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DISTRIBUTION OF DOWNWARD FLUX IN UNSATURATED HETEROGENEOUS HYDROGEOLOGIC ENVIRONMENTS

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Abstract

The finite element computer program UNSAT2 was used to investigate the horizontal distribution of unsaturated downward flux in porous tuff as a function of hydrogeologic heterogeneities under two different recharge rates. The distribution of downward flux is important because of its influence on groundwater travel time at a potential geologic repository for high-level radioactive wastes. Hydraulic properties of the Topopah Spring Member of the Paintbrush Tuff Formation at Yucca Mountain, Nevada, as reported by Peters et al. (1984) were selected for use in the eight simulations that were conducted. All simulations were run essentially to steady state. The simulations show that: 1) heterogeneities in an isotropic porous rock matrix will cause downward flux to be distributed nonuniformly; 2) zones in which saturated matrix hydraulic conductivity is less than the downward flux tend to develop positive pressures which may cause flow into fractures if they exist; 3) one-dimensional analysis of vertical flow in the unsaturated zone is insufficient to ensure that fracture flow does not occur even if the true magnitude of vertical flux is known; and 4) the true spatial distribution of hydraulic conductivity above the regional water table must be determined in order to obtain the true spatial distribution of downward flux; this analysis assumed constant spatial and temporal distribution of recharge for each simulation but the difference among simulations verify the fact that changing recharge rates also play a significant role in the distribution of downward flux due to the influence of recharge

rate on the development of positive pore pressures in the otherwise unsaturated rock.

The primary significance of this research is: 1) We have introduced a new method of UNSAT2 time step control that facilitates convergence even in complex, large-scale partially saturated hydrogeologic environments. Previous studies have experienced convergence problems with UNSAT2 under complex hydrogeologic conditions. 2) Nonuniform downward flow should be anticipated in heterogeneous hydrogeologic environments at a heterogeneity scale of 50 meters and a model scale of hundreds of meters, even if recharge is spatially uniform. 3) The impact of heterogeneities in the unsaturated zone on downward flux can now be quantified. 4) Hydrogeologic heterogeneities can create zones of positive pressure and consequent possible fracture flow in the unsaturated zone even when the recharge rate is less than the average saturated hydraulic conductivity, but most certainly when the recharge rate is greater; and 5) This type of study provides a basis for designing hydrogeologic property testing programs and recharge distribution testing programs that are compatible with the design of models that can characterize downward flux.

Introduction

A high level radioactive waste repository at Yucca Mountain, Nevada (Figure 1) is proposed for development in the unsaturated zone of the Topopah Spring Member of the Paintbrush Tuff Formation (Table 1 and Figure 2). A proposed conceptual model for water flow through this portion of Yucca Mountain as presented by Montazer and Wilson (1984), suggests that a portion of the natural downward flux above the Topopah

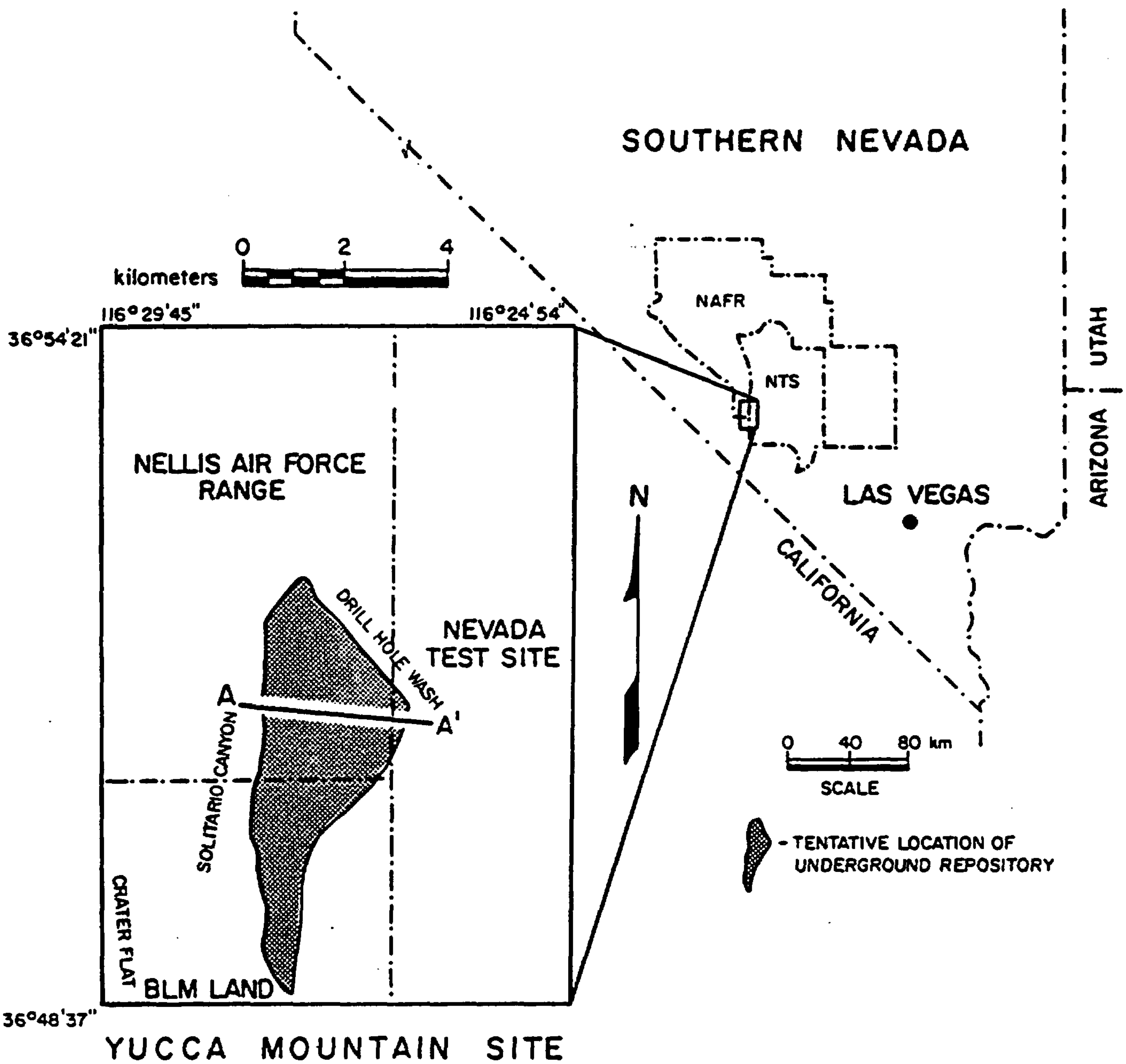

Figure 1. Location of the site for a possible radioactive-waste repository at Yucca Mountain in southern Nevada; A-A' shows the location of the geologic cross section in figure 2 (modified after Sinnock et al., 1984).

Table 1. Summary description of hydrostratigraphic units extending from the alluvium through the Bullfrog Member of the Crater Flat Tuff at Yucca Mountain (Montazer and Wilson, 1984, Table 1).

