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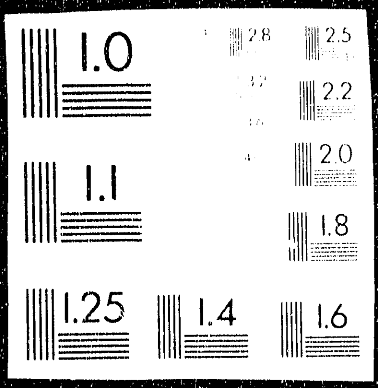

Conf-920430--69

LBL-31799

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

EARTH SCIENCES DIVISION

MAR 24 1992

To be presented at the International High Level Radioactive Waste Management Conference, Las Vegas, NV, April 12–16, 1992, and to be published in the Proceedings

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January 1992

Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098

LBL--31799

DE92 010459

Design of a Three-Dimensional Site-Scale Model for the Unsaturated Zone at Yucca Mountain, Nevada

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This work was performed under U.S. Department of Energy Contract DE-AC03-76SF00098 and DE-AI08-78ET44802, administered by the Nevada Operations Office, in cooperation with the U.S. Geological Survey, Denver.

ABSTRACT

A three-dimensional model of moisture flow within the unsaturated zone at Yucca Mountain is being developed. This site-scale model covers an area of about 30 km^2 and is bounded by major faults to the east and west. A detailed numerical grid has been developed based on locations of boreholes, different infiltration zones, hydrogeological units and their outcrops, major faults, and water level data. Different maps, such as contour maps and isopachs maps, are presented for the different infiltration zones, and for the base of the Tiva Canyon, the Paintbrush, and the Topopah Spring hydrogeological units.

I INTRODUCTION

The United States Geological Survey (USGS) is conducting site-characterization studies of Yucca Mountain, Nevada, the potential site for underground storage of high-level radioactive waste. The studies include the collection and analysis of geological, geophysical, hydrological, and geochemical data. All of these data will be integrated into a detailed conceptual model of the site and into a three-dimensional numerical model referred to in this paper as the "site-scale model". The site-scale model will quantify moisture flow within the unsaturated zone of Yucca Mountain and will evaluate the effects of gas flow and the geothermal gradient on the moisture flow. Ultimately, the site-scale unsaturated-zone model will be combined with a similar model for the saturated zone to yield an integrated model to be used for performance predictions.

The three-dimensional site-scale model of the unsaturated zone at Yucca Mountain is being developed by Lawrence Berkeley Laboratory (LBL) in collaboration with the USGS. The development of the model relies on previous modeling efforts, which began with the two-dimensional cross-section model developed by Rulon et al.[1] Rulon et al.[1] computed many steady-state moisture distributions for different infiltration rates and flow conditions (fracture- and matrix-dominated flow) and identified the potential for lateral flow due to dipping of the stratigraphic units. Wang and Narasimhan,[2] also using a two-dimensional cross-section model, showed that the degree of lateral flow depends strongly on assumed hydrological parameters of vertical fault zones, especially the characteristic curves. Similar conclusions were reached by Osnes and Nieland,[3] and their results also indicated perched water near major faults, when the faults are modeled "as a highly permeable fractured zone". Recently, three-dimensional models of the "natural state" of the unsaturated zone at Yucca Mountain were developed by Rockhold et al.[4] and Birdsell et al.[5] Rockhold et al.[4] studied the unsaturated zone in the immediate vicinity of the potential repository with their model extending 605 m in the N-S direction and 300 m in the E-W direction. They found considerable lateral flow due to the complex stratigraphy and perched water in some cases. The various cases they considered indicated mostly fracture-dominated flow in the shallow welded units (Tiva Canyon), but matrix dominated flow elsewhere. Birdsell et al.[5] considered a larger model area (4.5 km in N-S direction and 2.7 km in E-W direction), but concentrated on radionuclide transport, including retardation. They reported strong effects of the stratigraphy on the flow field. Both of the three-dimensional models used a large number of gridblocks (25,000 to 30,000), resulting in large computational efforts.

The primary objectives of developing the three-dimensional site-scale model, which are discussed in this paper, set:

(1) To investigate the feasibility for developing a detailed three-dimensional model of the moisture flow field at Yucca Mountain, that attempts to incorporate the geologic complexities and the non-linearities involved with unsaturated fluid flow in fractured rocks.

(2) If feasible, to use the model in the site characterization effort by evaluating temporal and spatial frequency of data needs.

(3) To quantify moisture flow within the unsaturated zone at Yucca Mountain and evaluate the effect of gas flow and the geothermal gradient on moisture flow.

In this paper, we primarily describe the development of the three-dimensional site-scale model in terms of the stratigraphy, structure, moisture infiltration, and rock properties. Numerical simulations using the model are currently (1991) being conducted.

II SITE DESCRIPTION

The hydrogeology at Yucca Mountain is controlled by fluid flow through heterogeneous layers of anisotropic, fractured volcanic rocks in an arid environment. The location of Yucca Mountain and the extent of the model area are shown in Figure 1.

