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THE USE OF TOUGH2 FOR THE LBL/USGS 3-DIMENSIONAL SITE-SCALE MODEL OF YUCCA MOUNTAIN, NEVADA

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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) and Bodvarsson et al. (1994, 1995).

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.

The computer code TOUGH2 developed by K. Pruess (1990) 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. In this paper, we also describe the three-dimensional site-scale model emphasizing the numerical grid development, and then show some results in terms of moisture, gas and heat flow.

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). 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 subsurface formation 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). Isopach maps of these most important hydro-geological units were prepared by Wittwer et al. (1992) based on all available borehole data at the time and these are used in the model with appropriate modifications as new data became available.

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., 1994). Fourteen different 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.

The fracture medium properties were developed using the equivalent continuum approximation developed by Klavetter and Peters (1986), which assumes capillary equilibrium between the fractures and the adjacent rock matrix blocks.

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 characteristic curves similar to the bedded tuffs of the Paintbrush units.

NUMERICAL GRID

The TOUGH2 computer code used in the site scale model study is based on the integrated finite-difference method and therefore, allows to create irregular gridblocks. The grid was designed in order to accommodate the spatial distribution of main hydrogeological units, the effects of major structural features, the sharp thermodynamic gradients at the boundaries between hydrogeological units, and relevant surficial information.

The three-dimensionnal numerical grid consisting of about 5000 elements and 20000 connections was designed in two steps. First, all available surficial information was used to create an horizontal two-dimensional grid. Then, data from isopach maps of hydrogeological units were integrated to vertically develop the horizontal grid between the ground-surface and the water table, thus creating the 3D grid. This step of grid generation required a lot of manual

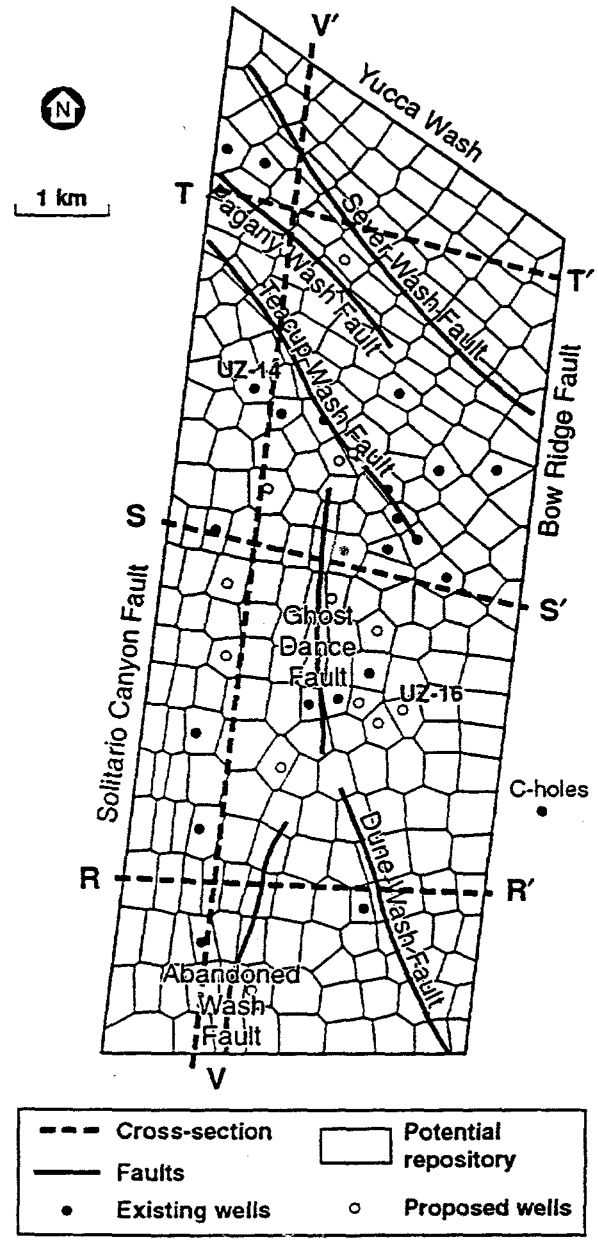

Figure 1. Areal extent and horizontal grid of the 3-D site-scale model. Also shown are some of the major faults in the area.

manipulation in order to handle small elements at interfaces and the fault offsets.