[fractures/m³, fractures per cubic meter; Std. dev., standard
NP, nonwelded to partially welded;

Stratigraphic unit		Tuff lithology	Hydrogeologic unit	Approximate range of thickness[1] (meters)	Fracture density[2] (fractures/m³)	Generalized permeability[3]	
						Matrix	Fracture
Alluvium		----	Alluvium	0-30	----	Generally substantial	----
Paintbrush Tuff	Tiva Canyon Member	MD	Tiva Canyon welded unit	0-150	10-20	Negligible	Substantial
Paintbrush Tuff	Yucca Mountain Member; Pah Canyon Member	NP, B	Paintbrush nonwelded unit	20-100	1	Moderate	Small?
Paintbrush Tuff	Topopah Spring Member	MD	Topopah Spring welded unit	290-360	8-40	Negligible	Substantial
Tuffaceous beds of Calico Hills		NP, B (V) (D) (in part zeolitic)	Calico Hills nonwelded unit	100-400	2-3	(V) Substantial (D) Small to negligible	Small?
Crater Flat Tuff	Prow Pass Member						
Crater Flat Tuff	Bullfrog Member	MD, NP, B (undifferentiated)	Water table; Saturated zone; Crater Flat unit	0-200	8-25	Variable	Variable

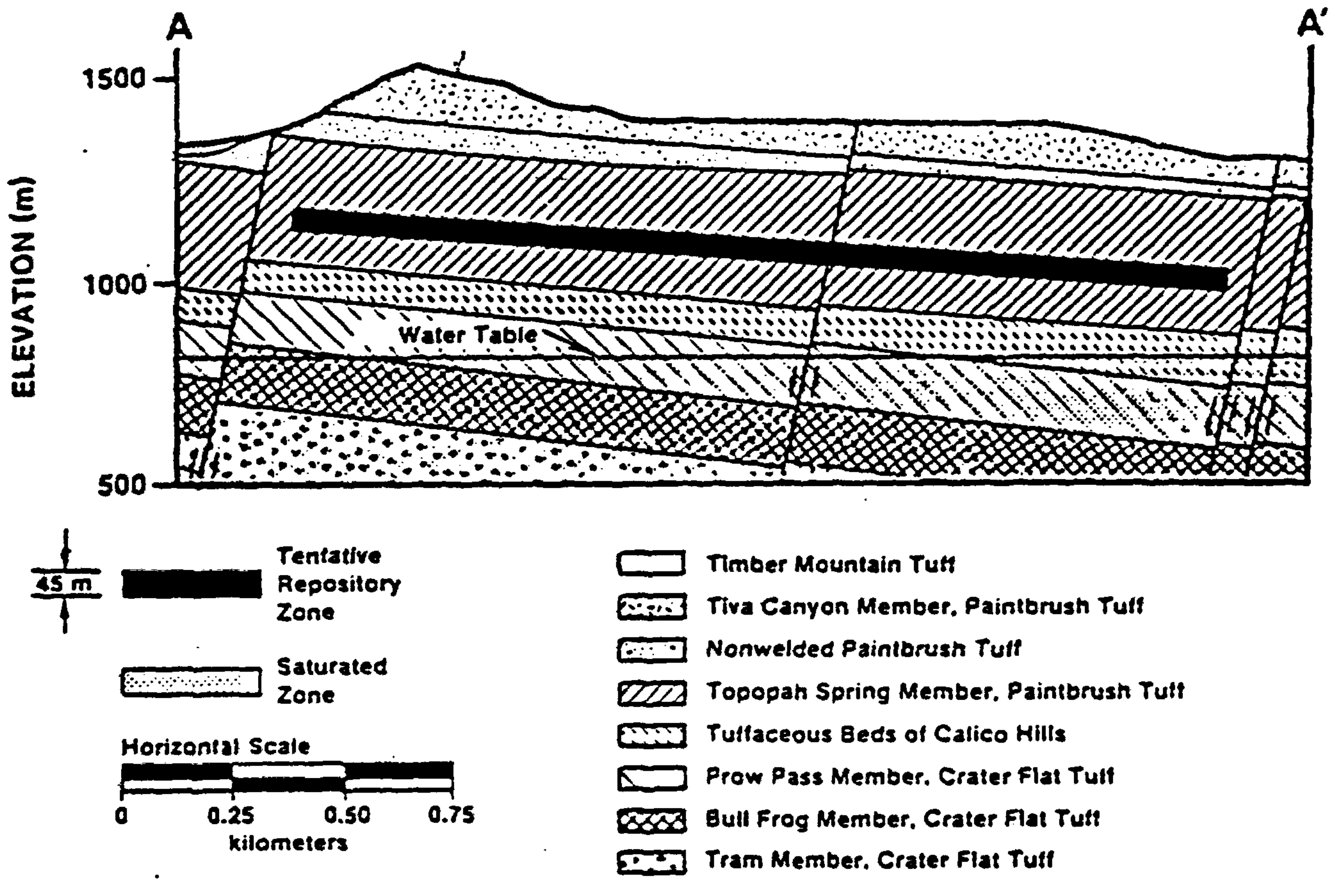

Figure 2. Geologic cross section of Yucca Mountain showing the tentative depth of a possible repository in the Topopah Spring Member of the Paintbrush Tuff (Sinnock et al., 1984).

Spring Member is diverted around the site by "capillary barriers." Montazer and Wilson assume that this diverted flux may flow laterally under the influence of a "capillary barrier" toward structural features at the edge of the repository but they provide no supportive information such as modeling. Peters and Klavetter (1988) present a method of viewing such a fractured geologic environment as a continuum. Sinnock et al. (1986) assume on the other hand that the downward flux is distributed uniformly in the horizontal plane. The evaluation of that important assumption is a primary goal of this paper.

The unsaturated model for flow in the Topopah Spring Member used in this study requires neither "capillary barriers," nor uniform distribution of downward flux. This conceptual model includes spatially varying hydraulic properties (heterogeneities) of the Topopah Spring tuff and the consequent variations in horizontal distribution of downward flux. Some of these heterogeneities may be envisioned as structural features such as faults. Others may be produced by random (or nonrandom) cooling processes that are not yet understood. All hydrogeologic heterogeneities discussed herein as possible structural features are treated as equivalent porous media. That is, the model does not simulate flow in discrete fractures.

Objectives of Study

The objectives of this unsaturated flow modeling study are as follows:

1. Quantify the effects that heterogeneous hydraulic properties have on the horizontal distribution of downward flux under unsaturated conditions in porous rock.

2. Quantify the effect of such heterogeneities on the pore water pressure within the porous rock matrix. Wherever the pressures are positive (greater than atmospheric), flow may occur in fractures or fracture zones, thereby greatly reducing ground water travel time to the saturated zone.
3. Present a conceptual framework for determining what kinds and amounts of data must be collected in hydrogeologic testing program that focus on unsaturated flow at Yucca Mountain.

Methodology

In partially saturated soil and rock the coefficient of saturated hydraulic conductivity in Darcy's Law is not a constant. It can be expressed as a function either of water content (degree of saturation) or of water tension (capillary pressure). The terms water tension, capillary pressure, matric suction or negative pressure in most cases are used synonymously. They all imply that the pressure on the water is less than atmospheric pressure. Negative pressures on the water in the unsaturated zone will cause the water to occur only in small pores; air will be present in the larger pores and in large aperture fractures.

Most computer models of the unsaturated flow process are based on the Richards equation, which can be derived by incorporating the Darcy equation for unsaturated flow into the equation for conservation of mass. The program UNSAT2 (Neuman, et al., 1974; Bloomsburg and Wells, 1978; and Davis and Neuman, 1983), which is used in this study, requires data on relative hydraulic conductivity as a function of water tension. The appropriate relative hydraulic conductivity versus water tension relationship was derived from experimental data presented in Peters et al. (1984) using the methods of Mualem (1976) and van Genuchten (1978). The saturated hydraulic conductivity is the maximum possible value of hydraulic conductivity.

During steady state downward flow under unsaturated conditions with homogeneous hydraulic conductivity, the water pressure will be negative and the magnitude of the unsaturated hydraulic conductivity will be the same as the existing flux value (i.e., h/ z = 1). Lateral variations in hydraulic properties can induce nonuniform downward fluxes as well as significant horizontal flow. The quantification of the spatial variations in downward fluxes calculated in our simulations is shown as graphs in Figures 3 through 10.

A synthesized vertical section of the Topopah Spring Member of the Paintbrush Tuff Formation was selected for modeling in this study. This section has dimensions of 700 meters (horizontal) by 300 meters (vertical). The finite element mesh used in UNSAT2 consists of 126 rectangular elements and 150 node points. All simulations were run until steady state was approached as demonstrated by the outflow rate approaching the inflow rate. In simulation 2, the difference between outflow and inflow is 5.7 percent; the difference is less than 2 percent in all other simulations.