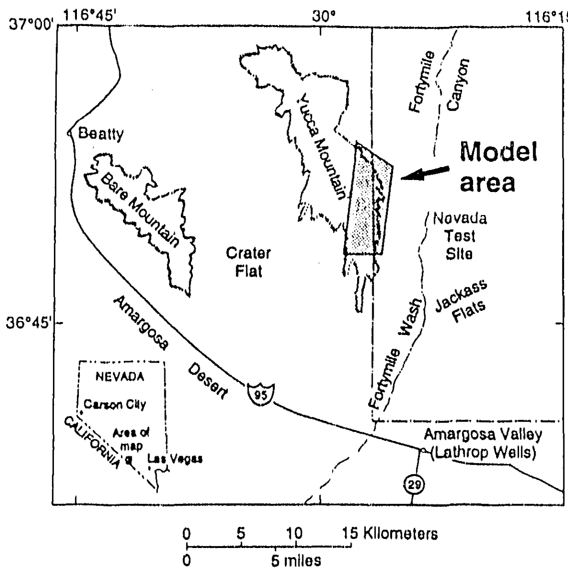


Fig.1 Location of Yucca Mountain and the site-scale model area. Modified from Montazer and Wilson. [6]

The model covers an area of about 30 km^2 centered around the popential repository area and is bounded by the Bow Ridge Fault to the east, and Solitario Canyon Fault to the west. The model extents to the north as far as Yucca Wash, where the topography suggests that a major northwest fault may be present. Figure 2 shows the areal extent of the model with the main faults at the boundaries, those faults located within the site-scale model area and the secondary smaller structural features. The various geologic structures were taken from maps and cross sections published by Scott and Bonk[7] and Nimick and Williams.[8] Reports by Tien et al.[9] and Montazer and Wilson[6] were used to obtain physical information about the faults. The major north to northeast striking faults are extensional features with steep westward dips. The vertical offset along these faults commonly ranges from ten to hundreds of meters and generally increases from north to south. For example, the vertical offset along the Ghost Dance Fault increases from a couple of meters at the northern end to about 30 m at the southern end. The northwest trending faults in the northern part of the model area are interpreted as strike-slip features with horizontal displacement ranging from almost zero to a few tens of meters. These major features penetrate the complete thickness of the unsaturated zone and possibly control the moisture flow and the saturation distribution. The secondary faults within the boundary of the site-scale model are features with less than 10 m vertical offset.[6,9]

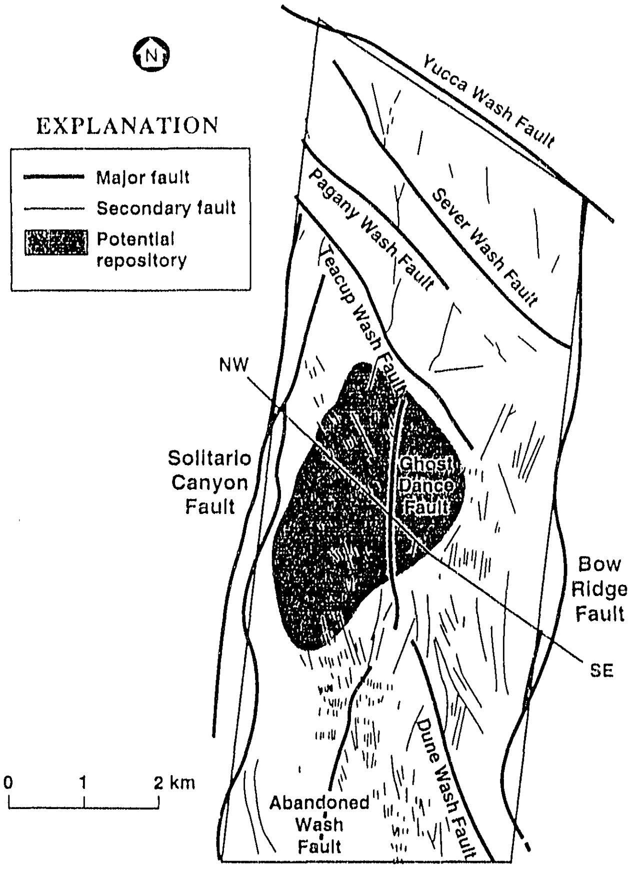


Fig. 2 Close-up of the extent of the model area showing major and secondary faults, and the potential repository location.

At smaller scales, the occurrence of fractures is correlated with increases in the degree of welding of the volcanic rocks, which in turn influences the mechanical response of the rock to stress. The unsaturated zone consists primarily of Tertiary tuff having a south to southeast dip of about 5 to 30°. The tuffs range from porous, nonwelded ash-flows and bedded tuff deposits, to massive, highly brittle welded ash-flow rocks, depending on their deposition mechanisms and cooling history.[6,9] Based on their hydrological characteristics, the geological units were regrouped into hydrogeological units, referred to below as Tiva Canyon, Paintbrush, Topopah Spring, and Calico Hills units.[6] Table 1 summarizes the relation between the major geological and hydrogeological units and gives a schematized description of the lithology. Due to cooling processes and different response to tectonic events, the brittle welded and porous nonwelded tuffs have vastly different mechanical and hydrological properties. The welded tuffs, such as the Tiva Canyon unit and Topopah Spring unit, are characterized by relatively low porosities (10 to 15%)[6], low saturated matrix hydraulic conductivities (2 to 4 10^{-11} m/s)[6] and high fracture densities (8 to 40 fractures per cubic meter).[10] On the other hand, nonwelded and bedded tuffs, such as the Paintbrush nonwelded unit, have higher matrix porosities (25 to 50%),[6,11] saturated hydraulic conductivities (10^{-6} to 6 10^{-8} m/s),[6,11] and lower fractures densities (about 1 fracture per cubic meter).[10] Zeolitic alteration appears in the lower part of the Topopah Spring Member, and in the Calico Hills hydrogeologic unit, and results in a decrease of the porosity and hydraulic conductivity of the tuffs. Thus, the Calico Hills unit has been divided into vitric and zeolitic zones. The fracture density is similar in both zones (2-3 fractures per cubic meter),[10] but the porosity of the vitric zone (25-40%) is slightly higher than that of the zeolitic zone (15-35%).[11] Similarly, the saturated hydraulic conductivity of the vitric matrix blocks is considerably higher (10^{-9} m/s) than that of the zeolitic matrix blocks (10^{-11} m/s).

