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PRELIMINARY ANALYSIS OF THREE-DIMENSIONAL MOISTURE FLOW WITHIN YUCCA MOUNTAIN, NEVADA

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March 1994

This work was prepared under U.S. Department of Energy Contract No. DE-AC03-76SF00098, and DE-A108-78ET44802 administered by the Nevada Operations Office in cooperation with the U.S. Geological Survey, Denver.

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ABSTRACT

The continuous development of the three-dimensional site-scale model of Yucca Mountain Nevada is described. Three-dimensional moisture flow simulations are conducted, that show how the stratigraphic units and fault offsets and properties at Yucca Mountain create complex three-dimensional flow patterns. Even for areally uniform infiltration rates, these geological complexities result in large lateral flow components and often concentrated flow into the water table. When the major faults are assumed to act as capillary barriers, moisture buildup occurs close to the faults. Conversely, when the faults are assumed to readily absorb water and allow for vertical migration, lateral flow is greatly enhanced and relatively dry conditions are found in the rock matrix adjacent to the faults. These results suggest that careful observations of saturations and rock matrix conditions in rock masses near major faults may help determine the hydrological characteristics of the faults. The site-scale model has been used to predict conditions in wells UZ-16 and other wells, in order to investigate the predictive capabilities of the model. Gas flow and the geothermal gradient have been incorporated into the model.

INTRODUCTION

The three-dimensional site-scale numerical model of the unsaturated zone at Yucca Mountain is under continuous development and calibration through a collaborative effort between Lawrence Berkeley Laboratory (LBL) and the United States Geological Survey (USGS). The site-scale model covers an area of about 30 km^2 and is bounded by major fault zones to the west (Solitario Canyon Fault), east (Bow Ridge Fault) and perhaps to the north by an unconfirmed fault (Yucca Wash Fault). The model consists of about 5,000 grid blocks (elements) with nearly 20,000 connections between them; the grid was designed to represent the most prevalent geological and hydro-geological features of the site including major faults, and layering and bedding of the hydro-geological units. Further information about the three-dimensional site-scale model is given by Wittwer et al. (1992, 1993, 1994).[1,2,3]

Previous large scale model studies of natural conditions at Yucca Mountain include those of Rulon et al. (1986),[4] Wang and Narasimhan (1987),[5] Osner and Nieland (1990),[6] Rockhold et al. (1990),[7] Birdsell et al. (1990),[8] Wittwer et al. (1992, 1993, 1994),[1,2,3] and Tsang et al. (1993).[9] Two-dimensional models by Rulon et al,[4] Wang and Narasimhan,[5] and Osner and Nieland,[6] showed the potential for significant lateral flow in the bedded units due to dipping of the stratigraphic units, and that the degree of lateral flow depends to a large degree on the hydrological characteristics of the major faults intersecting these units. Tsang et al.[9] and Wittwer et al.[3] performed two-dimensional simulations to show how important the fault characteristic curves (moisture tension, saturation and effective permeability curves) are in determining the water intake and subsequent vertical migration down a fault zone. Three-dimensional site-scale models of Yucca Mountain have been developed by Birdsell et al.,[8] Rockhold et al.[7] and Wittwer et al.[1,2] All of these models consider the complex geological conditions of the site to some degree, but with variable detail and accuracy of representation. They also vary in the extent of the model area and volume considered, and in the number of grid blocks and modeling approach because of the different purposes of the models.

The general approach used in the development of the current site-scale model is to start with a detailed three-dimensional representation of the geology and hydro-geology of the site and to incorporate the different important processes and components (e.g., water, gas, heat) in stages. The model is designed to readily accommodate future requirements and complexities, as additional data are collected, and as important features of the basic underlying conceptual model are identified or changed. Submodels are used to investigate specific hypotheses and their importance before incorporation into the three-dimensional site-scale model. The primary objectives of the three-dimensional site-scale model are to:

(1) quantify moisture, gas and heat flows in the ambient conditions at Yucca Mountain,
(2) help in guiding the site-characterization effort (primarily by USGS) in terms of additional data needs and to identify regions of the mountain where sufficient data have been collected, and
(3) provide a reliable model of Yucca Mountain that is validated by repeated predictions of conditions in new boreholes and the ESF and has therefore the confidence of the public and scientific community.

In this paper we discuss the three-dimensional flow of moisture within Yucca Mountain on the basis of modeling results. The computer code TOUGH2 developed by K. Pruess (1990)[10] at LBL was used along with the three-dimensional site-scale model to generate these results. We have also incorporated gas flow and the geothermal gradient into the site-scale model. Some of the results obtained to date are described in terms of two-dimensional submodels of the site-scale model.

