary is driven by unit-pressure gradient.

The following section will show that this concept may be useful in significantly reducing the computational effort required to simulate two-dimensional flow by the assumption of unit-gradient flow at boundaries. The use of one-dimensional calculations in conjunction with the unit-gradient boundary concept and down-dip information to generate two-dimensional flow path lines will be discussed.

3.1 Unit-Gradient Boundary Conditions

Two demonstrations of the feasibility of unit-gradient boundary conditions will be presented. In the first study, Eaton and Hopkins (1992) used the LLUVIA-II code to compare results obtained using the unit-gradient boundary conditions to results obtained using the more conventional zero-flux boundary conditions. In this demonstration, the use of unit-gradient boundary conditions on the sides of the region give results similar to the no-flow boundary condition only at large distances from the side boundaries, thus implying that the choice of boundary conditions has a strong influence on the computed results.

A second demonstration is given using the two-dimensional Yucca Mountain PACE geometry (Barnard and Dockery, 1991) and the NORIA-SP code (Hopkins et al., 1991). The PACE results show that if no-flow side boundary conditions are used, unit-gradient flow exists far from the boundaries only in the geologic layers above the unit which has relatively high conductivity. In the region of the high-conductivity material, the no-flow boundary conditions used in NORIA affect the flow at all horizontal locations.

The unit-gradient boundary condition results in constant flow parallel to the geologic-unit interfaces and path lines that are similar when the material is assumed homogeneous along these units. This implies that, under these ideal conditions, two-dimensional flow path lines can be generated using an extremely simplified one-dimensional computational mesh. This approximation can reduce computational times required to generate two-dimensional path lines by one to two orders of magnitude. Application of the unit-gradient condition will be demonstrated below to illustrate the concept and its usefulness.

3.1.1 Geometry and Numerical Grid

The problem domain in the first demonstration is a rectangular grid, Figure 3.2, with the down-dip of the geologic units approximated by rotating the gravitational force vector by 6.25 degrees. A numerical grid consisting of 20 by 22 mesh points in the x and z directions, respectively, was used. The 500-m-wide domain considered started ~ 500 m east of Drillhole H-5 at Yucca Mountain. The material properties for the four geologic regions are shown in Table 3.1. Conductivity values are generated using the van Genuchten (1978) formulation. The expression of saturation and conductivity used in this study, as given by van Genuchten, are

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

and

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

where: $\lambda = 1 - 1/\beta$, K_s = saturated conductivity, ψ = water pore pressure, and α and β are given in Table 3.1.

Figure 3.2 Two-Dimensional Computational Domain for LLUVIA-II Calculations.

Table 3.1 Material Properties

Layer	Porosity Total	K_s (m/s)	α (1/m)	β	S_r	Fractures (1/m ³)
1	0.11	2×10^{-11}	0.00567	1.798	0.080	28.3
2	0.09	3×10^{-12}	0.0033	1.798	0.052	35.6
3	0.21	8×10^{-11}	0.0265	2.223	0.164	2.0
4	0.41	3×10^{-12}	0.0220	1.236	0.010	1.6

3.1.2 Boundary Conditions

Steady-state solutions were obtained using evenly distributed steady-state infiltration rates of 0.01, 0.1, and 1.0 mm/yr across the top boundary. Unit-gradient boundary conditions were specified at the left, right, and bottom boundaries. These conditions are similar to the second type boundaries discussed by McCord (1991). A second set of solutions was obtained by replacing the side unit-gradient conditions with no-flow conditions while maintaining the unit-gradient condition along the bottom.

3.1.3 Description of the Unit-Gradient Boundary Condition

The unit-gradient condition specifies that the velocity component exiting the boundary be computed by assuming that the head gradient in the direction of the gravity vector at the boundary is unity. Consequently, at boundaries where the unit-gradient condition is specified, the flux components leaving the region, are equal to

$$q_x = -K_x \sin \theta$$

and

$$q_z = -K_z \cos \theta$$

where

q_x = Darcy flux along the x-coordinate direction (m/s), q_z = Darcy flux along the z-coordinate direction (m/s), K_x and K_z = Hydraulic conductivity as a function of pore pressure (m/s), and θ = Angle of the geologic down-dip.