Most of the surface of the site-scale model area consists of welded ash-flow tuffs of the Tiva Canyon welded unit. Along the western slope of Yucca Mountain Crest and in the northern part of the site-scale model area, the nonwelded and bedded tuffs of the Paintbrush unit, and the welded tuffs of the Topopah Spring unit are exposed.

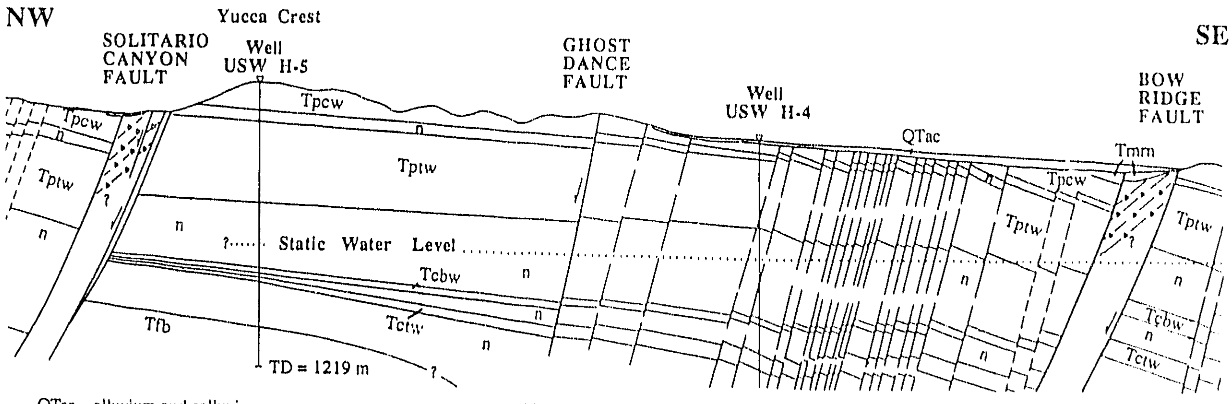
A NW to SE vertical cross-section through the middle of the model area is presented in Figure 3 and shows the major normal fault zones along the western (Solitario Canyon Fault) and eastern (Bow Ridge Fault) model-area boundaries. The slightly east dipping hydrogeological units are cut by the major Ghost Dance Fault and many secondary faults. This cross-section illustrates the complexity of the geological and hydrogeological features, all of which need to be considered in the site-scale model.

Table 1 Schematic description of the relation between major geological and hydrogeological units.

	GEOLOGICAL UNIT	LITHOLOGY	HYDRO-GEOLOGICAL UNIT
PAINTBRUSH TUFF	TIVA CANYON Member	densely welded tuff moderately welded tuff	TIVA CANYON
		partially welded tuff nonwelded tuff bedded tuff	PAINTBRUSH
	YUCCA MOUNTAIN Member	non- to moder. welded tuff bedded tuff	
	PAH CANYON Member	non- to moder. welded tuff bedded tuff	
	TOPOPAH SPRING Member	nonwelded tuff	
		moder. to densely welded tuff densely welded tuff vitrophyre	TOPOPAH SPRING
		moder. to partially welded tuff bedded tuff	CALICO HILLS
TUFF. BEDS CALICO HILLS		non- to partially welded tuff	
CRATER FLAT TUFF	PROW PASS Member	non- to partially welded tuff bedded tuff	
	BULLFROG Member	non- to densely welded tuff bedded tuff	
	TRAM Member	non- to moder. welded tuff	

III MODELING APPROACH

In the development of a site-scale model of Yucca Mountain, one must consider and incorporate all the important complexities of the site. Table 2 identifies some of the site-scale modeling issues that need to be addressed. Perhaps the most critical issue at present (1991) time is the poorly known flow characteristics of the major faults. Previous studies have indicated that assumptions made regarding the conditions and hydrological parameters of the faults greatly affect the results in terms of lateral flow and perched water. The smaller fractures and matrix flow are probably of less importance because they can be considered (at least initially) by using composite characteristic curves.[12,6]



QTac alluvium and colluvium
Tmm Rainer Mesa Member
Tpcw Tiva Canyon Member
n non-welded tuff (e.g. Paintbrush and Calico Hills)
Tptw Topopah Spring Member
Tcbw Bullfrog Member
Tctw Tram Member
Tfb Lava Flows and Breccias
TD Total Depth

Fig.3 NW-SE vertical cross section through the site-scale model area. Modified from Scott and Bonk.[7]

Table 2 Some site-scale modeling issues.

