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TESTING CONCEPTUAL UNSATURATED ZONE FLOW MODELS FOR YUCCA MOUNTAIN, NYE COUNTY, NEVADA

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ABSTRACT

An important component of site characterization and suitability assessment of the proposed nuclear waste repository at Yucca Mountain, Nevada is determination of the most appropriate conceptual model of the hydrologic mechanisms governing saturated and unsaturated flow for the site. As observers in the INTRAVAL Unsaturated Zone Working Group, L. Lehman & Associates conducted a modeling exercise which numerically examined alternative conceptual flow models. Information was provided to the Working Group by the US Geological Survey. Additional published data were utilized to fill in data gaps and to provide additional confidence in results.

Data were modeled utilizing one and two dimensional matrix and fracture numerical models. Good agreement was obtained using a 2-dimensional dual porosity fracture flow model. Additional measures are needed to constrain the field conditions enough to validate conceptual models using numerical models. Geochemical data on tritium, chlorine-36, or carbon-14 concentrations or temperature profiles which can give estimates of time since recharge for water in the unsaturated zone, are needed to eliminate the non-uniqueness of various model solutions.

INTRODUCTION

Yucca Mountain is currently being investigated as a potential nuclear waste repository. One of the main questions regarding the performance of a repository at Yucca Mountain has been the determination of water flux through the unsaturated zone. An international group called the International Transport Code Validation Study (INTRAVAL) was formed to examine the question of validation for flow and transport models. The INTRAVAL test case for the unsaturated zone was performed using data specific to Yucca Mountain and attempted to validate site flow models. The state of Nevada participated in the INTRAVAL process as an observer as part of their technical role. The independent modeling exercises performed for the state of Nevada are presented in this paper.

SITE DESCRIPTION

Located in southwestern Nevada, approximately 150 km northwest of Las Vegas, Yucca Mountain lies within the southern Basin and Range Province. The climate is arid with yearly precipitation ranging from 150 to 200 mm/yr. Vegetation is sparse and concentrates near the bottoms of washes and ravines.

Yucca Mountain is composed of a north-south trending block of volcanic tuff bounded on the east and west by normal faults. The tuff units were deposited during discrete events upon pre-existing Paleozoic carbonates. Basin and Range type faulting has broken the bedrock into north-south trending irregular blocks. The blocks between faults contain numerous fractures predominantly oriented toward the northwest.[1] Figure 1 shows a generalized cross-section of the area being considered for the waste repository. The water table within these rocks exists at more than 400 meters below the surface and may be locally confined.

AVAILABLE DATA

Data were provided to the INTRAVAL working group by the USGS in the form of a composite stratigraphic column based on samples collected from surface transects, with hydrologic properties for each lithologic unit. As part of the site characterization program at Yucca Mountain shallow and deep wells have been drilled using air methods though the unsaturated zone. Data from the shallow wells UZN-53, 54 and 55 including density, porosity, water content and lithology were supplied to depths of 100-120 meters. These data were to be used to calibrate the numerical models in order to predict a water content profile for an adjacent deep hole, UZN-16. A blind prediction was to be done with access to stratigraphy and porosity data from UZN-16, but without access to water content data. Water contents were provided after the predictions were submitted.

MATRIX MODEL DESCRIPTIONS

For the 1-dimensional and dual porosity fracture models, an integrated finite difference computer code V-TOUGH,[2] which is an enhanced version of the TOUGH code,[3] was used. This simulator calculates multi-phase fluid flow in unsaturated porous media under non-isothermal conditions. For this study isothermal conditions were assumed and enforced upon the model simulations.

A. 1-D Matrix Models

The initial conceptual model of unsaturated flow at Yucca Mountain was 1-dimensional and included uniform infiltration along the upper surface of the volcanic tuff stratigraphy. Flow was assumed to occur predominately through the matrix from the surface, through the repository horizon at the Topopah Springs Member, continuing to the water table.

The 1-dimensional simulations consisted of 4, 7 and 11 hydrologic unit configurations representing the stratigraphic column at Yucca Mountain. They are based on the composite data provided by the USGS. Hydrologic units were inferred from the composite data based on a qualitative grouping of similar-valued measured properties. Conductivities were estimated as the geometric mean of measured conductivities from inferred units. Porosity and other properties were taken as the standard mean. Parameters used in the V-TOUGH Sandia Function (modified van Genuchten Equation) to represent the water retention characteristics were fitted to the available water retention data by minimizing the sum of the squared error between the function and the data.