The x and z coordinates are parallel and perpendicular to the geologic unit boundaries.

The velocity components at the boundaries, parallel to the geologic-unit boundaries are computed using the pressure gradients computed by the code. This is essentially the same method as is used at all internal mesh points. It is important to note that for computational geometries that are not parallel and perpendicular to the unit boundaries a coordinate rotation must be applied.

3.1.4 Results of Varying Applied Boundary Conditions

Figure 3.3 shows steady-state Darcy velocity vectors for infiltration rates of 0.01mm/yr, 0.1mm/yr, and 1.0 mm/yr. For the purpose of comparison, the Darcy velocity vectors using no-flow side boundaries are given in Figure 3.4. These figures clearly show, as expected, that the no-flow conditions noticeably redirect the flow near the sides of the mesh. The flow near the middle of the mesh is not significantly affected (Figure 3.5). This implies that, if the mesh were made considerably longer, the side boundary conditions may not significantly affect the results in regions adequately removed from these boundaries. Particle-path lines for the 0.01mm/yr and 1.0 mm/yr cases are given in Figures 3.6 and 3.7 for the no-flow and unit-gradient conditions. Comparison of these path lines for the 0.01 mm/yr case show that considerably more relative lateral particle movement is calculated using the unit-gradient boundary conditions. When the infiltration rate is increased to 1.0 mm/yr, little lateral motion is calculated regardless of the boundary condition.

3.1.5 A Demonstration of Unit-Gradient Flows Using NORIA-SP

A second demonstration of the existence of unit-gradient flow will be given using the two-dimensional Yucca Mountain PACE geometry (Barnard and Dockery, 1991) and the NORIA-SP code (Hopkins et al., 1991). Computed results of PACE geometry show that when no-flow side boundary conditions are used, unit-gradient flow exits far from the boundaries only in the layers above the geologic unit of relatively high conductivity ($z < 900$ m). In the region of the high-conductivity material, the no-flow boundary conditions used in NORIA-SP affect the flow at all horizontal locations.

Figure 3.3 Darcy Velocity Vectors, Using Unit-Gradient Boundary Conditions.

Figure 3.4 Darcy Velocity Vectors, Using No-Flow Boundary Conditions.

Figure 3.5 Horizontal Velocity Profiles with $z = 250$ m, 0.01 mm/yr.

Figure 3.6 Particle Path Lines, 0.01 mm/yr.

Figure 3.7 Particle Path Lines, 1.0 mm/yr.

The problem domain considered is the Yucca Mountain configuration used in the PACE exercise (Figure 3.16).

Figure 3.8 Two-Dimensional Yucca Mountain Geometry (Barnard and Dockery, 1991).

The material properties for the nine geologic regions are shown in Table 3.2. Conductivity values are generated using the van Genuchten (1978) formulation.

3.1.6 Boundary Conditions Using NORIA-SP

Steady-state solutions were obtained using an evenly distributed infiltration of 0.01 mm/yr across the top boundary. No-flow boundary conditions were applied at the left and right boundaries. Fixed pressure was applied at the bottom boundary to simulate the water table.

Table 3.2 Material Properties (PACE)

Layer	Porosity Total	K_s (m/s)	α (1/m)	β	S_r	Fractures (1/m ³)
-TM	0.10	2×10^{-11}	0.005	1.9	0.10	5
-TD	0.06	5×10^{-12}	0.004	2.0	0.15	5
-TDL	0.18	2×10^{-12}	0.005	1.52	0.0	3
TML	0.12	2×10^{-11}	0.005	1.52	0.0	5
-TM	0.08	2×10^{-11}	0.005	1.49	0.0	5
-TV	0.04	4.0×10^{-11}	0.005	1.46	0.0	10
-TNV	0.33	3.0×10^{-10}	0.02	4.0	0.20	3
t-TN	0.36	3.0×10^{-12}	0.02	1.2	0.0	3
BT	0.24	7.0×10^{-12}	0.003	1.65	0.06	3
-TN	0.36	2.0×10^{-11}	0.005	1.37	0.0	3