- UNCERTAINTIES IN FLUX DETERMINATION
- DENSELY FRACTURED WELDED UNITS; MILLIONS OF FRACTURES AND MATRIX BLOCKS
- FLOW CHARACTERISTICS OF MAJOR FAULTS (E.G. GHOST DANCE FAULT)
- MATRIX VS. FRACTURE FLOW
- GAS FLOW (AIR + WATER VAPOR)
- THERMAL EFFECTS ON FLUID FLOW
- LATERAL FLOW AND PERCHED WATER
- FRACTURE AND CAPILLARY BARRIERS

Our general approach is initially to develop a three-dimensional site-scale model for moisture flow only, neglecting gas flow and the geothermal gradient. The model is designed to readily accomodate in future refinements and complexities as additional data are collected, and as important features of the conceptual model are identified or changed. The main moisture-flow model will be extended in a next stage to include the effects of the prevailing geothermal temperature gradient, and gas-flow will also be added. Figure 4 presents a flow chart of the site-scale modeling approach and its relation to the data-collection and the performance-prediction tasks.

The site-scale model will incorporate all available geological, geochemical and hydrological data in order to estimate moisture, gas, and chemical transport within the unsaturated zone at Yucca Mountain. Data collection and analysis that will continue to be performed by USGS and other scientists feed directly into the conceptual model, and also impact the choice of numerical codes and their development and modifications for the site-scale modeling effort. The results of the selection and development of numerical codes, and the refinement of the conceptual

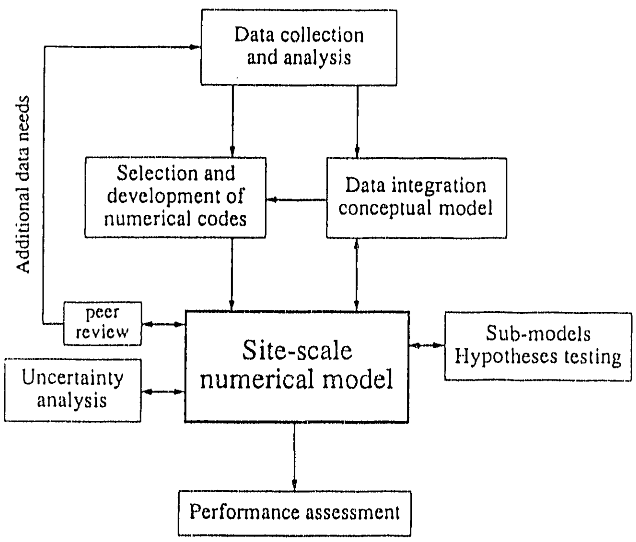


Fig.4 Simplified flow chart of the site-scale modeling approach.

model, are very important ingredients of the evolving site-scale model. Various numerical submodels will be used to investigate specific hypotheses and approximations, such as the influence of the grid resolution and orientation on the numerical results, the effect of spatial and temporal variation of infiltration, the effect of short- and long-term barometric variations, or the influence of the geothermal gradient on moisure and gas flow. The results from the submodels will be incorporated as needed into the main three-dimensional site-scale model to allow determination of processes that control the transport of moisture, chemicals and gas at Yucca Mountain.

The site-scale model is also intended to help guide the site characterization effort at Yucca Mountain, especially in the type and amount of data needed. For example, sensitivity studies using the model may suggest that more detailed moisture-tension data are needed. Conversely, the simulations may show that a certain model parameter is of less importance, and, therefore, significantly reduce the number of field measurements for this parameter. The site-scale model will therefore provide a valuable tool to facilitate interactions between the collectors and the users of field data.

Peer review of the model results and the data collection process will be an essential part of the site-scale modeling effort. The peer review will be at different levels, including model consistency and accuracy review, review of the input data to the model to ensure that it accurately consider field data and observations, review of additional data requirements or over-abundance of data, and review of technical validity of the approach and the overall model results.

IV DESIGN OF THE THREE-DIMENSIONAL SITE-SCALE MODEL

The design of the numerical grid used in the simulations must consider the effects of the normal faults, the spatial distribution of the infiltration, the sharp thermodynamic gradients at the boundaries between hydrogeological units, the locations of existing and proposed wells, and the possible occurrence of lateral flow and perched water.

The locations of the nodal points for the horizontal grid were determined, based on the following criteria to:

(1) Coincide with the locations of existing or proposed boreholes. This allows direct comparison of model results with actual field data.
(2) Align along known major faults, such as the Ghost Dance Fault, Dune Wash Fault and Abandoned Wash Fault. This alignment allows one to explicitly prescribe "faults properties" to the elements represented by the faults, and also allows subsequent (when sufficient data are collected) incorporation of a subgrid of fine elements to represent the small thickness (perhaps 1 m or less) of the fault zones more accurately.
(3) Be areally distributed to reflect properly the different infiltration zones for ease in describing surface flux conditions that depend on the different infiltration zones.
(4) Be areally distributed to reflect propc ly the areas where different rock types are exposed.

(5) Have gradual changes in element sizes to minimize errors in representing gradients in thermodynamic conditions, hence minimizing model inaccuracies.

At Yucca Mountain, moisture infiltration is believed to be morphologically dependent, whereas different mechanisms control the net infiltration from rainfall. Because of variations in soil cover and exposed fractures, the model area can be divided into three infiltration zones, alluvium (24%), sideslopes (60%) and ridgetops (14%). Figure 5 shows the areal distribution of the different infiltration zones which have to be considered in the design of the horizontal grid of the model. After all the nodal points had been located, a numerical grid generator was used to develop the horizontal grid shown in Figure 6.