The initial negative pressure condition throughout the mesh was set at 1.4 meters of water, which corresponds to a saturation level of 99.9 percent. In accordance with Montazer and Wilson (1984) a constant recharge boundary of 0.5 mm/yr is prescribed on the upper boundary except in simulation 7 in which the recharge rate is 0.6 mm/yr. The sides of the mesh are no-flow boundaries; the lower edge of the mesh is the water table (atmospheric pressure) in all cases. The flow properties of the tuff were obtained from Peters et al. (1984). The values used are derived from laboratory analysis of core hole samples obtained from borehole G-4; however, samples from borehole GU-3 have comparable properties. Relative permeability vs. pressure data were obtained from Peters et al. (1984).

In the first simulation, the entire flow region is homogeneous and isotropic with a saturated hydraulic conductivity of 0.601 mm/yr. This value was obtained by Peters et al. (1984) by testing core sample G4-5; it is approximately the geometric average of the measured values of saturated hydraulic conductivity for the Topopah Spring Member. The unsaturated permeability and soil moisture values are those reported by Peters et al. (1984) for this sample of rock. This porous medium is referred to herein as "average conductivity" rock.

The remaining simulations have this average conductivity of 0.601 mm/yr assigned to the majority of the isotropic elements in the mesh. However, in cases 2 through 8 various arrangements of elements are assigned either a high conductivity (1.26 mm/yr) or low conductivity (0.211 mm/yr). These two values are referred to herein as "high conductivity" and "low conductivity" rock. The saturated conductivities reported by Peters et al. (1984) for samples from the two boreholes (G4 and GU-3) range from 0.047 to 14.19 mm/yr; therefore, the values used herein do not reflect the full range of values known at this time. We elected subjectively not to use the extreme values on either end of the spectrum.

Detailed hydrogeologic heterogeneity has not been mapped in the Topopah spring Member, but several faults have been mapped. The volcanic tuff in the Topopah Spring Member consists of a compound cooling unit composed of as many as four separate ash-flow sheets (U.S. DOE, 1986); consequently even without structures such as faults the Topopah Spring Member could display wide variations in all hydraulic properties because of variations in flow conditions at the time of deposition and because of variations in the rate of cooling of the ash.

A table of random numbers was used to select the locations of the high and low conductivity elements in Cases 6, 7 and 8; even so, the resulting distribution of hydraulic properties among the elements shows some spatial correlation (i.e., some of the high or low conductivity elements are clustered). Detailed characterization is needed to identify the actual correlation scale.

The scale of variation of flow properties will not be known until the Topopah Spring Member is characterized in great detail. The scale of variation of hydrogeologic properties in our simulations is on the order of 50 meters (the width of each element). Diagonal, vertical and "random" arrangements of the low and high conductivity elements were used in the various simulations. A more detailed description of the various simulations conducted in this study follows.

Case 1

In Case 1, the hydraulic properties of each element within the modeled region were set equal to the properties measured for sample G4-5 (K=0.601 mm/yr) of Peters et al. (1984). The constant uniform flux at the upper surface was set at 0.5 mm/yr. The simulation was run for 1,000 years before essentially steady state was attained. The results of this simulation are shown in Figure 3. At steady state the outflow is distributed uniformly across the lower edge of the region modeled. Under these conditions all simulated nodal pressures are negative.

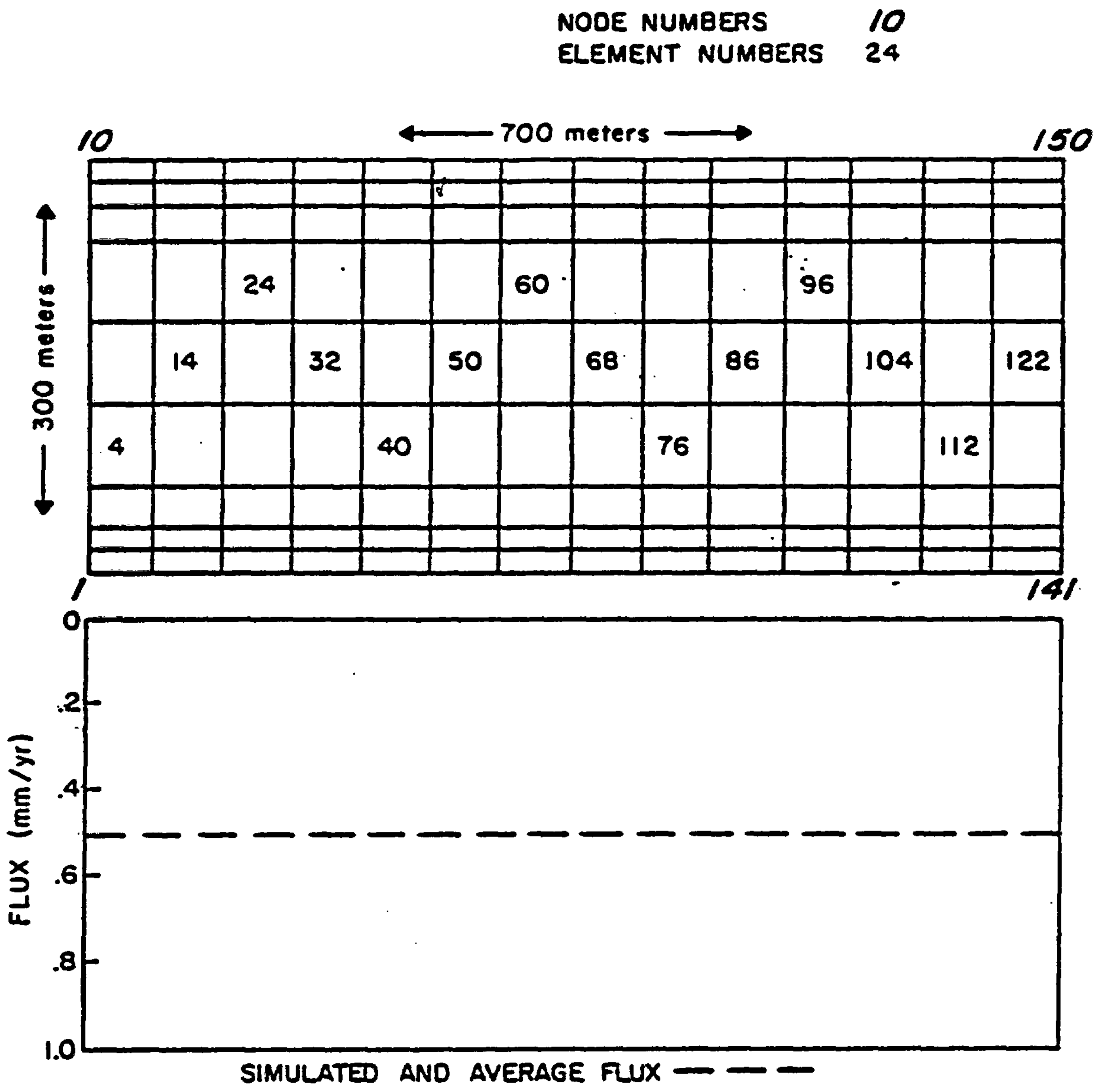

Figure 3. Finite element mesh and computed fluxes at bottom of mesh for Case 1; homogeneous distribution of hydraulic conductivity. All nodal pressures computed by the model are negative.