3.1.7 Results Using NORIA-SP

Calculated velocity vectors and path lines for an infiltration rate of 0.01 mm/yr and no-flow side boundary conditions are given in Figures 3.9 and 3.10. Large amounts of lateral flow are generated as a result of the relatively large conductivity of the third geologic unit above the water table (Tpt-TNV). The path lines far from the vertical boundaries ($200 < z < 700$ m) and above this high-conductivity unit are approximately similar (Figure 3.10). This is a characteristic of unit-gradient flow. The velocity components calculated by NORIA-SP are in the vertical and horizontal directions. A coordinate rotation is applied to these velocities to obtain velocity components along the geologic unit interfaces. These velocities are compared to the unit-gradient components calculated using the geologic down-dip angles and the conductivities calculated by NORIA-SP. These results are given in Table 3.3.

Table 3.3 shows results at the vertical midpoint of each geologic unit for $x = 500$ m. Comparing the components of calculated velocities (NORIA-SP) along the geologic units with unit-gradient velocity values based on the NORIA-SP calculated conductivities, we note that the velocities obtained using both procedures compare within a factor of two for all of the geologic units above the high-conductivity region, Tpt-TNV, $z > 900$ m. Thus unit-gradient flow is present in these regions. However, in the vicinity of this high-conductivity region, the unit-gradient velocities are considerably larger than those calculated by NORIA-SP using the no-flow boundary conditions.

Figure 3.9 Velocity Vectors for Infiltration Rate of 0.01 mm/yr.

Figure 3.10 Path Lines for Infiltration Rate of 0.01 mm/yr.

Table 3.3 NORIA-SP Velocities Compared With Unit-Gradient Velocities

Elevation (m) at $x = 500$	U_{NORIA} (m/s)	U_{unit} (m/s)
795	4×10^{-14}	2×10^{-15}
801	7×10^{-11}	3×10^{-8}
811	*	14×10^{-14}
962	2×10^{-14}	3×10^{-14}
1034	8×10^{-14}	4×10^{-14}
1093	5×10^{-14}	7×10^{-14}
1120	10×10^{-14}	12×10^{-14}
U_{unit} is the velocity component calculated using the unit gradient equations. U_{NORIA} is the velocity component in the direction parallel to the geologic unit interfaces * indicates that NORIA calculated flow up the geologic down-dip and is therefore dominated by the no-flow boundaries.		

These results imply that the flow above Tpt-TN, at $x = 500$ m, is approaching the unit-gradient condition and is not significantly affected by the applied no-flow boundary condition. However, in the vicinity of the high-conductivity region, the no-flow boundaries significantly affect the flow.

3.1.8 Implications for Simplified Two-Dimensional Flows

There is an interesting aspect regarding the use of the unit-gradient boundary condition that may be extremely useful for reducing computational times required to approximate two-dimensional flows. That is, the flow of water is constant along each geologic unit if each geologic layer is assumed to be homogeneous. Under these assumptions the fluid particle path lines are similar to each other.

Thus using information regarding the average down-dip angle of each geologic unit, a minor extension may be made to any one-dimensional code which allows the calculation of a single path line. Because of the similar nature of scenarios with these constraints, this path-line configuration is applicable at all horizontal locations along the geologic unit. Significant savings in computer execution times can be realized by approximating two-dimensional flow using this concept. Our current plan is to demonstrate this concept by making the appropriate modifications to the one-dimensional code TOSPAC (Dudley et al., 1988.)

4.0 NONISOTROPIC CONDUCTIVITY EFFECTS

In all numerical calculations of the flow through Yucca Mountain to date, the conductivity parallel and normal to layering have been done using a fixed value for this ratio within a geologic unit. Most calculations have assumed the ratio equal to one. Values as large as 500 were considered by Prindle and Hopkins (1990). Considerable experimental data exist which imply that the conductivity ratio is a strong function of saturation and down-dip angle of the geologic strata (Yeh et al., 1985). LLUVIA-II has been used to predict the nonisotropic nature of equivalent hydraulic conductivities as a function of pore pressure (saturation) and geologic down-dip angle (Eaton and McCord, 1992). The numerical results for layered regions are compared with semi analytical expressions presented by Yeh et al (1985). Good agreement was obtained for conductivity ratios $K_{parallel}/K_{normal}$ for wet and moderately dry conditions.