The vertical grid was designed based on the spatial distribution of the hydrogeological units, such as the welded units (Tiva Canyon and Topopah Spring) and nonwelded units (Paintbrush, Calico Hills, Prow Pass). The hydrogeological units were divided vertically so that thin elements would surround the unit boundaries. Because the thicknesses of the units vary considerably throughout the model area, a fixed number of vertical elements was chosen for every unit, each of the elements having a percentage of the whole unit thickness. This approach allowed for a lateral

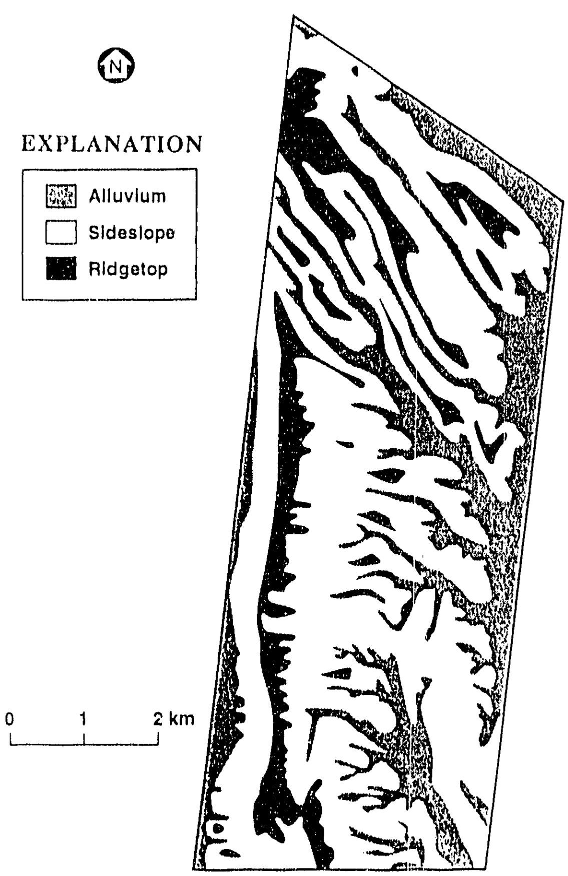


Fig.5 Approximate view of the different infiltration zones used in the site-scale model.

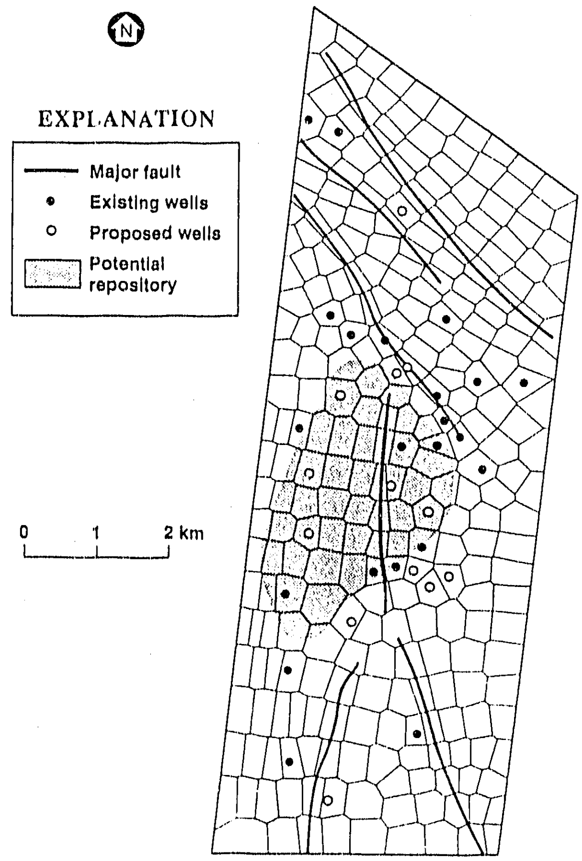


Fig.6 Horizontal grid for the site-scale model showing the location of faults, and existing and proposed exploratory wells considered in the design.

continuity of the element layers. The three normal faults located within the model area (Ghost Dance, Abandoned Wash and Dune Wash Faults) were simulated in an explicit manner by accounting for their vertical offset in the design of the vertical grid. On the other hand, regions with many faults of smaller displacement were modelled in an implicit manner by modification of the characteristic curves of the relevant grid blocks.

A geometrical three-dimensional representation of the hydrogeologic units between the ground surface and the water table was developed to obtain the spatial location of the unit boundaries. Once these surfaces were determined, the z-coordinates of the center of the vertical elements were calculated using the previously determined vertical gridding of each hydrogeological unit. Surficial data, such as fault offsets, dips and strikes of the beds, and the lithology of the wells, were laterally and vertically extrapolated to design contour maps of the boundaries of the hydrogeological units and the water table. The hydrogeological-unit boundaries also were determined from the lithologic logs of the wells.

The contour map for the base of Tiva Canyon welded unit (Figure 7) was developed by taking into account the offsets along the three major normal faults. These offsets were determined from the geological maps and cross sections published by Scott and Bonk,[7] and Nimick and Williams.[8] The hydrogeological unit boundary elevations, taken from twenty three boreholes lithologic data, were used with data on the dips and strikes of the volcanic-rock layers to obtain consistency between surficial data and subsurface data. The outcrop elevations of the boundaries of the units were determined from geological maps and also were included to obtain more data points in the northern and western part of the model area. The contour map of the base of the Tiva Canyon unit shown in Figure 7 agrees reasonably well with a map based on geologic boundaries previously published by Carr,[13] which considered less well data but a greater number of faults.