The upper boundary of the matrix elements simulate atmospheric conditions. Gas pressure at the upper boundary was fixed at 100,000 Pa (1 atm) and saturation near 0 for the simulations. Pressure at the lower boundary was fixed at 100,000 Pa and saturation at 1. The left and right domain boundaries were modeled as no flow boundaries.

The initial state of the model elements is such that the column is nearly in equilibrium with about 0.005 mm/yr of downward infiltration. Two different infiltration scenarios were assumed. In the first, a steady state infiltration rate of 0.01 mm/yr was used. The second was a transient "pluvial" infiltration signal. The pluvial infiltration history is based on work done by Spaulding.[4] It was modeled with a pluvial maximum at about 18,000 years ago with infiltration of 0.054 mm/yr.

B. 2-D Matrix Models

A 2-dimensional model of a vertical cross-section of the Yucca Mountain site was constructed. The vertical section contains seven distinct porous media with hydraulic properties represented by the van Genuchten equation for both the fluid retention and the hydraulic conductivity. The vertical section was taken to be 750 meters wide and 488 meters deep with the water table as the lower boundary. The left vertical boundary was taken to be a faulted zone beneath the Solitario Canyon west of Yucca Mountain. A vertical line of symmetry was selected at a distance of 375 meters due east of this fault and a cross-section between these vertical boundaries modeled.

The finite element method was used to solve the 2-dimensional form of the Richards equation for the 2-

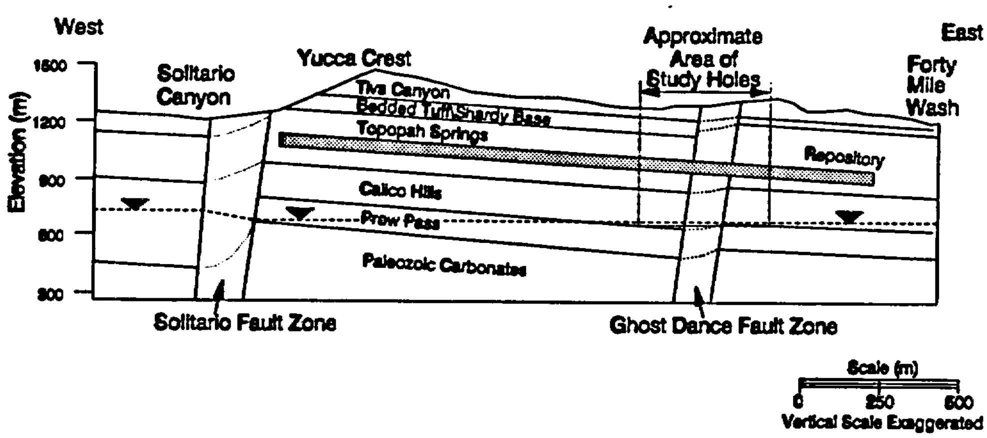

Figure 1. Generalized cross-section of the proposed repository at Yucca Mountain Nevada showing general stratigraphy and study location.

dimensional model. A computer program implementing the finite element solution, called TWOD[4] was applied in the analysis.

The initial condition for all 2-D runs was assumed to be that of static equilibrium or no flow and simulations were performed to steady state. It was assumed that water infiltrated at a mean rate of 0.1 mm/year through the top boundary of the region, while water infiltrated through the length of the fault boundary on the west at two rates; 0.1 mm/year for run E-1 and 1.0 mm/year for run E-2.

MATRIX MODEL RESULTS

The results of some typical 1-dimensional simulations are shown in Figure 2. The modeled water content profiles are plotted versus depth and compared to measured data 95% confidence intervals. The measured water content confidence intervals are found by grouping the data to include all measurements found in each 5 meter span. Statistics were then calculated for each 5 meter span. 95% confidence intervals were calculated as 2 standard deviations above and below the mean. Simulated water content profiles are shown nearly at steady state except for the run using the pluvial infiltration signal which covers 45,000 years then terminates.