The use of analytical expressions for these conductivity ratios would simplify the implementation of layered effects in global calculations where it is impractical to include detailed geologic structure.

4.1 Analytical Model

The Yeh et al. (1985) expression for the equivalent effective conductivity of an arbitrarily oriented layered medium is given by

$$K_p = K_m \exp \left(\frac{\sigma_f^2 + \sigma_\alpha^2 \Psi^2}{2 [1 + A \lambda \cos(\beta)]} \right)$$

where K_p is the effective conductivity in the direction parallel to the material layering, and

$$K_n = K_m \exp \left(- \frac{\sigma_f^2 + \sigma_\alpha^2 \Psi^2}{2 [1 + A \lambda \cos(\beta)]} \right)$$

where K_n is the effective conductivity in the direction normal to the layering. The parameters in the above equations are defined by: K_m is the geometric-mean of the saturated conductivity, σ_f^2 is the variance of the $\ln(K_{sat})$ field, σ_α^2 is the variance of the slope of the $\ln(K)$ versus Ψ random field, Ψ is the mean pressure head, A is the mean α (see conductivity equation below for definition of α), λ is the correlation length normal to layering, and β is the dip of the soil layering. The form of unsaturated conductivity used in the Yeh et al. analysis is given by

$$K(\Psi) = K_{sat} e^{-\alpha \Psi}$$

One important aspect of these effective conductivity expressions is that they indicate that the anisotropy of layered media can vary (by orders of magnitude) as the hydraulic state (pore pressure) changes. This behavior could have a significant impact on flow and transport predictions.

4.2 Numerical Approach

The problem geometry and applied boundary conditions used in the LLUVIA-II numerical calculations are given in Figure 4.1. Geologic down-dip is approximated by rotation of the gravitational vector with respect to the z axis. In all calculations, the top boundary (maximum z) was set to a fixed pore pressure. The unit-gradient boundary condition was applied at the remaining three boundaries. A 31- by 31-node grid was used. Steady-state solutions were obtained for pore pressures varying from -2m to -6 m and down-dip angles ranging from 10 degrees to 70 degrees. These represent dry to very dry saturation conditions. Hydraulic conductivities vary by up to four orders of magnitude over this pressure range. For pore pressures of -6m, the conductivity values are as much as 7 orders of magnitude lower than their corresponding values at saturated conditions.

Figure 4.1 Problem Geometry and Numerical Boundary Conditions.

The randomly generated saturated-conductivity fields used in this study were typical of layered soil since considerable soil data are available. Typical values of the quantities required by the Yeh et al. equation are: mean of $\ln K_{sat} = -1.1 \times 10^{+1}$, variance of $\ln K_{sat} = 1.5$, $A =$ mean of $\alpha = 3.0$, and geometric mean $K_{sat} = 1.291 \times 10^{-6}$. The effective conductivity result was calculated using two different methods. In the first, the effective conductivity was calculated by the following equation using the numerically calculated fluxes

$$K_{eff_x} = \frac{flux_x \Delta x}{\Delta P_x}$$

where $flux_x$ = mass flux in the x direction, Δx = width of region, ΔP_x = average change in effective pressure across the region in the x direction, and Δz = height of region. The K_{eff_z} value is calculated by interchanging x and z values in the above equation.

In the second method, effective conductivities were approximated using the calculated conductivities along a single column at $x = x_{max}/2.0$ while assuming one-dimensional series flow in the z-direction and one-dimensional parallel flow in the x-direction. These equations give

$$\frac{\Sigma (\Delta z)}{K_n} = \frac{\Delta z_1}{K_1} + \frac{\Delta z_2}{K_2} + \dots = \Sigma \frac{(\Delta z_i)}{K_i}$$

and

$$K_p = \frac{\Delta z_1 K_1 + \Delta z_2 K_2 + \dots}{\Sigma \Delta z} = \frac{\Sigma (\Delta z_i K_i)}{\Sigma (\Delta z_i)}$$