Because some of the boreholes are rather shallow, there were not sufficient data points for the deeper units to reproduce the offsets along the faults. Therefore, isopach maps were developed for the hydrogeological unit boundaries between the Paintbrush nonwelded and Topopah Spring welded units, and between the Topopah Spring and Calico Hills units. Lithologic logs from twenty nine boreholes located inside and around the border of the model area were used to develop the isopach map of the Paintbrush nonwelded hydrogeological unit (Figure 8). Because of the lack of data in the northern part of the model area, the thickness of the unit was estimated from the geologic map.[7]

Isopach maps based on thicknesses of the geological units have been published for the Yucca Mountain and the Pah Canyon Members by Tien et al.[9] These maps were only used as guidelines for the main deposition features of the tuffs because they do not consider the hydrogeological division of the volcanic sequence.

The isopach map for the Topopah Spring hydrogeological unit was based on data from twenty three boreholes (Figure 9). An isopach map for the geological unit previously published by Tien et al.[9] was compared to the new hydrogeological unit map. Because of the different data considered and the different area covered by the past studies, the two interpretations agree only for the most central part of the model area. Other isopach maps have been published by Ortiz et al.[14] for various sections of the Topopah Spring Member, e.g. the lower lithophysal zone, and the vitrophyre zone, but these maps consider only certain parts of the whole unit and cannot, therefore, be compared to our new isopach map of the Topopah Spring unit.

The bottom of the site-scale model is assumed to coincide with the water table. Previous reports from

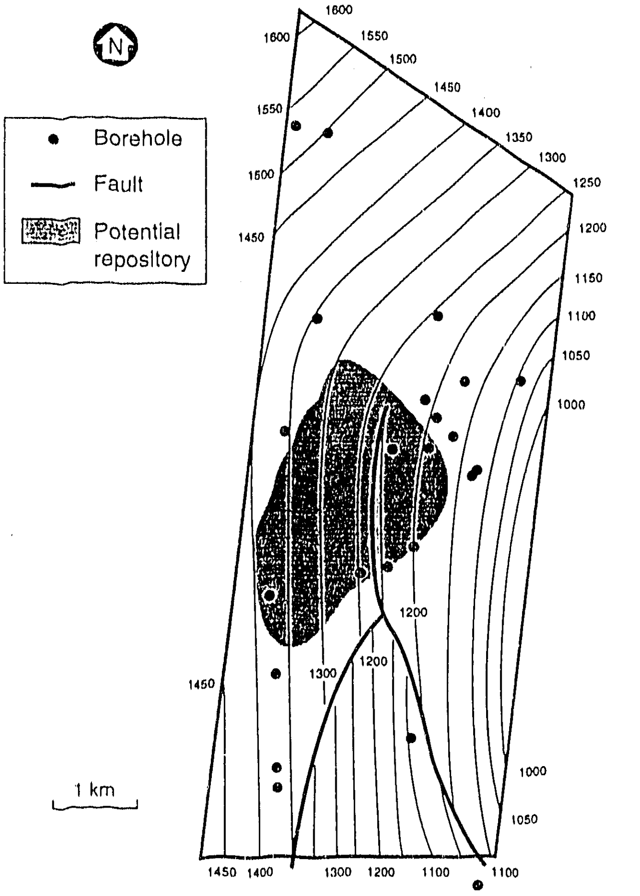


Fig.7 Contour map of the base of the Tiva Canyon hydrogeological unit (m. above sea level).

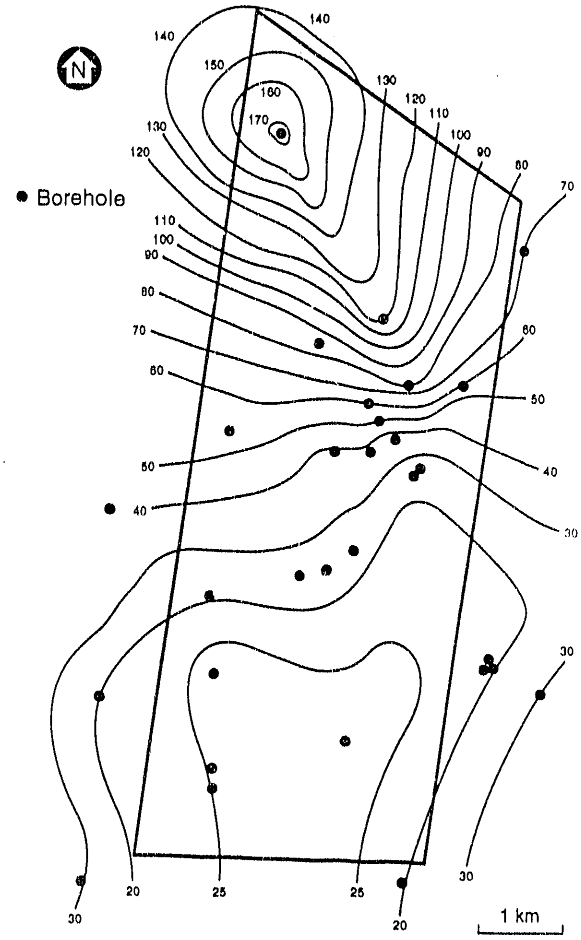


Fig.8 Isopach map for the Paintbrush hydrogeological unit (m).