Horizontal Grid

The locations of the nodal points for the horizontal two-dimensional grid were determined based on different data. They are the locations of existing or proposed boreholes, the major faults, such as the Ghost Dance fault, Dune Wash fault and Abandoned Wash fault, the distribution of the different infiltration zones properties and rate, and different exposed rock types. The grid blocks are also designed to have gradual changes in element sizes in order to minimize errors in representing gradients in thermodynamic conditions, hence minimizing model inaccuracies.

After all the nodal points were located, an automatic numerical grid generator was used to develop the horizontal grid. Later (1994) this 2D horizontal grid was modified to include the trace of the ESF by aligning elements along it.

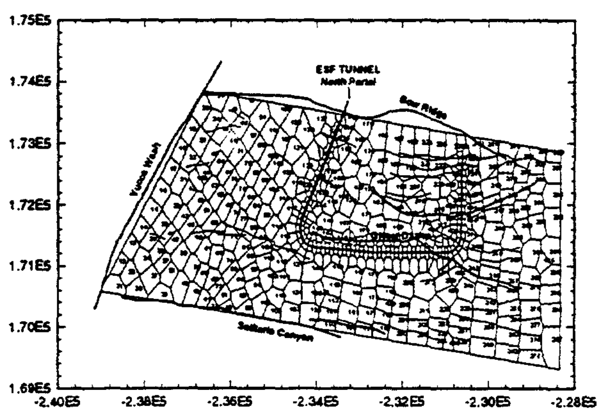

Figure 2. Horizontal grid for the site-scale model including the trace of the ESF tunnel.

Vertical Grid

The vertical grid (Fig. 3) has seventeen layers of grid-blocks which represent, as closely as possible, the lithological variations within the main units. The offsets along the three fault zones (Ghost Dance-, Abandoned Wash-, and Dune Wash faults) were explicitly represented within the three-dimensional grid. The grid blocks along the fault horizontally connect the sublayers on each side of the faults through a double number of gridblocks. This model geometry is consistent with the complex geology of this heavily faulted region.

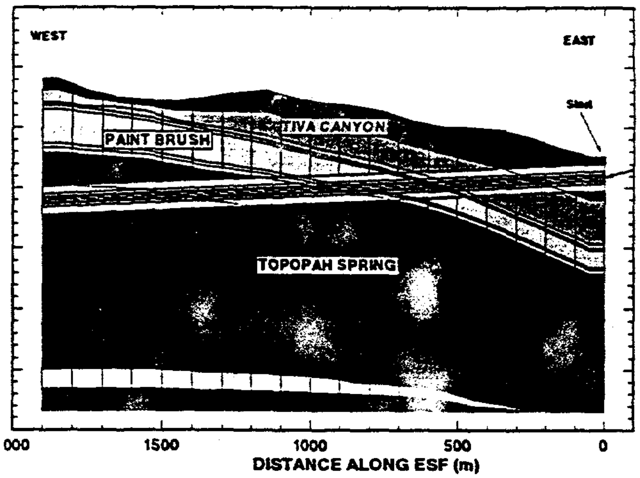

Fig. 3. Vertical cross section including the ESF Tunnel.

Gridblocks with Offsets

A major problem for gridblocks along the fault traces was the proper way to connect the sharp offsets of the units on two sides of the fault through the fault itself.

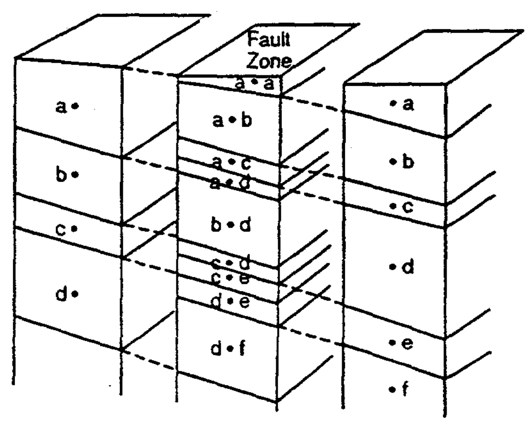

Figure 4. Example of grid design by fault zones.

This was solved by creating a double number of sublayers for the fault-gridblocks, and modifying the mesh generator to connect them by their common interfaces to the adjacent gridblocks. A schematic representation of this grid design is given in Figure 4. To obtain the right volumes and interfaces, dummy elements were introduced in the faults and in the columns adjacent to fault columns. These dummy elements helped generate the proper connections and maintain the observed fault offsets.