4.3 Results

Effective conductivity ratios as a function of pore pressure are given for an average of eleven calculations in Figures 4.2 and 4.3 for down-dip angles of 10 degrees and 70 degrees. Each calculation used a different set of randomly generated values of K_{sat} and α data typical of soil material. The three curves represent results from the three calculation methods: (1) mass balance and Darcy's equation, (2) parallel and series analogy and (3) the Yeh et al. analytical relations. Good agreement is obtained for $-4 < \psi < -2$ m. At the pressure level of -4 m, the ratio of saturated conductivity to conductivity is on the order of 10^5 , indicating dry conditions. For the extremely dry conditions, $\psi < -4$ m, agreement between the numerical and analytical results is not good.

Effective conductivity ratios, as a function of the down-dip angle, are given for an average of 11 calculations in Figures 4.4 and 4.5.

These results show that the conductivity ratio is relatively insensitive to the down-dip angle. The series and parallel equations show no dependence on the angle. The LLUVIA-II and Yeh et al. results show reasonable agreement for a pore pressure of -2.0m and poor agreement at a pore pressure of -6.0 m. This disagreement is not critical because the conductivity ratio is reasonably insensitive to the down-dip angle for all cases. Additionally, in most situations the down-dip angle is fairly well known and does not vary appreciably between layers.

In order to make this concept directly applicable to Yucca Mountain, this study should be repeated using the best available Yucca Mountain material characteristics.

Figure 4.2 Conductivity Ratio as a Function of Boundary Pore Pressure for an Average of Eleven Realizations, Down-dip = 10 degrees.

Figure 4.3 Conductivity Ratio as a Function of Pore Pressure for an Average of Eleven Realizations, Down-dip = 70 degrees.

Figure 4.4 Conductivity Ratio as a Function of Down-dip Angle for a Boundary Pore Pressure of -2.0 m.

Figure 4.5 Conductivity Ratio as a Function of Down-dip angle for a Boundary Pore Pressure of -6.0 m.

5.0 SUMMARY OF INFORMATION

Presented in this report are various aspects of numerical modeling that help define the bounds of applicability of using one-dimensional numerical calculations for approximating the water flow through two-dimensional, nonhomogeneous, partially saturated porous regions. This information can be particularly helpful when making abstractions in support of the one-dimensional calculations in a total systems performance analysis study. The results of these studies are itemized below.

1. It is demonstrated that the effect of low-conductivity meter scale obstructions can, in many cases, be accounted for by the use of effective conductivities. In unsaturated flows where the material characteristics are extremely nonlinear, the presence of low-permeability obstructions (Figure 2.2) provide little flow resistance over and above that resulting from the high-conductivity background material (Eaton and Dykhuizen, 1988).
2. For most fracture/matrix material combinations, the presence of unconnected unsaturated fracture arrays (Figure 2.6) generate little resistance to infiltrating water (Martinez et al., 1992).
3. Effective conductivities for materials comprised for meter scale random binary mixtures of high and low conductivities can be represented using the analytical model of Kirkpatrick (Figure 2.8) (Dykhuizen and Eaton, 1991).
4. The unit-gradient boundary concept can be used in conjunction with one-dimensional modeling to effectively approximate two-dimensional flow path lines on a mountain scale in layered geologic media when the media are nonhomogeneous in the direction normal to the layering.
5. The effect of nonisotropic conductivity can possibly be included through the use of analytical expressions which provide $K_{\text{parallel}}/K_{\text{normal}}$ as a function of material saturation and down-dip angle. This was shown to be true for soils on meter-scale problems. It remains to be determined for Yucca Mountain materials (Eaton and McCord, 1992).

In summary, with the incorporation of the above concepts, it is possible to use one-dimensional modeling to approximate two-dimensional flow path lines in layered systems while accounting for, to some extent, low-conductivity obstructions, unsaturated fractures, random mixes of material conductivities, and nonisotropic conductivities. These phenomena are accounted for without explicitly including them in the geometry of the numerical model. Additionally, the effect of lateral flow, resulting from geologic down-dip, can be accounted for by the use of the unit-gradient boundary conditions.

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APPENDIX

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