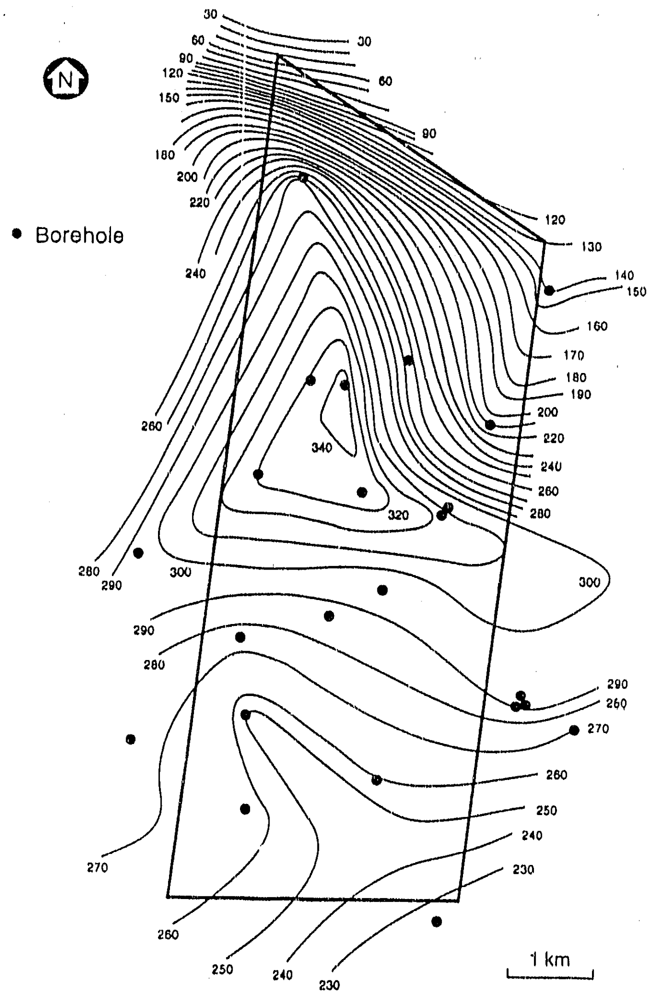


Fig.9 Isopach map for the Topopah Spring hydrogeological unit (m).

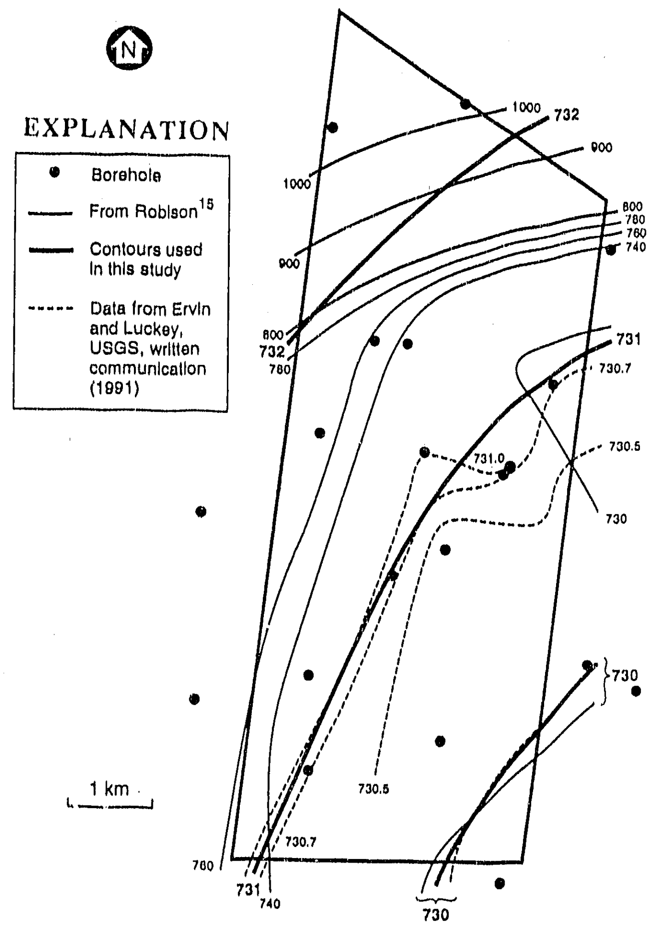


Fig.10 Water-table map used in the design of the three-dimensional model (m. above sea level).

Robison[15] suggest the presence of a steep hydraulic gradient in the northern part of the model. Because the available data about this steep gradient are very limited and subject to new interpretation, we considered only the water elevations measured in the wells located in the low-gradient zone and extrapolated this gradient for the entire model area. Our approximate map of the water table therefore is located at depths ranging from 380 to 860 m below ground surface is presented in Figure 10.

V PRELIMINARY NUMERICAL SIMULATIONS

The integrated finite-difference computer code TOUGH2[16] is being used to simulate the steady-state moisture flow, the liquid-saturation distribution and the matric-potential distribution between the land surface and the water table. The relationship between permeability and liquid saturation for the unsaturated hydrogeologic units is simulated through composite characteristic curves that combine the effects of the porous matrix and the fractures.[2,6] The available data measured on cores from deep boreholes, which were compiled by Montazer and Wilson[6] are used for the properties of the rock matrix of the different units.[6] Recent measurements of rock properties published by Flint and Flint,[11] such as porosities, air and water hydraulic conductivities, and grain densities, are used to refine the properties of the nonwelded hydrogeological units. Because zeolitization greatly reduces the hydraulic conductivity of the rock, the influence of zeolitization is considered in the model by changing the hydraulic parameters for areas where the rocks are highly altered.