THE SITE-SCALE MODEL AND ITS PARAMETERS

Figure 1 shows the horizontal grid used in the three-dimensional site-scale model; the grid was designed based on locations of existing and proposed boreholes, traces of selected major faults and spatial distributions of infiltration zones and outcrops (Wittwer et al., 1992).[1] The major faults explicitly considered in the model include the Ghost Dance Fault, the Abandoned Wash Fault and the Dune Wash Fault. These three faults have large offsets and may therefore greatly affect the three-dimensional moisture flow within the mountain. The vertical grid consists of seventeen layers representing the subsurface formation that consists of a series of fractured welded ashflow tuffs (Tiva Canyon, Topopah Spring tuffs) and porous non-welded ashflow and ashflow tuffs (Yucca Mountain-, Pah Canyon, Calico Hills, Prow Pass, Bullfrog tuffs, bedded tuffs).[11,12] Isopach maps of these most important hydro-geological units were prepared by Wittwer et al., 1992[1] based on all available borehole data at the time and these are used in the model with appropriate modifications as new data became available.[13]

For the numerical simulations one requires hydrological property values for the rock matrix blocks and the fractures for each gridblock. The most important hydrological parameters include formation porosities, permeabilities and characteristic curves (relationships between saturations, capillary pressures and relative permeabilities). In this work we use hydrological parameter values similar to those employed in earlier work (Wittwer et al., 1993).[3] Fourteen dif-

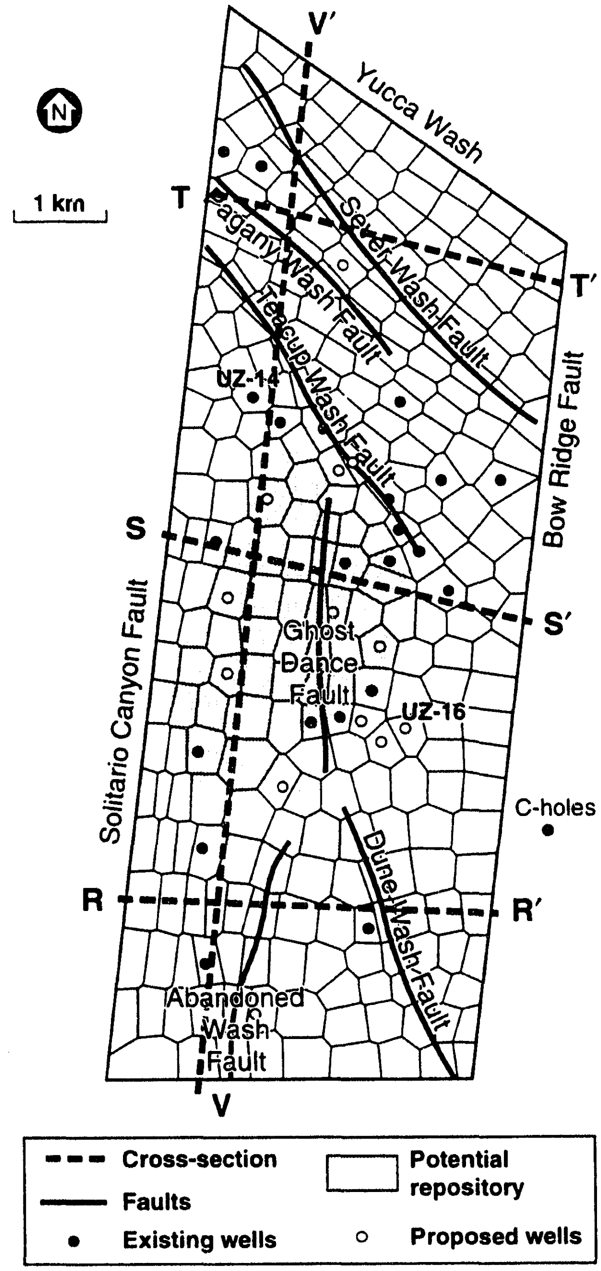

Figure 1. Areal extent and horizontal grid of the 3-D site-scale model. Also shown are some of the major faults in the area.

ferent hydrological properties are used for the seventeen model layers with two sets of values representing the Tiva Canyon unit, three for the bedded non-welded tuffs (Paintbrush), five for the Topopah Spring welded unit and four sets representing the vitric and zeolitic portions of the Calico Hills formation. In general, rock matrix permeabilities of the welded units, the Tiva Canyon and Topopah Spring formations are low or on the order of 10^{-18} m^2, whereas higher permeabilities are used for the non-welded tuffs of the Paintbrush unit (~ 10^{-13}m^2) and the Calico Hills (10^{-13}m^2 for the vitric part and 10^{-16} m^2 for the zeolitic part). Matrix porosities also vary greatly among and within the different formations. In the current work the porosity values assigned are insignificant as the steady state results presented here are insensitive to "storage-type" parameters such as porosities, compressibilities, matrix rock densities and heat capacities. Detailed descriptions of the parameter values used are given in Table 1 in Wittwer et al. (1993).[3] Some localized changes in parameter values were necessary to match observed thermodynamic conditions near some of the recent boreholes (e.g., well UZ-16). The table also gives the van Genecten parameter values (α, m, n) used to represent the characteristic curves assumed for the seventeen model layers.

The fracture medium properties were developed using the equivalent continuum approximation developed by Klavetter and Peters (1986),[14] which assumes capillary equilibrium between the fractures and the adjacent rock matrix blocks. The overall saturated fracture permeability was assumed to be 10^{-11} m,[2] and fracture flow is only evoked at very high liquid saturations (above 98%) or equivalently very low moisture tensions (1,000 to 3,500 Pa). Fracture flow conditions were only considered for the welded tuff units (Tiva Canyon and Topopah Spring), and only occur in these units when high infiltration rates (>0.5mm/year) are assumed at ground surface.