All of the 1-dimensional modeling attempted in this exercise did a poor job of matching the observed water content profiles. Additional units did not improve the fit. Rather, fit seemed to deteriorate with the addition of more units. The relatively wet conditions measured within the upper high conductivity unit (40-70 meters depth), co-existing with the unsaturated conditions in the low conductivity units, such as the Tiva Canyon Unit and the Topopah Springs Unit below, could not be modeled with 1-dimensional geometry and realistic infiltration input and while keeping properties within measured bounds. The water retention properties in the Bedded/Shardy Base Unit at 40-70 meters depth, causes water to be held at higher saturation in the units above and below. This is due to the fact that at similar pressures the equilibrium saturation for this unit is much lower.

The infiltration rate and vertical flux through a 1-dimensional matrix only flow model is limited by the saturated conductivity of the tightest unit. Higher flux rates result in high pressure gradients and extensive perched water or saturated zones in the matrix, conditions not observed in the data available for this exercise. This meant that infiltration magnitudes for 1-dimensional matrix models were limited to maximums of from about 0.01 mm/yr to 0.10 mm/yr. Varying the infiltration rate did not reconcile the difference in degree of fit between the units. Unsatisfactory fit of the 1-dimensional model to the data for many model configurations led to the development of a 2-dimensional model.

Two water content profiles are given in Figure 3, one for each of the fault flux rates. These profiles are for a vertical transect taken along the line of symmetry of the 2-dimensional domain. The 2-dimensional model results were similar to the 1-dimensional results. Conditions near 40-70 meters depth (Shardy Base, Non-Welded, Bedded Tuffs) were modeled consistently drier than the data measurements. When higher infiltration rates were modeled areas of perched water appeared at the top of the Topopah and base of the Tiva Canyon Units.

Two-dimensional effects do not seem to be able to account for the relatively wet conditions measured in the high conductivity zone. Water movement laterally through the matrix was insufficient to overcome the water retention relationships between this unit and the adjacent units.

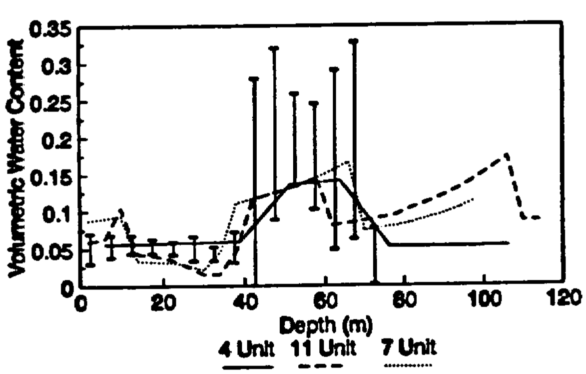

Figure 2. Comparison of simulated water contents using the 1-dimensional, matrix only models with confidence intervals for working group data from the shallow calibration holes UZN-53, UZN-54 and UZN-55.

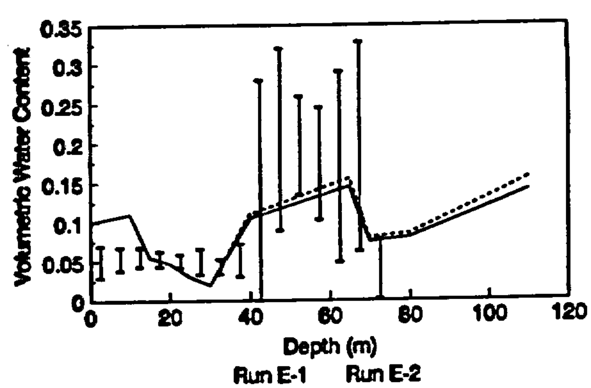

Figure 3. Comparison of 2-dimensional 7 unit runs with confidence intervals for working group data from the shallow calibration holes UZN-53, UZN-54 and UZN-55.

Using the recharge maps of Harrill[8] for Nevada, recharge water volume within the Yucca Mountain drainage was calculated at about 6 mm/yr/m^2. Hokett et al.[9] simulated precipitation on bare and vegetated plots of alluvium near Yucca Mountain and found that 40-50 mm/yr of water infiltrated to a depth of 1.2 meters. The Depression Focused Recharge Model, (DFR)[10] was also used as part of our study to estimate recharge to valley bottoms and faulted areas. The model incorporates simplified topography, surface material hydrologic properties and statistically simulated weather to perform a water balance. Estimates of recharge to wash and valley bottoms based on this model ranged from 8 mm/yr to 160 mm/yr.