Case 2

In Case 2, one column of elements representing high hydraulic conductivity rock (K=1.26 mm/yr from Peters et al., 1984) was placed in the center of the mesh. This column can be viewed as analogous to a vertical, relatively permeable fault zone like that shown near the middle of cross sections A-A', (Figure 2). A hydraulic conductivity of 0.601 mm/yr was assigned to the other elements. The constant uniform recharge rate at the upper surface was set at 0.5 mm/yr. The simulation was run for 1,200 years before steady state was attained. The results are quantified in Figure 4. The flux is not distributed uniformly. Specifically about 15 percent of the flow occurs through the high conductivity column, which comprises only 7 percent of the outflow boundary. Adjacent to the center column of elements computed fluxes are below the average value at distances as great as 300 meters from the column. The flux varied spatially from 0.42 mm/yr to 0.77 mm/yr throughout the region modeled; all nodal pressures computed by the model are negative. One intuitively might have expected the general aspects of this result but without such a modeling effort the impact of the fault could not have been quantified.

Case 3

In Case 3 hydrogeologic properties of three columns of elements (Figure 5) were set equal to the properties measured for sample G4-2 (K=1.26 mm/yr; Peters et al., 1984). These columns are located at the left side, the right side, and the middle of the modeled region. These columns could be viewed as three relatively permeable vertical fault zones cutting the Topopah Spring Member. The simulation was run for 1,500 years before steady state was reached. The results are quantified

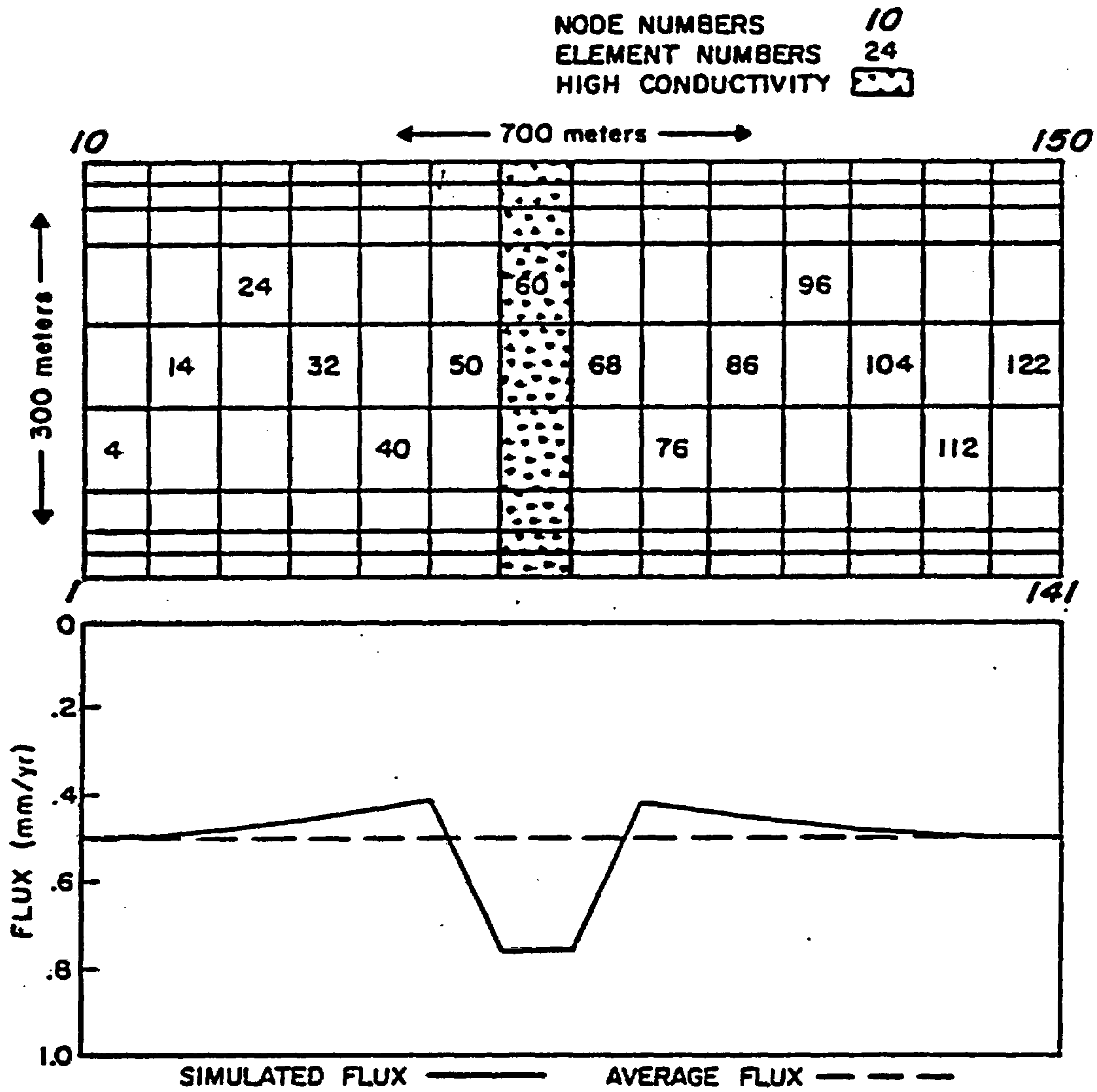

Figure 4. Finite element mesh and computed fluxes at bottom of mesh for Case 2. All nodal pressures computed by the model are negative.

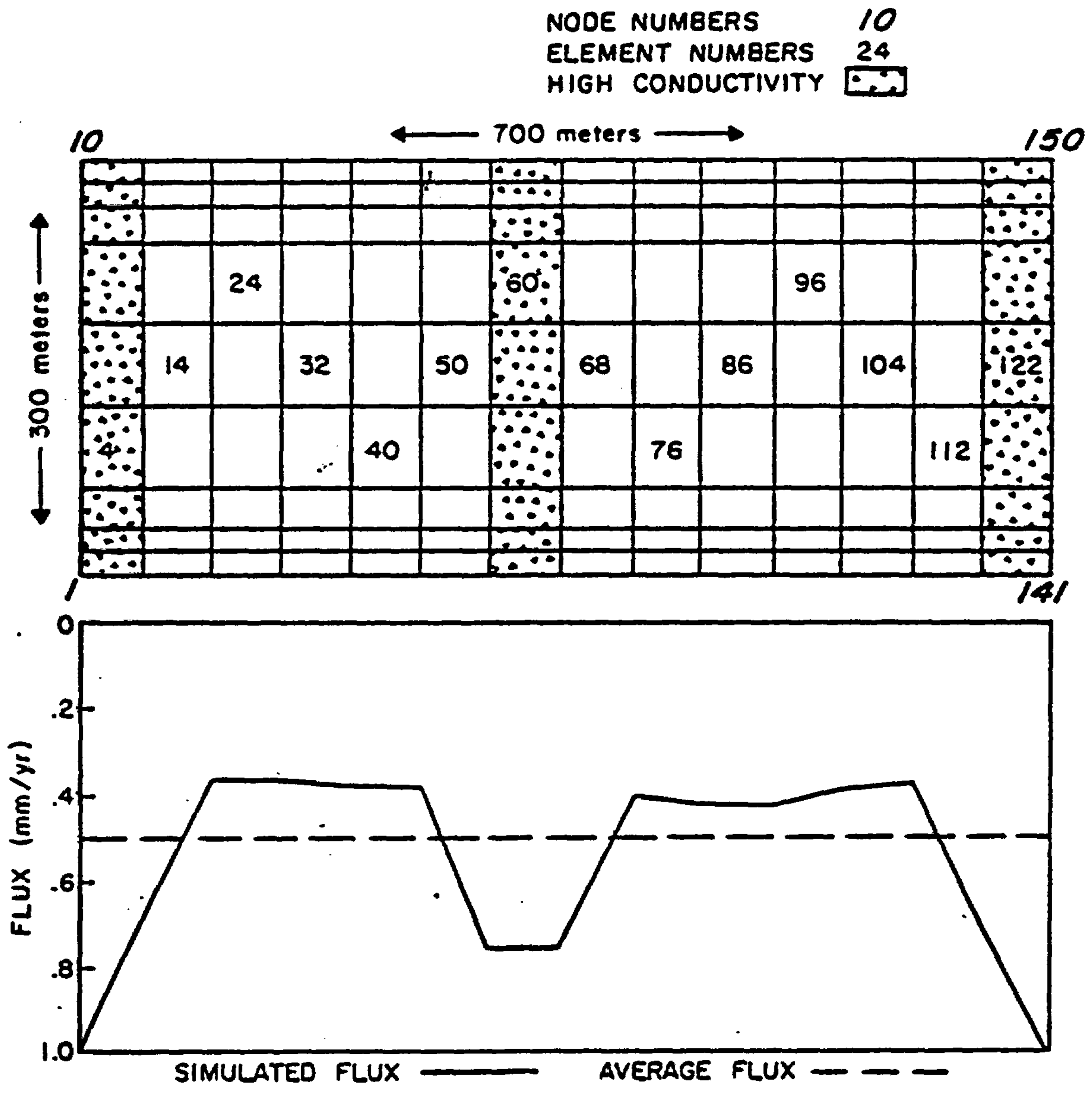

Figure 5. Finite element mesh and computed fluxes at bottom of mesh for Case 3. All nodal pressures computed by the model are negative.