Three faults are represented discretely in the site-scale model (Ghost Dance, Abandoned Wash and Dune Wash faults), using rather coarse elements. The elements representing the faults have lateral widths in the range of 200 to 300 m, so that they represent fault zones rather than individual faults. This is consistent with recent geological observations made by Spengler et al. (1993),[15] who found that the Ghost Dance fault zone has a lateral width of hundreds of meters. Also, our numerical grid is designed to be readily modified for finer revolution near major components of these fault zones, if need be. Due to lack of hydrological information on fault properties at Yucca Mountain, we have taken the approach of assuming extreme hydrological properties in order to understand the importance of the faults and their properties. Three different assumptions regarding the hydrological behavior of the faults are made as follows:

(1) the faults are capillary barriers,
(2) the faults are impermeable, and
(3) the faults are permeable and have similar characteristic curves to the bedded tuffs of the Paintbrush units.

In case (1), the faults are assumed permeable, but due to their large "openings," their capillary suction capability is low, hence, little water enters the faults. In case (2), the faults are assumed to be sealed with fine-grained low-permeability material, hence, have low permeability and large suction potential. In general, the results obtained using cases (1) and (2) are very similar except for simulations when gas flow was important. In case (3), the faults accept water because of the assumed capillary functions (same as those of the Paintbrush unit) and are able to transmit the water downward because of the assumed relatively high permeability. Case (3) conceptualizes the faults as filled with granular material similar to that found in the Paintbrush unit. The results for case (3) representation of the faults will be labeled "permeable fault" whereas those for cases (1) and (2) are labeled as "capillary barrier fault" and "impermeable fault," respectively. Similar approaches for representing faults at Yucca Mountain are presented in Tsang et al.[9] and Wittwer et al.[3]

MOISTURE FLOW SIMULATIONS

We have conducted a series of three-dimensional moisture flow simulations in order to investigate possible patterns of moisture flow within Yucca Mountain. The approach used is to assume a given average infiltration rate (usually 0.1mm/year, although there is no definite evidence for this value), then assume an infiltration distribution (either uniform or spatially variable) and finally use the three-dimensional site-scale model to compute the moisture flow within the mountain, for assumed hydrological characteristics of the major faults. All of these assumptions have to be made in the current work, because the site-characterization effort has only recently started and the various model input parameters, such as the effective infiltration rates and distributions, hydrological fault property values, etc., are poorly known at best, but will be much better quantified as the site-characterization effort progresses.

A. Uniform Infiltration Rate

A series of simulations were conducted using the three-dimensional site-scale model assuming an uniform (areally) infiltration rate. Different average uniform infiltration rates ranging from 0.001 to 0.5 mm/year were considered. In these simulations the faults were modeled assuming either "capillary barrier" behavior or "permeable fault" behavior. Figure 2 shows typical results of the simulations in terms of two-dimensional cross-section S-S', which location is shown in Figure 1. Cross section S-S' extends across Yucca

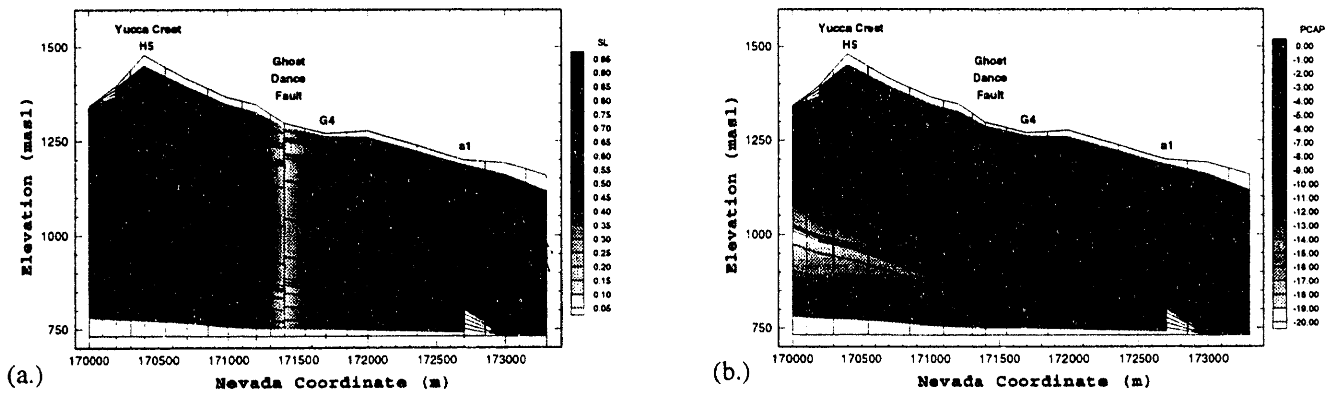

Figure 2. Two-dimensional cross section S-S' showing calculated distributions of liquid saturation (2a) and capillary pressure (2b).