New 3D Grid Generator

We are developing a new flexible grid generator with arbitrary 3D grids and fault offsets (Fuller et al., 1995). The

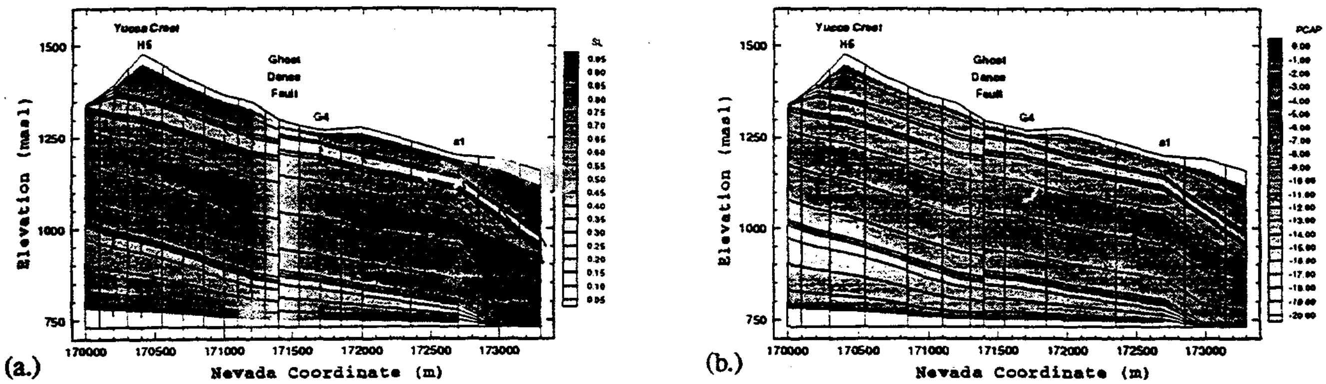

Figure 5. Two-dimensional cross section S-S' showing calculated distributions of liquid saturation (2a) and capillary pressure (2b).

data input for the generator will be a combination of the following:

(1) Surface and subsurface location of wells and tunnels. Location, dip, strike and offset of faults as well as the thickness of fault zones.
(2) Description of each layer or horizon (hydrogeologic) unit: depth to each unit (isopach), dip of layers, thickness of layers, elevation of layers.

Given the combination of the above data of a flexible 3-D finite element mesh, element and connections information is generated for input to a numerical simulation routine e.g. TOUGH2. We require for all the elements (including the fault and boundary elements), the interface areas, the interface distances, the element volume at each xyz coordinate.

The grid generator is now completed to the point that the site-scale model grid can be automatically generated in less than a minute using several input files containing the data listed above. New faults can readily be added to the model with arbitrary offsets.The grid generator is now being extended to the explicit modeling of tunnels and wells in which transition from radial to rectangular geometry is desired.

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. In these simulations the faults were modeled assuming either "capillary barrier" behavior or "permeable fault" behavior. Figure 5 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 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. Typically steady-state results, with insignificant changes in saturation (<0.001) are reached after about 1016 to 1017 seconds (3x108 years) of simulation time.

The results shown in Figure 5 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. 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. 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 5b).

Figure 6 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 6a 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 6b, 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 6a. 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 model). In the horizontal slice representing the bottom of the Topopah Spring units (Figure 6c), 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 6d).