in Figure 5. The flux through the high conductivity columns is about twice the average flux. About 42 percent of the flow moved through 21 percent of the area. The flux values vary spatially from 0.36 mm/yr to 1 mm/yr throughout the region modeled; all nodal pressures computed by the model continue to be negative.

Case 4

This simulation was designed to test the effects of flow through a medium with columns of rock that display less than average hydraulic conductivity (K=0.211 mm/yr). This value of hydraulic conductivity was obtained for sample G4-1F of Peters et al. (1984). The left, right, and center columns of elements inserted into the model of Case 4 represent rock with this average value of conductivity (Figure 6). These three columns of relatively low hydraulic conductivity elements could be viewed as three fault zones that contain relatively low unsaturated hydraulic conductivity gouge (e.g., Figure 2). The simulation was run for 1,000 years prior to reaching steady state. The results are quantified in Figure 6. The flux values vary spatially from 0.21 mm/yr to 0.6 mm/yr throughout the region modeled. Most of the elements that contain the lower conductivity rock, as well as many of the neighboring node points, developed positive pressures by the time steady state was reached. The areas of positive pressure also are shown in Figure 6. This result would not have been expected.

Case 5

Two relatively high hydraulic conductivity (K=1.26 mm/yr) inclined columns of elements were used in this simulation. These relatively high hydraulic conductivity elements were arranged diagonally in the otherwise

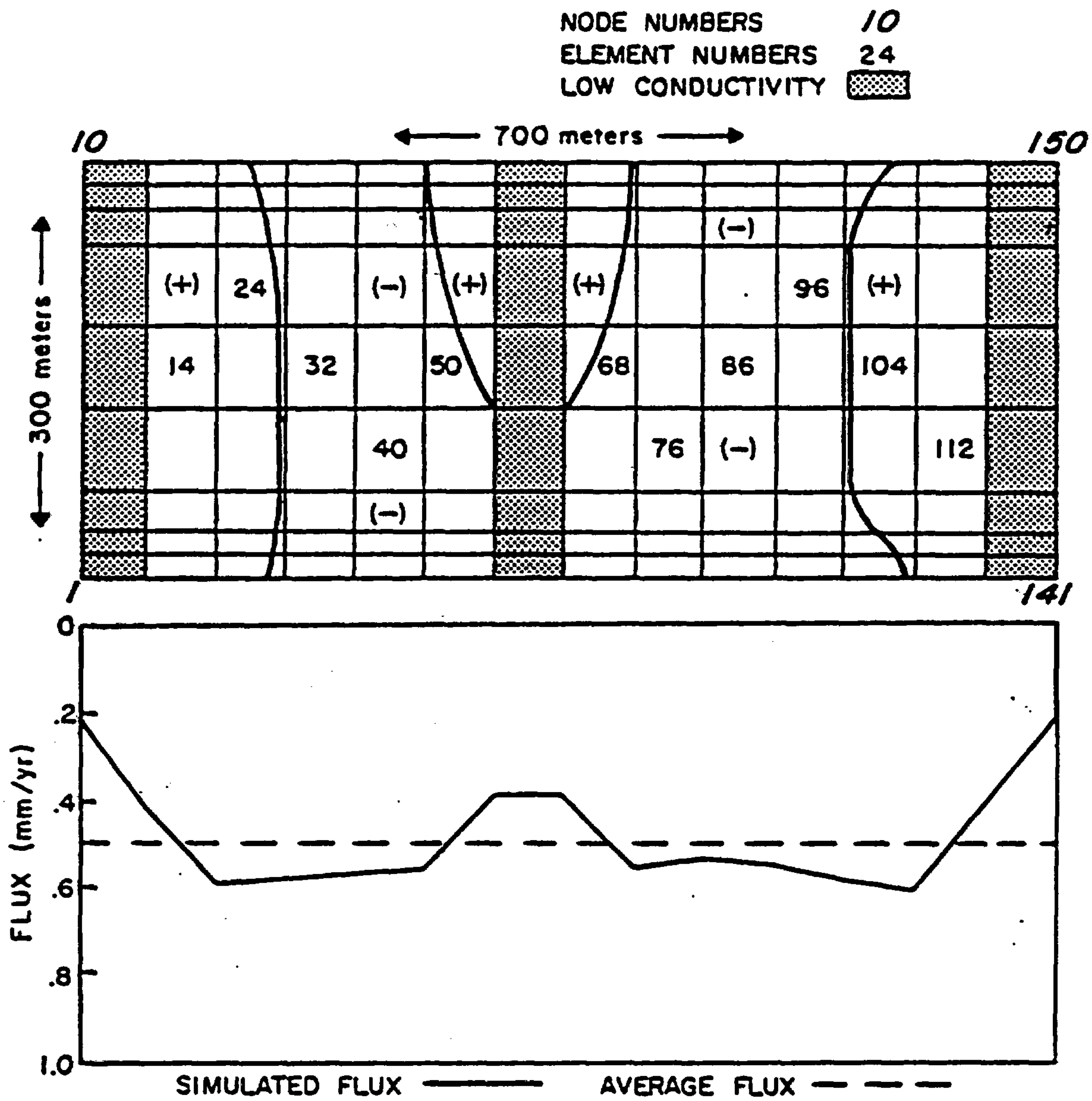

Figure 6. Finite element mesh and computed fluxes at bottom of mesh for Case 4. The contour line on the finite element mesh is the zero atmospheric contour that separates regions of positive (+) pressures from regions of negative (-) pressures as computed by the model.

average hydraulic conductivity matrix. The relatively permeable inclined columns begin at each of the upper corners of the region modeled and dip to the center of the base of the region modeled as shown in Figure 7. This configuration is analogous to two relatively permeable fault zones that dip and intersect. The simulation was run for 1,500 years prior to reaching steady state. The results are quantified in Figure 7. The flux is greatest along the aforementioned diagonal, high conductivity elements. The net result is greater flux at the center of the discharge face. The flux varies spatially from 0.43 mm/yr to 0.58 mm/yr throughout the region modeled. Two nodes show positive pressures; however, these are the result of round off errors in the program and are only slightly positive. The pressures at the remainder of the nodes are negative.

Case 6

In this case, a high hydraulic conductivity value of 1.26 mm/yr (Peters et al., 1984) was assigned to 22 elements throughout the flow region as shown in Figure 8. These elements were selected using a random number table. The remaining elements were assigned a hydraulic conductivity value of 0.601 mm/yr. Geologically this case could reflect differential depositional patterns or variable cooling rates near the surfaces of strata that are distributed throughout the formation. Flow was simulated for 1,500 years prior to achieving steady state conditions. In this particular case, even though the locations of the rock represented by the elements with high hydraulic conductivity were generated randomly, the high hydraulic conductivity elements tend to group at the left and right sides of the region. This grouping produces the nonuniform distribution of downward flux shown in Figure 8. The outflow varies spatially from 0.44 mm/yr to 0.61 mm/yr among nodes.