Mountain from west to east through wells H5, G4 and a1, and intersects the Ghost Dance fault. An average uniform infiltration rate of 0.1 mm/year is used for the calculations shown in Figure 2, that represent steady-state results for moisture flow. Typically steady-state results, with insignificant changes in saturation (<0.001) are reached after about 10^{16} to 10^{17}seconds (3×10^8 years) of simulation time. This time estimate varies somewhat, but not largely, by the initial thermodynamic conditions assumed for the three-dimensional flow volume of the site-scale model.

The results shown in Figure 2 illustrate low saturation in the Ghost Dance fault, which is to be expected because of the assumed "capillary barrier" nature of the fault. Low liquid saturations, on the order of 40% or so, are found in the Paintbrush unit and in the vitric portion of Calico Hills formation. These relatively low liquid saturations result from the relatively high saturated permeabilities of these units. On the other hand, the welded tuff such as Tiva Canyon and the Topopah Spring units show liquid saturation exceeding 80% for almost the entire formation, again reflecting the relatively low matrix permeabilities of these units. High liquid saturations are also found in the zeolitic portions of the Calico Hills formation. The flow vectors shown in Figure 2a illustrate near vertical flow in the Tiva Canyon unit, significant lateral flow in the Paintbrush non-welded tuff formation, some lateral component of flow in some of the sub-units of Topopah Springs and near vertical flow in the Calico Hills formation. In general, the dipping of the formations in the model leads to significant lateral flow in the Paintbrush unit and various sub-units of the Topopah Spring formation. Capillary pressures are mostly above -10 bars for most of the layers except the bottom part of Topopah Springs and the top part of Calico Hills vitric, near the western boundary of the model (Figure 2b). High capillary pressures are found in some of the sub-units of Topopah Spring due to significant lateral flow in the overlying bedded tuffs. The results shown in Figure 2 are consistent with simulation results by other investigators.[1-8]

In general, it is difficult to show a complex three-dimensional distribution of saturation, capillary pressures or fluid flow, especially without the benefits of color graphics. Figure 3 is an attempt to show one example of calculated three-dimensional liquid saturation within Yucca Mountain using data from four different cross-sections. The cross-sections used are R-R', S-S', T-T' and V-V', all shown in Figure 1. Figure 3 shows well the obvious features of the model results including the low saturation conditions in the faults and the Paintbrush tuff, as well as the complex stratigraphic effects on the saturation distribution. It is not possible, however, to show with this representation the detailed effects of the stratigraphic sublayers, on moisture flow, or saturation conditions within the mountain. It should be noted that the bottom boundary in Figure 3 represents the water table.

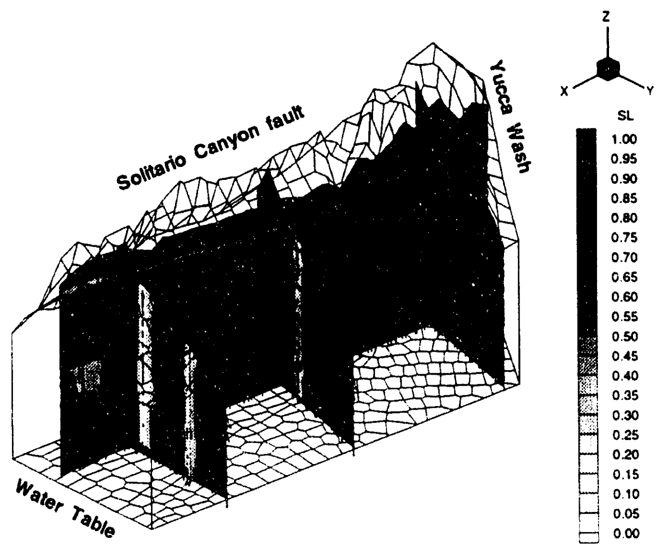

Figure 3. A quasi-three-dimensional calculated liquid saturation at Yucca Mountain shown using data for cross sections R-R', S-S', T-T' and V-V' (see Figure 1)

One of the important objectives of the current study is to investigate where in Yucca Mountain near vertical one-dimensional flow dominates, where somewhat more complex two-dimensional moisture flow occurs, and finally, where the most complex three-dimensional flow regime is expected. This type of information is of utmost importance when decisions have to be made regarding locations of holes for surface-based testing and locations of tunnels and drifts for subsurface tests and analysis. It is certainly not cost effective to place additional boreholes in regions where sufficient understanding of flows and rock properties is already achieved because of the relatively simple one-dimensional moisture flow field that occurs in that region.