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

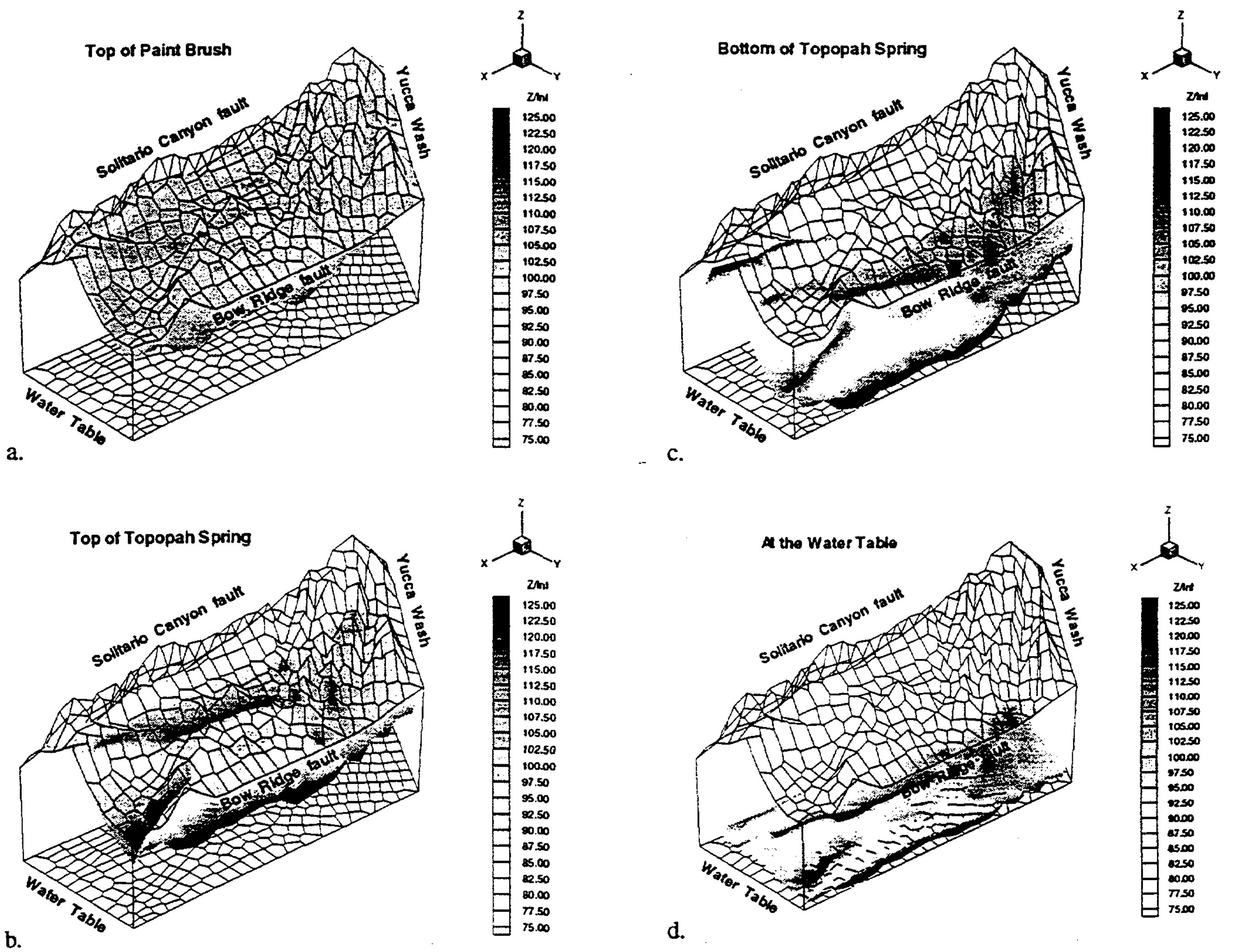

Figure 6. Calculated normalized vertical moisture fluxes (% of infiltration at ground surface) at different depths in the site-scale model for the case of "capillary barrier" faults, and an uniform areal infiltration rate of 0.1 mm/year.

some regions north of Ghost Dance Fault near one-dimensional vertical moisture flow is exhibited from these model calculations.

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.

A series of numerical simulations were also performed using non-uniform distribution of infiltration at the ground surface. Due to space limitations, these simulations are not described here, but the reader is referred to Bodvarsson et al. (1994).

MODEL EFFICIENCY

In order to investigate the model efficiency, we performed 1-D, 2-D, and 3-D simulations using the TOUGH2 standard version as well as a decoupled version which only solves for moisture flow. We used a 0.1mm/year uniform moisture infiltration at the top for all of these runs. An additional layer was put on the top of the mountain to simulate the atmospheric condition for the fully coupled runs. The observed temperature gradient of Yucca Mountain was prescribed in the simulations.

For all of the cases considered, the problem was simulated to steady state conditions. In general, steady state conditions were considered to be reached after the outflow of water at the water table equalled within a fraction of a percent the total infiltration prescribed at the ground surface. For cases with gas flow, similar mass balance was performed for this component. In most cases, steady state conditions were reached after 10^{13} seconds (3×10^6 years). As expected, this was the case independent of the dimensionality of the model (1-D, 2-D and 3-D). The computer execution time (CPU time) to reach steady state varied from less than a minute for the 1-D runs, typically 30 minutes for the 2-D runs and 2 to 15 hours for the 3-D runs. These runs were made on a Pentium (90MHz) personal computer.

The single component moisture flow runs reach steady state in around one hour, whereas the fully coupled gas, moisture and heat flow runs take 10-20 hours of CPU time to reach steady state. It should be noted that one must be very careful in prescribing boundary conditions in order to get meaningful simulation results.

SUMMARY

The development of the three-dimensional site-scale model of Yucca Mountain continues with the purpose of guiding the site characterization effort. A large effort has been devoted to the development of an automatic grid generation for complex geological settings such as Yucca Mountain. 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 model has been modified to include the Exploratory Studies Facility (ESF) and is being extended in all directions to include more wells.

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