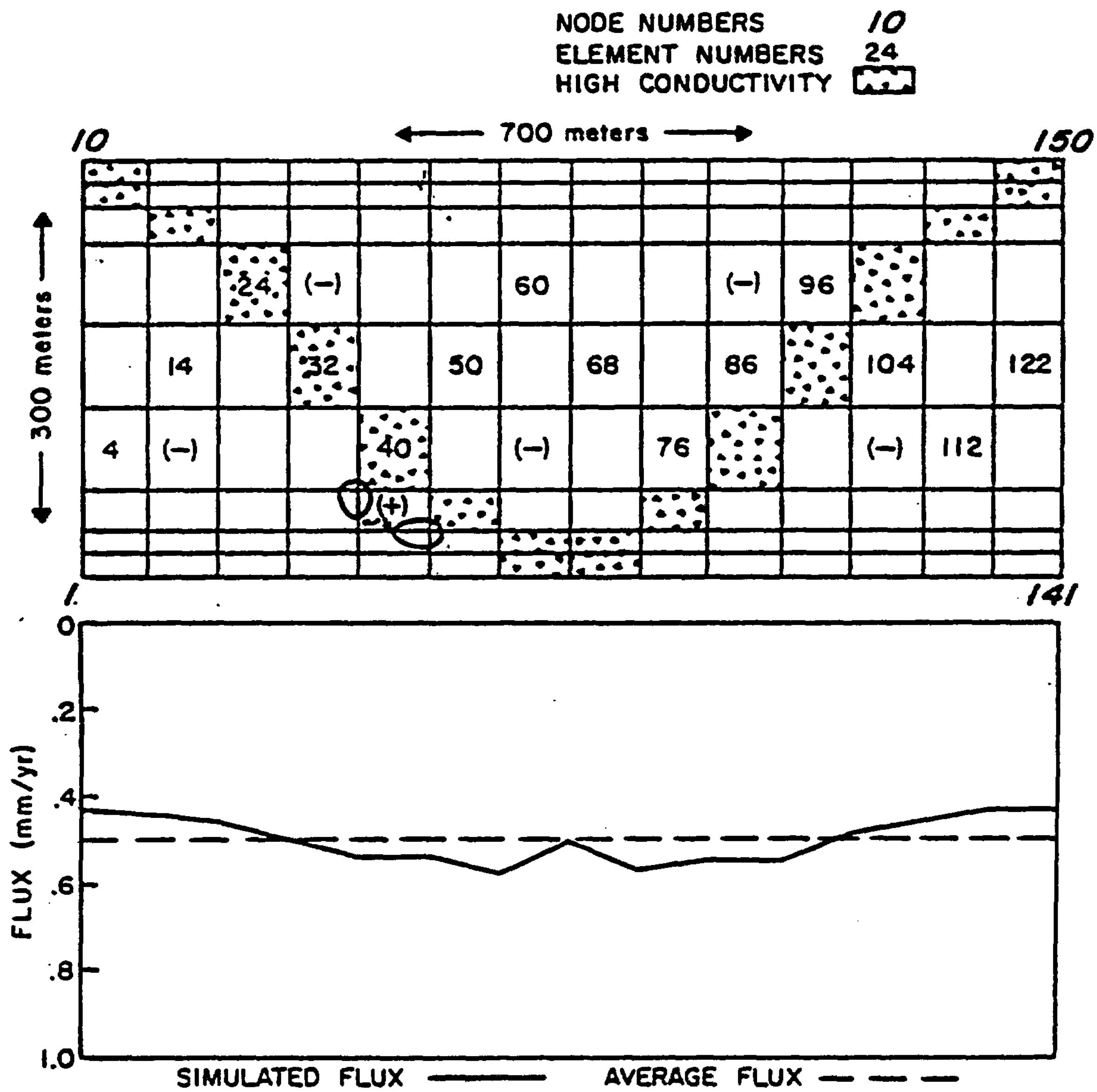

Figure 7. Finite element mesh and computed fluxes at bottom of mesh for Case 5. The contour line on the finite element mesh is the zero atmospheric contour that separates regions of positive (+) pressures from regions of negative (-) pressures as computed by the model.

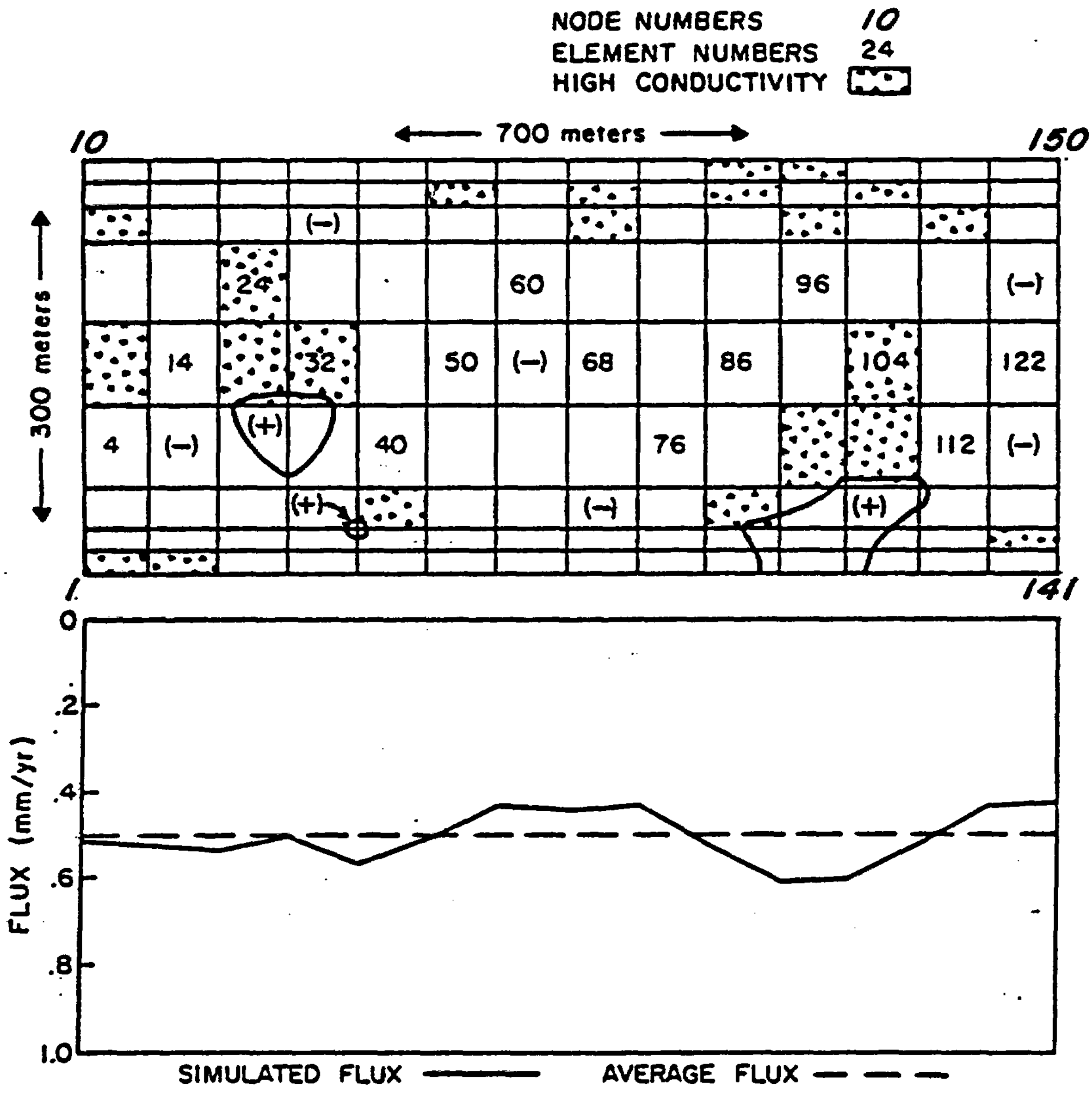

Figure 8. Finite element mesh and computed fluxes at bottom of mesh for Case 6. The contour line on the finite element mesh is the zero atmospheric contour that separates regions of positive (+) pressures from regions of negative (-) pressures as computed by the model.