Figure 4 shows four nearly horizontal slices of normalized vertical moisture flow within the mountain. Here we define the normalized vertical moisture flow as the vertical moisture flow at any location (x, y, z) normatized (divided by) the assumed average infiltration rate at the ground surface (in this case, 0.1mm/year). These horizontal slices are shown for locations above the Paintbrush non-welded units (bottom of Tiva Canyon), right below the bedded units (top of Topopah Spring), bottom of Topopah Spring, and at the water table. Figure 4a shows that the moisture flow in the Tiva Canyon unit is near vertical with almost no variation in normatized vertical flux (everywhere about 100% of the net infiltration-rate at the ground surface). Figure 4b, which represents a location below the Paintbrush unit, shows the large degree of variations due to lateral flow within that unit when compared to Figure 4a. In general, lateral flow occurs towards the east due to the dipping of the layers, with moisture accumulation close to major faults (assumed to be capillary barriers in this case) and model boundaries (e.g., Bow Ridge Fault is assumed to be an impermeable boundary in the mod-

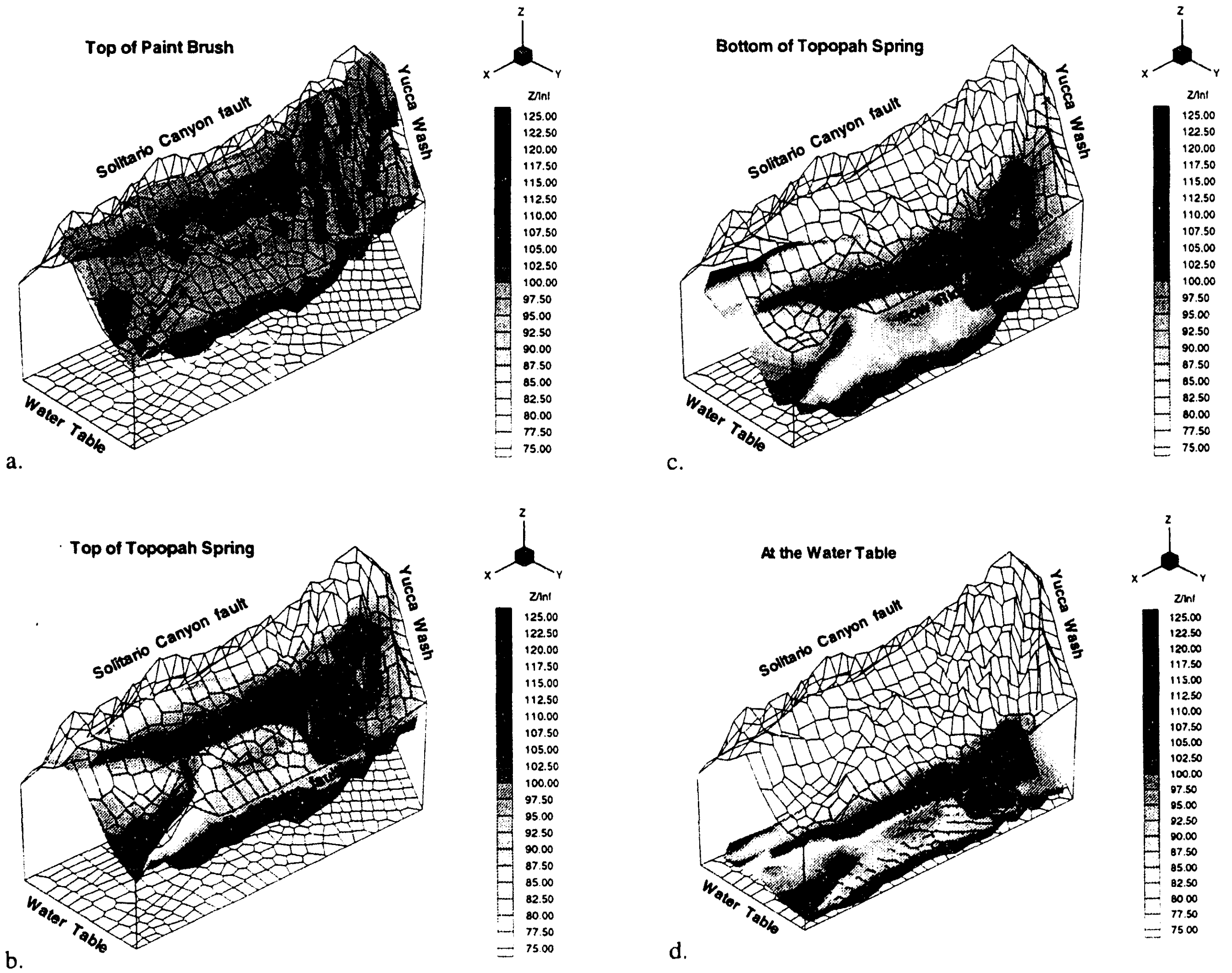

Figure 4. Calculated normalized vertical moisture fluxes (% of infiltration at ground surface) at different depths in the site-scale model for the case of "capillary barrier" faults, and an uniform areal infiltration rate of 0.1 mm/year.

el). In the horizontal slice representing the bottom of the Topopah Spring units (Figure 4c), additional lateral flow is evident with drying of regions west of major faults and moisture accumulation near the faults. This trend is further enhanced at the water table (Figure 4d).

Several important conclusions can be drawn from these results keeping in mind the underlying assumptions of uniform infiltration of 0.1mm/year and faults acting as "capillary barriers":

(1) Most of the lateral moisture flow occurs in the Paintbrush non-welded units;
(2) There is considerably more lateral flow in the southern part of Yucca Mountain than the northern part, mostly because of steeper dipping layers in the southern part. In some regions north of Ghost Dance Fault near one-dimensional vertical moisture flow is exhibited from these model calculations.
(3) Large vertical flow is found near major faults due to lateral flow and moisture accumulation near the faults because of their "capillary barrier" nature in these simulations. Hence, measurements of saturations and capillary pressures in rock matrix blocks near faults may give as much information about flow characteristics of the faults, as measurements of these quantities in the faults themselves.