These high rates of recharge have not been previously utilized in unsaturated zone modeling efforts for Yucca Mountain. Previous estimates have been based on inverse modeling using 1-dimensional matrix only flow models and so have been limited to 0.01 to 0.1 mm/yr. If the high estimates of recharge are reasonable then some mechanism other than 1-dimensional or 2-dimensional matrix flow, such as fracture flow, must prevail at the mountain.

FRACTURE MODEL DESCRIPTION

The conceptual model upon which our fracture model is based can be outlined as follows. Yucca Mountain consists of four subhorizontal hydrologically distinct matrix zones with distinct properties as shown in Tables 1 and 2. Three of the four units are significantly fractured while Unit 2 is not.[1] The fracture surfaces are coated with minerals that reduce the conductivity between the matrix and fracture to 1/10 or less of the non-coated value.[5] The fractures are vertically continuous in the units where they exist and are open to the atmosphere at the top and water table at the bottom of the column.

Table 1. Fracture Model Hydrologic Properties.

Model Unit	Geologic Unit	Depth Interval (m)	K_s (m/s)	Porosity
1	Tiva Canyon	0 - 44	5.25E-11	0.076
2	Bedded/Shardy Base	44 - 68	2.64E-6	0.388
3	Topopah Springs	68 - 396	6.18E-11	0.118
4	Calico Hills	396 - 476	4.78E-11	0.240
FRACTURE A*	Fracture	0-44, 68-476	8.15E-3 - 0.130	0.990
FRACTURE B	Fracture	0-44, 68-476	8.15E-3 - 0.130	0.990
FRACTURE C	Fracture	68-476	8.15E-3 - 0.130	0.990

Matrix data from working group composite data and holes UZN-53, UZN-54 and UZN-55.
* Fracture parameters based on Wang & Narasimhan (1985), and Spengler & Chornack (1984).

Table 2. Fracture Model V-TOUGH Sandia Function Parameters.

Unit	λ	S_{lr}	S_s	$1/P_o$ (1/Pa)	P_{max} (Pa)
1	0.21	0.04	1.0	1/130,000	5.0e+9
2	0.24	0.04	1.0	1/22,000	5.0e+9
3	0.24	0.04	1.0	1/150,000	5.0e+9
4	0.24	0.15	1.0	1/150,000	5.0e+9
FRACTURE A*	0.45	0.04	1.0	1/600	1.0e+9
FRACTURE B	0.45	0.04	1.0	1/10,000	1.0e+9
FRACTURE C	0.45	0.04	1.0	1/30,000	1.0e+9

Matrix data from working group composite data and holes UZN-53, UZN-54 and UZN-55.
* Fracture parameters based on Wang & Narasimhan (1985).

It is assumed rain water and snow melt generally runoff too rapidly to infiltrate much into the upper matrix unit and so tend to run into fractures open at the bedrock surface. Flow within fractures is initiated when input is higher than matrix conductivity. Water may also infiltrate areas of alluvium at canyon bottoms eventually reaching highly fractured fault zones below. While there is a net inflow of water to the fractures, the upper matrix experiences net evaporation. This is due to the tendency of water to run off these tight rock units when it is available causing evaporation to dominate the mass balance of the upper matrix.

Figure 4 shows the geometry of the dual porosity fracture model. The matrix stratigraphy is represented as a block of 4 hydrogeologic units, identical to those used for the 1-dimensional matrix only model. Except for Unit 2, the block is penetrated by regularly spaced vertical fractures. The fractures are spaced 3 per horizontal meter with average apertures ranging from 200-400 microns (0.0002-0.0004 m). The no flow boundary at left represents the centerline of an average matrix block, which is attached at the right to fracture elements. The fracture element is also bounded by a no flow boundary at its right. The width of the matrix elements represents a characteristic matrix half length of 0.15 meters between fractures. Fractures do not penetrate Unit 2 but are vertically connected to it.