Nodes with positive pressures also are shown in Figure 8. This simulation demonstrates that even with a hydraulic conductivity field selected randomly, the distribution of vertical flux may not be uniform and that positive pressures can develop.

Case 7

Simulation number 7 employed the same arrangement of hydraulic conductivity as the simulation for Case 6 but with a recharge rate of 0.6 mm/yr at the upper surface. The simulation was run for 1,500 years prior to reaching steady state. The results are quantified in Figure 9. The higher recharge rate produced fully saturated conditions in many of the average hydraulic conductivity elements (K=0.601 mm/yr). The regions which developed positive pressures are shown in Figure 9. Pressures as great as 7.6 meters of water developed at some node points. The flux varies spatially from 0.53 mm/yr to 0.69 mm/yr throughout the region modeled. The distribution of flux is very similar to that of Case 6, even though about one-third of the node points developed positive pressures.

Case 8

In Case 8 the same random distribution of hydraulic conductivities as discussed in Case 6 was used. However, low hydraulic conductivity (K=0.211 mm/yr) values (rather than high conductivity values) were assigned to the randomly selected elements. The input flux was set at 0.5 mm/yr, as in Case 6. The results are quantified in Figure 10. The flux varies spatially from 0.4 mm/yr to 0.61 mm/yr throughout the region modeled. The regions with positive pressures also are identified in Figure 10. This simulation shows that the existence of low conductivity

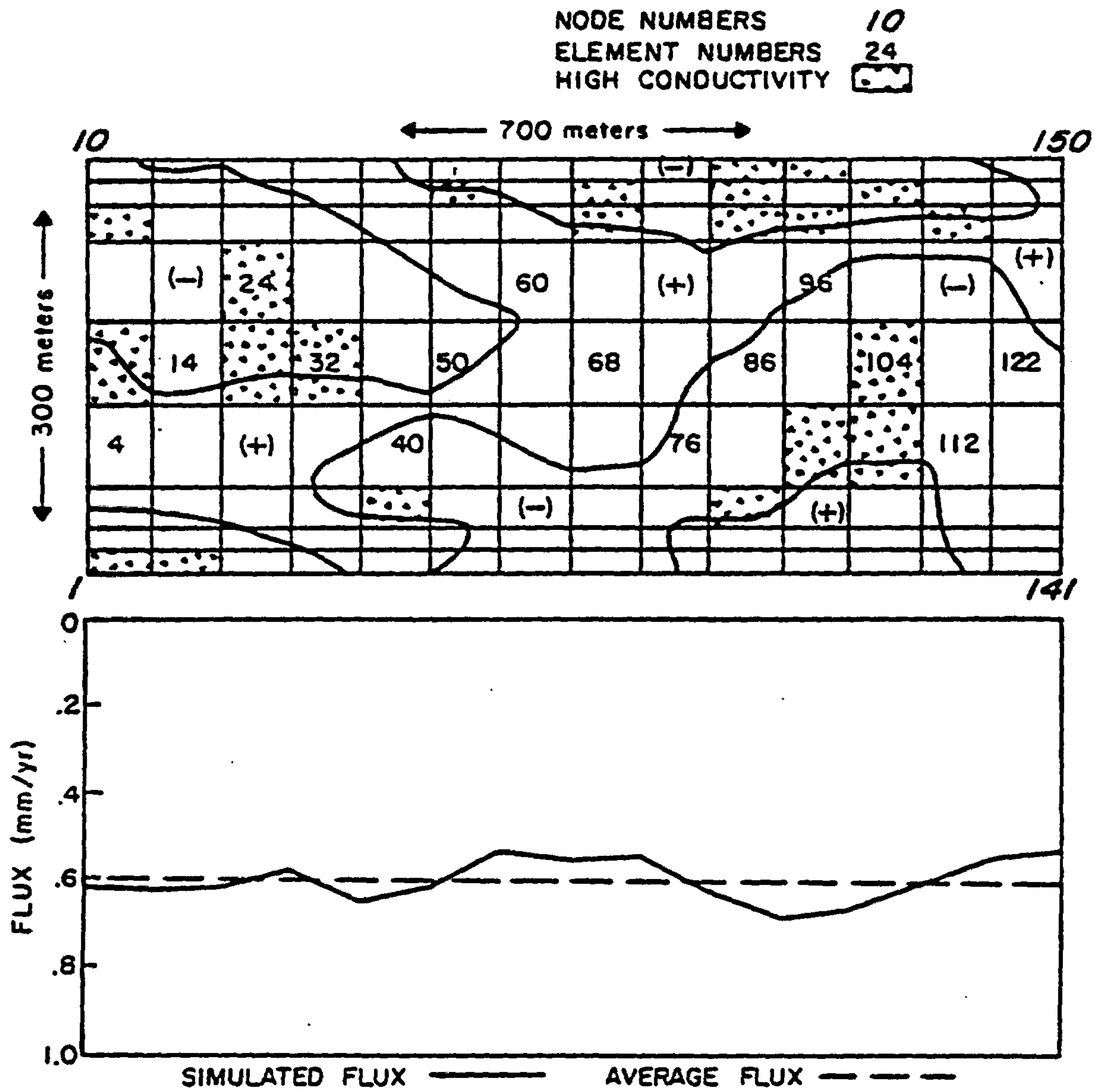

Figure 9. Finite element mesh and computed fluxes at bottom of mesh for Case 7. The contour line on the finite element mesh is the zero atmospheric contour that separates regions of positive (+) pressures from regions of negative (-) pressures as computed by the model.