Figures 5a through 5d show similar horizontal slices for the case of a "permeable fault" (still uniform infiltration rate of 0.1mm/year). Figure 5a shows that for most of the mountain the moisture flow within Tiva Canyon will be near-ver-

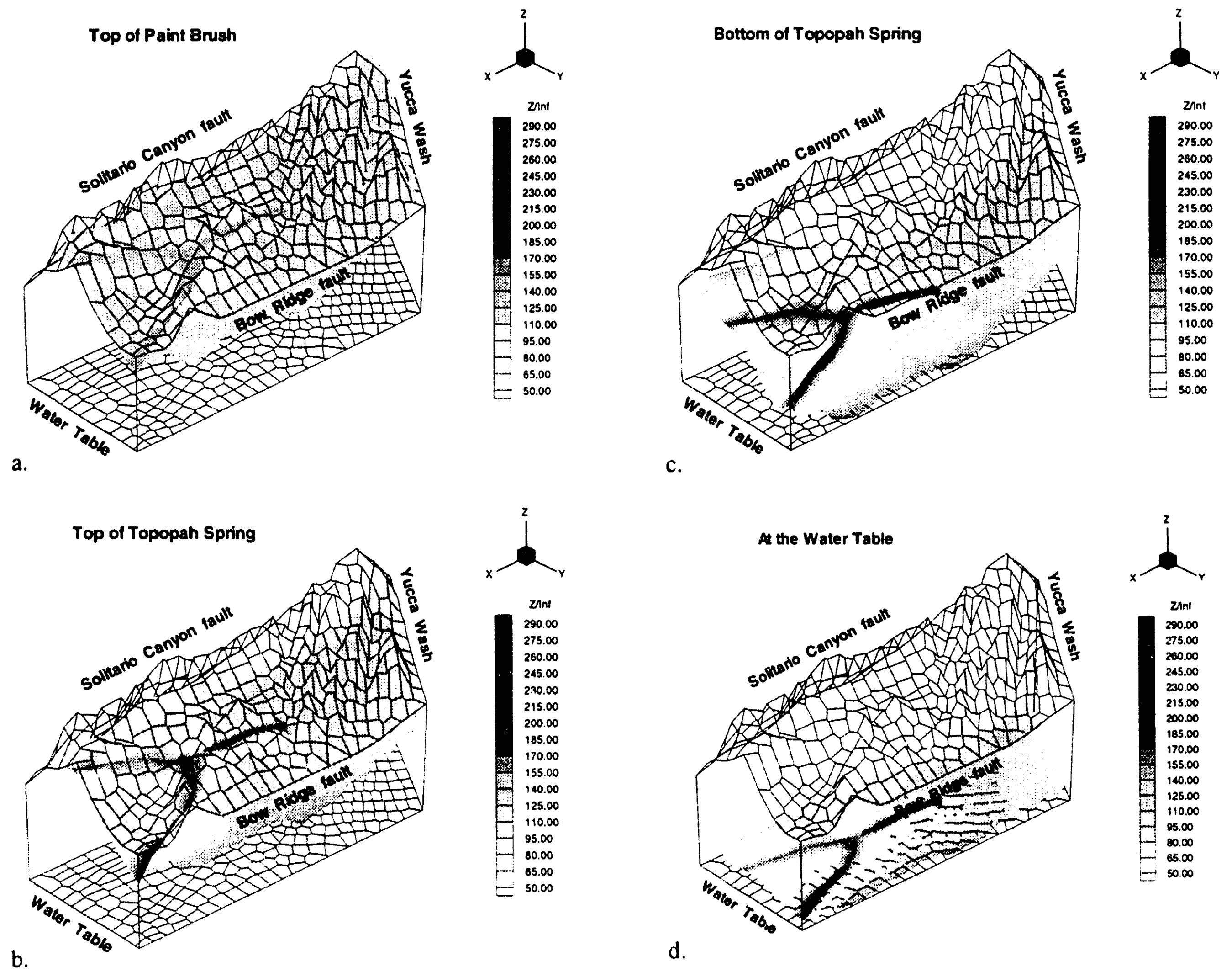

Figure 5. Calculated normalized vertical moisture fluxes (% of infiltration at ground surface) at different depths in the site-scale model for the case of "permeable" faults, and an uniform areal infiltration rate of 0.1 mm/year.

tical except for some lateral infiltration into the major faults and subsequent vertical drainage. Again, the large lateral flow potential of the Paintbrush tuffs is evident when Figures 5a and 5b are compared. In this case the major faults clearly establish themselves as major vertical pathways for flow. Similar conclusions can be reached about subsequent deeper horizontal slices as greater portions of the vertical flow occur through the major faults. It is interesting to note that again some of the area north of Ghost Dance Fault exhibits very little evidence of lateral flow with near uniform vertical flow in this area. The major faults in the northern part of the model region (Sever-Wash, Pagany Wash and Teacup Wash faults) are strike-slip type faults with little offsets. One should also note that for this case the vertical moisture migration away from the three faults that are modeled discretely are near-uniform, so that measurements of important rock matrix thermodynamic conditions away from faults may give crucial information about the hydrological characteristics of the faults.