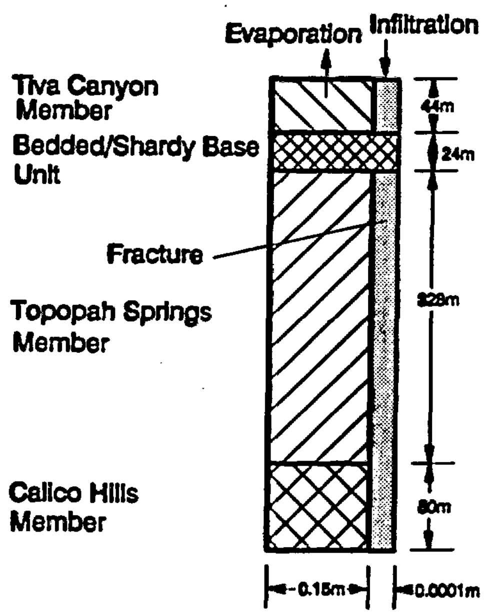

Figure 4. Schematic of conceptual geometry for the dual porosity fracture model of unsaturated flow at Yucca Mountain simulated using the V-TOUGH computer code[1].

The fracture conductivity is calculated based on the "cubic law" for flow within two parallel plates.[7] Several apertures were used for calculation of the saturated conductivity to explore sensitivity. Three different characteristic curves for fracture water retention were also used due to lack of measurements of these properties for fractures at Yucca Mountain. For these three curves, Sandia Functions were used to model fracture properties. The air entry value was varied from 600 Pa to 30,000 Pa while other parameters were held constant.

The uppermost fracture element contains a water source which may be varied in time to simulate transient infiltration. A water sink simulating net evaporation is placed in the uppermost matrix element. Table 3 outlines the features of the 4 calibration simulations presented here. The initial state of the model elements is approximately in equilibrium with the water table.

Table 3. Features of the Fracture Model Calibration Runs.

Run	Infiltration History	Aperture for Conductivity (μm)	Fracture Water Retention Curve
F-1	Pluvial	100	A
F-2	Pluvial	100	B
F-3	5 mm/yr	200	A
F-4	5 mm/yr	400 (upper) 800 (lower)	A (upper) C (lower)

FRACTURE MODEL RESULTS

The results of the fracture model calibration simulations are shown in Figure 5. The modeled water content profiles are taken from the matrix elements of the model. Simulated water content profiles are shown approximately at steady state except for the runs using the pluvial infiltration signal which covers 45,000 years then terminates.

Simulation F-4 produced the best fit and combines higher fracture apertures with distinct characteristic curves for the upper fracture (above 40 m) and the lower fracture (below 70 m). Water retention for the lower fracture is modeled with a higher air entry value which makes it more like the matrix than the upper fracture. This will cause the lower fracture to hold more water at higher capillary suction than the upper fracture. The physical basis for assuming distinct water retention curves for fractures in the upper unit and the lower units is that fractures within these units probably have different densities, amounts of fillings, surface roughness, and aperture distributions all of which will effect the unsaturated properties.

The fracture models show that the high saturation existing in the area of Unit 2 may be explained by infiltration greater than the matrix will allow. This flow arrives through the highly fractured units above. It causes storage in the relatively unfractured Unit 2 to increase until it is wet enough to allow the flow to continue down the fractures below. The relationship between the fracture and matrix hydrologic properties is crucial to this analysis. Much good matrix data are available but information on fracture properties is limited and so assumptions were made regarding them in this study.

For prediction of the water content at the deep hole UZN-16 the configuration of simulation F-4 was used. Figure 7 shows the 95% confidence intervals for water content data calculated at 10 meter groupings compared to the fracture model simulation. An air entry value of 10,000 Pa was used for the lower fracture elements. In the Bedded/Shardy Base Unit (40-70 meters) our profile captures the highest values. In the deep Calico Hills Unit below the repository horizon, the simulated profile is drier than the data. The simulated profile did not include the Prow Pass Unit at 450 meters depth. This simulation matches up well with the Tiva Canyon Units and the Topopah Springs Unit.