Simulations were performed using a one-dimensional submodel to evaluate the effect of the element size on the numerical results. These studies were conducted to determine the sensitivity of the results to the number of vertical elements and their fineness, especially around unit boundaries. The rock properties were taken from a previous report by Rulon et al.,[1] and infiltration rates of 0.1 and 1.0 mm/yr were used. Further simulations, with element thicknesses of 1 m around the unit boundaries, produced very similar results and indicated that the vertical grid consisting of nineteen elements gives sufficiently accurate results. Figure 11 shows an example of saturation profiles obtained for a 710-m-thick section. An infiltration rate of 0.1 mm/yr was used and the entire section was divided into a coarse grid (19 blocks) and a fine grid (46 blocks).

Steady-state numerical simulations are currently (1991) being performed to evaluate the occurrence and magnitude of lateral flow within the various blocks delineated by major faults and to evaluate the formation of perched-water bodies at the lithologic and structural boundaries between different hydrogeological units. The influence of fault zones and the infiltration distribution on the liquid-water flow through the potential repository unit and to the water table will also be evaluated for various cases.

VI CONCLUDING REMARKS

Lawrence Berkeley Laboratory, in collaboration with USGS, is developing a three-dimensional numerical model of the unsaturated zone at Yucca Mountain. Current studies have focused on the design of the vertical and horizontal grid systems, which will form the framework for subsequent simulations. The nodal distribution in the model is based on the locations and distribution of: boreholes, varying infiltration characteristics, hydrogeologic units, major faults, and water-level data. Horizontal nodal points are designed to allow direct comparison of model results and field data, to explicitly describe fault properties, and to accurately depict the aerial distribution of zones of infiltration. These infiltration zones are divided into uncovered ridgetops, talus covered sideslopes, and alluvial filled washes. The numerical grid is aligned along surface traces of high-angle faults, such as the Ghost Dance, Abandoned Wash, and Dune Wash Faults, and along northwest-trending strike-slip features to facilitate inclusion of fault-zone properties as more data become available during characterization efforts. The vertical grid appears adequate to accomodate variability in the properties of hydrogeological units. Fine elements are used near boundaries of hydrogeological units where abrupt thermodynamic gradients, lateral flow, and zones of perched water are likely to occur.

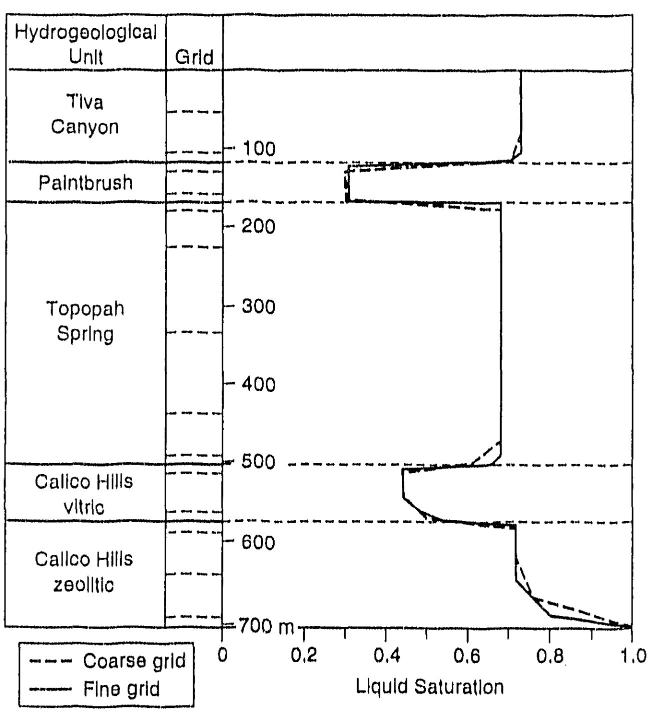


Fig.11 Liquid-saturation profiles for a schematic vertical column of elements from the site-scale model (infiltration rate 0.1 mm/yr).

Major hydrogeological units within the unsaturated zone throughout the site-scale model area include, in descending order, the Tiva Canyon welded unit, the Paintbrush nonwelded unit, the Topopah welded unit, and the Calico Hills nonwelded unit. The Tiva Canyon welded unit crops out over most of the model area and dips to the east by 5° to about 30°, except in the northern part of the area where the unit dips southeastward. The Paintbrush nonwelded unit ranges in thickness from about 25 m to 170 m and is thickest in the northwestern part of the site-scale model area. The Topopah Spring welded unit ranges in thickness from about 60 m to 340 m. This unit is thickest near the central part of the model area and thins abruptly to the northeast. The establishment and refinement of the site-scale unsaturated zone model is anticipated to become an important tool to help guide and test future data needs.

ACKNOWLEDGMENTS

This work was performed under U.S. Department of Energy Contract No DE-AC03-76SF00098, and DE-AI08-78ET44802 administered by the Nevada Operations Office, in cooperation with the U.S. Geological Survey, Denver. The authors thank Y.W.Tsang and K.Karasaki for reviewing this paper.

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5/06/92