B. Non-Uniform Infiltration

A series of numerical simulations were also performed assuming non-uniform distribution of infiltration at the ground surface. Due to space limitations, only one of these simulations will be described here. The base case considered is shown in Figure 6a through 6d. In this case, the major washes in the northern part of the mountain are assumed to accept the bulk of the infiltration, with additional infiltration in the washes is the south-eastern part of the model. Figure 6a shows basically the areas where the concentrated infiltration occurs; zero met infiltration is assumed elsewhere. This

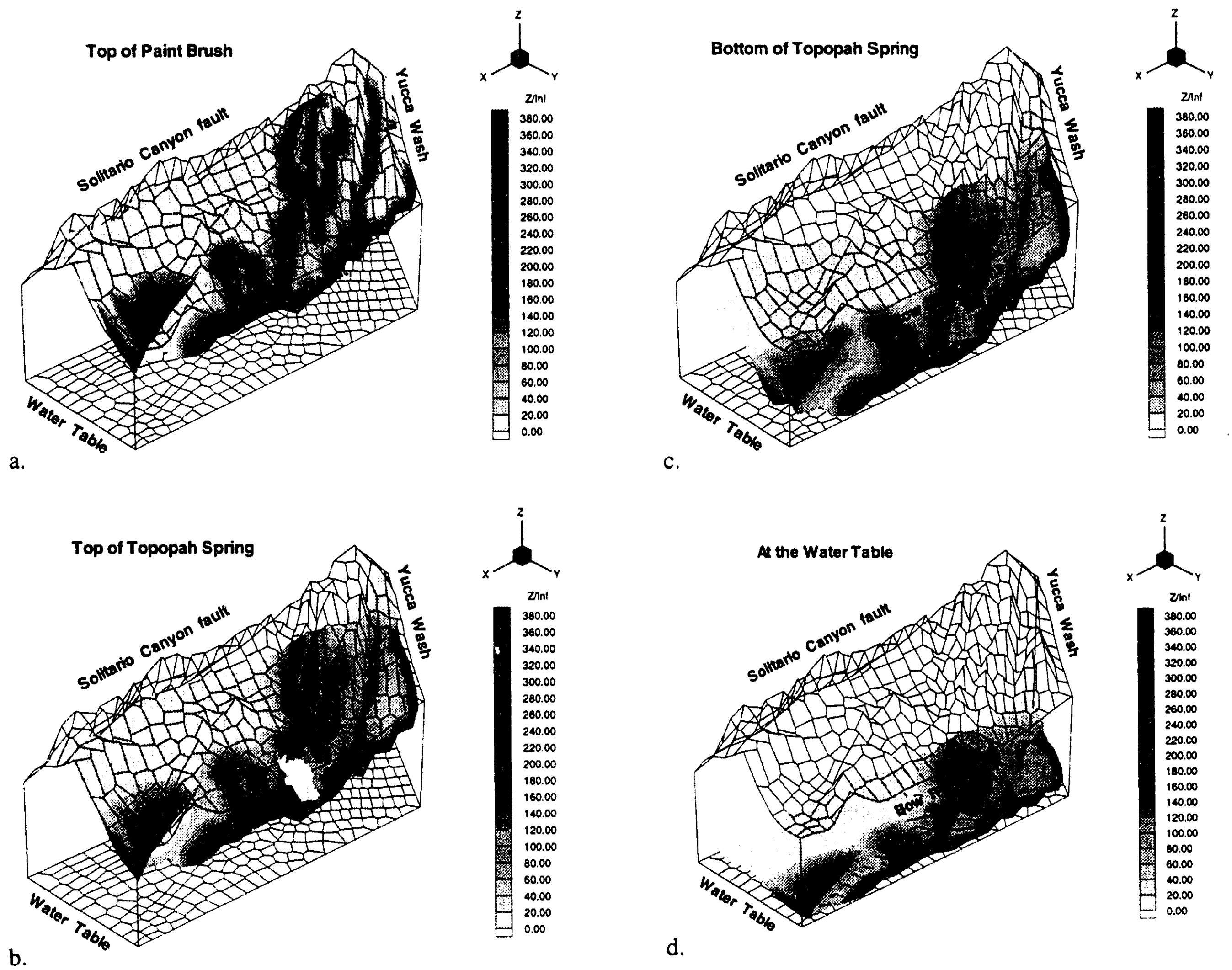

Figure 6. Calculated normalized vertical moisture fluxes (% of average net infiltration) at different depths in the site-scale model for the case of "capillary barrier" faults, and non-uniform infiltration (average 0.1 mm/year).