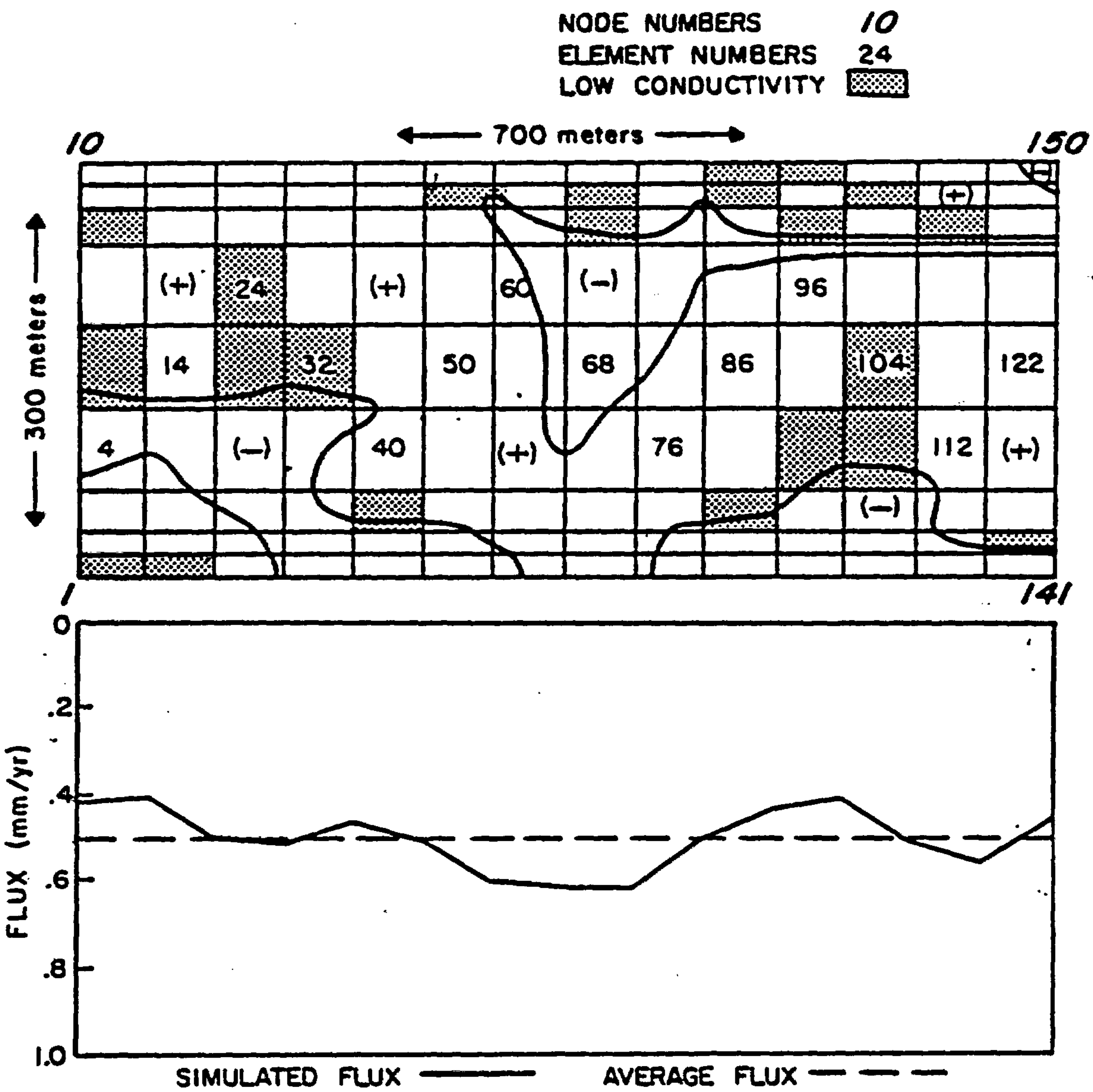

Figure 10. Finite element mesh and computed fluxes at bottom of mesh for Case 8. The contour line on the finite element mesh is the zero atmospheric contour that separates regions of positive (+) pressures from regions of negative (-) pressures as computed by the model.

(K=0.201 mm/yr) rock in 22 out of 126 elements produces positive pressures in well over half of the region modeled at a recharge rate of 0.5 mm/yr.

Discussion of Results

Vertical fault zones or other geologic features of higher or lower hydraulic conductivity rock of the size used in simulations 2 and 3 (50 meters) have not been mapped in Yucca Mountain. However, the range of conductivity values used in the study is less than the range that has been measured within Yucca Mountain by Peters et al. (1984). Consequently our simulations may not reflect the maximum possible effects of heterogeneities within the Topopah Spring Member.

The results of the first three simulations show that water moves laterally because of pressure gradients induced by vertically oriented high-permeability heterogeneities in the rock. The result is a nonuniform horizontal distribution of downward flux. Flux is greater through the elements of relatively high conductivity than through the elements of average conductivity; areas of positive pressure do not develop with the first three cases with a recharge rate of 0.5 mm/yr. Pressures become greater than atmospheric pressure (positive) if the flux is greater than the saturated conductivity of the low conductivity elements (Case 4); as a portion of the rock becomes saturated, water moves toward adjacent areas. In Case 4, the greater flux in the elements of average conductivity also causes positive pressures to develop in the average conductivity material (Figure 4).

Cases 5 through 8 are perhaps less hypothetical than the first four cases because the latter reflect vertical variations in hydraulic properties in addition to horizontal variations. The results of simulations 5 through 8 illustrate that variability of hydraulic conductivity in the vertical direction often will produce positive pressures in the lower conductivity rock where it underlies higher conductivity rock. Positive pressures occur because the high conductivity rock at a higher elevation will carry more flux than the lower conductivity rock. When this greater flux moves downward into the lower conductivity rock it causes complete saturation and positive pressures. These positive pressures then must dissipate horizontally as the flux is redistributed in the horizontal plane. This situation is shown in Figures 6, 8, 9 and 10.

Positive fluid pressures are important because all pores (including fractures or open fault zones) will accept flow under such conditions. Consequently, much shorter travel times through the profile may occur compared to the case where only matrix flow occurs. Our study shows that it will be necessary to consider the heterogeneities of rock properties in order to predict the distribution of downward flux. It also will be necessary to delineate the scale of heterogeneities in order to select a mesh size for simulation. If this procedure is not followed, simulations may not account for regions of positive pressure and fracture flow.

The following factors should be emphasized with respect to the results of this series of simulations.

1) Only matrix flow of liquid water is simulated; flow through discrete fractures, vapor flow, and heat flow are not included specifically. If the vertical columns of elements discussed herein

are envisioned to be fault zones they must be filled with gouge or other porous rock. Discrete fracture flow is not treated in the models discussed in this paper. Faults that display open fractures will not function hydraulically like the heterogeneities described herein (see Wang and Narasimhan, 1984).

2) Only flow in the Topopah Spring Member of the Paintbrush Tuff Formation is considered, as analyzed by Montazer and Wilson (1984), Wilson (1985) and Peters et al. (1984). The bedding of the rocks is assumed to be horizontal. The true dip (see Figure 2) of the Topopah Spring Member was not simulated.

3) Three of the eight conditions simulated are analogous to fault or fracture zones that contain either relatively higher or lower permeability. Hydraulic conditions simulated around these zones are realistic if any fracture flow that may be present can be treated as an equivalent porous medium.

4) We have assumed uniform spatial distribution of recharge in accordance with Montazer and Wilson (1984). In reality the recharge rate will vary with permeability. However the recharge flux should redistribute according to permeability soon after it enters the Topopah Spring Member. Investigation of the true effect of nonuniform recharge is left to future work.

5) We have simulated the bottom of the Topopah Spring Member as the water table. The only alternative is to input measured pressures at the bottom of the Topopah Spring Member. The insertion of real pressures is left to future work after the appropriate pressures have been measured.

Conclusions

These computer simulations using UNSAT2 justify the following conclusions.

1) Heterogeneities in a porous rock matrix will cause downward flux in the unsaturated zone to be distributed nonuniformly in the horizontal plane.

2) Positive pressures tend to develop in some zones in which the saturated hydraulic conductivity of the matrix is less than the downward flux (see for example Figure 6). This condition, where it occurs, will produce preferential flow paths. Flow into fractures may occur at such locations if discrete, open fractures intercept these zones of positive pressures; however, we did not simulate such flow. Continuous fracture flow through the entire unit, if it occurs, could reduce the ground water travel time to the accessible environment considerably. Flow through fractures could also reduce some pressures to atmospheric.

3) The effect of heterogeneities on flow in the unsaturated zone cannot be predicted intuitively. Quantification by a modeling process such as the one used herein is required.

4) A one-dimensional analysis of flow in the Topopah Spring Member of the Paintbrush Tuff Formation within Yucca Mountain is insufficient to ensure that nonuniform downward flux or fracture flow do not occur.

5) If the spatial average downward flux is 0.5 mm/yr as expressed by Montazer and Wilson (1984) (or greater) and if the permeability values presented by Peters et al. (1984) are representative, then regions of positive pressure probably exist in the tuffs of Yucca

Mountain. If the values are valid, positive pressures will develop wherever the saturated hydraulic conductivity is less than 0.5 mm/yr. This result illustrates the necessity for measuring recharge rates and hydrogeologic properties at the appropriate scale.

6) The results of the simulations presented herein illustrate the necessity for delineating in detail the spatial distribution of hydraulic conductivity in the unsaturated zone within Yucca Mountain. The results quantified herein illustrate that modeling of the downward flux should be conducted in at least two dimensions. Delineation of populations of hydraulic conductivity values according to spatial distribution may be feasible using the statistical procedure discussed by Steinhorst and Williams (1985).

7) Documentation of the absence of regions of positive pressure would constitute the best evidence in support of the concept of exclusive matrix flow rather than a combination of matrix flow and fracture flow in the Topopah Spring Member of the Paintbrush Tuff Formation.

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