infiltration pattern is based on personal communication with A. and L. Flint (1992). The total infiltration rate amounts to 0.1 mm/year when averaged over the entire region. A similar infiltration pattern, but with different infiltration rates is given in a paper in this issue by Flint and Flint (1994).[16] For this infiltration pattern only the Dune Wash Fault has important hydrological contributions as it blocks lateral flow toward the east in the southern part of the model. Figures 6a through 6d show how the relatively concentrated infiltration flux is dispersed laterally as well as vertically. Observations of moisture migration close to the water table show that it is near uniform over areas of several square kilometers, although the concentrated flux was in regions with characteristic lengths of only a few hundreds of meters. Some of this may be due to grid effects. Current work on the non-uniform infiltration studies involves investigating cases with the new estimated infiltration map developed by Flint and Flint (1994).[16]

MODEL PREDICTIONS

The quality and accuracy of complex three-dimensional models such as the site-scale model can only be tested and verified by model predictions, and later comparisons with observed field data. We have started this process for wells UZ-16 and UZ-14. In the case of well UZ-16, we made predictions of liquid saturation and capillary pressure profiles versus depth. In general, the predictions were reasonable compared to the subsequently measured saturations and capillary pressure profiles, but significant differences were found in both the Topopah Spring and the Calico Hills units. The major discrepancy was due to differences in locations of predicted geological units and those found during drilling, especially in the Calico Hills with the vitric and zeolitic units. The model predictions also indicated high liquid saturations (> 80%) in the entire Topopah Spring unit, whereas the measured values show gradual increase in liquid saturation below the bedded (Paintbrush) units from about 50 to 80% over a depth interval of about 125 m. The best comparison between the observed and predicted liquid saturation profiles for UZ-16 were obtained when an infiltration rate of about 0.1 mm/year was assumed. We are currently calibrating the three-dimensional site-scale model to match accurately the observed conditions in UZ-16, and also predicting liquid saturation profiles for well UZ-14.

GAS COMPONENT AND GEOTHERMAL GRADIENT

Gas flow and the geothermal gradient have been incorporated into the three-dimensional site-scale model. At this time, the gas boundary conditions at the ground surface assume a gas-static pressure profile between the water table and the ground surface. An average annual temperature at Yucca Mountain of about 16°C is prescribed uniformly at the ground surface, and an average temperature of 33°C at the water table. These ground surface boundary conditions neglect important near surface variations and processes such as barometric pressure variations, yearly and areal temperature variations, wind effects and others. These type of variations have been found extremely important in the upper 100 m of the mountain (mainly within Tiva Canyon) as indicated by large gas flows in these regions of the mountain (Weeks, 1990).[17]

Current studies of gas and heat flow include two-dimensional cross-sectional model studies to investigate the various processes and their sensitivities including the barometric effects, wind effects, ground surface temperature variations and areal variations in temperature and heat flow at the water table. The result of these sub-model calculations will be used to determine the most appropriate boundary conditions to be incorporated into the site-scale model for gas and heat flow at the ground surface, as well as at the water table.

SUMMARY AND CONCLUSIONS

The development of the three-dimensional site-scale model of Yucca Mountain continues with the purpose of guiding the site characterization effort. Various three-dimensional moisture flow simulations have been carried out by assuming different infiltration patterns, and using various assumptions regarding hydrological characteristics of major faults. The site-scale model has been used to predict saturation conditions in recent boreholes. Gas flow and the geothermal gradient have been incorporated into the model. The following conclusions can be reached from this study:

(1) Even when uniform infiltration rates are assumed at the ground surface, lateral flow and three-dimensional effects due to the complex stratigraphy at the site, and major fault offsets, cause highly variable areal distributions of discharge at the water table.

(2) When the major faults are assumed to act as capillary barriers, lateral flow causes build-up of moisture close to the faults and subsequent vertical migration. Conversely, when the faults are assumed to readily absorb water and migrate it downward, lateral flow is greatly enhanced and relatively dry conditions are found near the faults.

(3) The hydrological characterization of major faults at Yucca Mountain is extremely important as the three-dimensional moisture flow depends strongly on the hydrological behavior of the faults. Careful measurements of saturation and capillary pressure conditions in the rock masses near the faults may yield as much informa-

tion about hydrological characterizations of the faults as direct measurements in the faults themselves.

(4) Non-uniform distribution of infiltration is likely at Yucca Mountain and leads to enhanced lateral flow in different parts of the mountain, more complex three-dimensional flow patterns, and more likely existence of perched water in different parts of the mountain.

(5) The use of the site-scale model (and other models) to predict conditions in new boreholes as well as in the Exploratory Studies Facility is critical for understanding the site, ensuring the quality and accuracy of the model as well as for securing confidence by the public and the scientific community in the model. This process has started with use of the model for predicting conditions in wells UZ-16 and UZ-14.

(6) Gas flow and the geothermal gradient have been incorporated into the site-scale model, and calibrations of these components against known gas and thermal conditions are underway.

ACKNOWLEDGMENTS

This work was prepared under U.S. Department of Energy contract no. DE-AC03-76SF00098, and DE-A108-78ET44802 administered by the Nevada Operations Office in cooperation with the U.S. Geological Survey, Denver. Review of this paper by J. Wang and Y. Tsang of LBL, is greatly appreciated. The authors also appreciate the contributions of M. Chornak, A. Flint, L. Flint, E. Kwicklis, and R. Spengler from the U.S. Geological Survey, as well as R. Bhogeswara of LBL to this work.

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