Figure 8 shows a comparison of the saturations predicted for UZN-16 compared to the saturations calculated from the measured data. The predicted saturations err on the conservative side (high), for the Bedded/Shardy Base Units but reflect an average range throughout the Topopah Springs Unit. The discrepancies are assumed to be due to the porosity

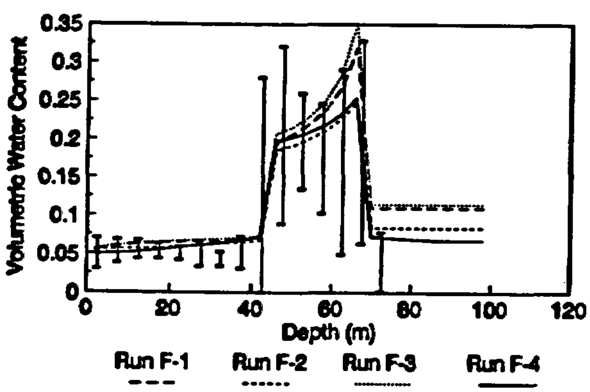

Figure 5. Comparison of water contents modeled in matrix elements for the dual porosity fracture model with confidence intervals for working group data from the shallow calibration holes UZN-53, UZN-54 and UZN-55.

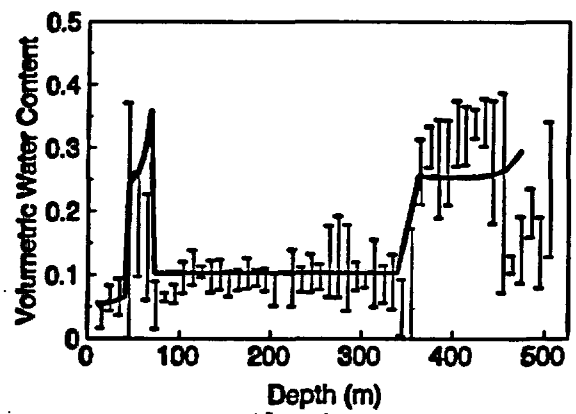

Figure 7. Predicted water content profile using the fracture model for UZN-16 compared with 95% confidence intervals of measured UZN-16 water content data.

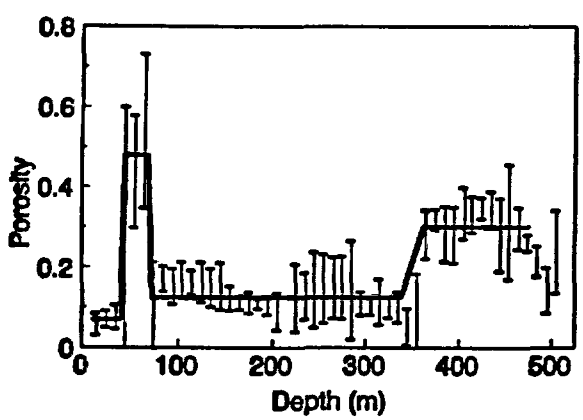

Figure 6. Porosity used for the fracture model prediction of the UZN-16 measured water content profile compared with 95% confidence intervals for the UZN-16 data.

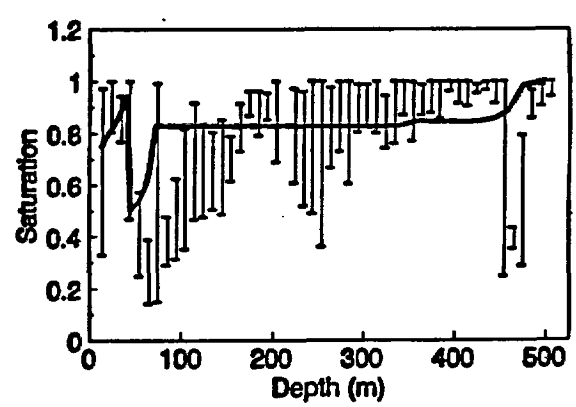

Figure 8. Predicted saturation profile using the fracture model for UZN-16 compared with 95% confidence intervals of saturation based on UZN-16 measurements.

values used for each layer. Had these runs been calibrated against saturation, then a different layering scheme would likely have been developed.

It is worthwhile to note the differences between the calibration set and the UZN-16 data. The most noticeable difference is that the water content profile is much drier in the Bedded/Shardy Base Unit at UZN-16 than in the calibration set. Further the porosity values for this unit were 25% higher at UZN-16. UZN-16 is located at the bottom of the wash while the calibration holes were located upstream and off the wash bottom. Alluvial cover was also much thicker at UZN-16. These differences may indicate different hydrologic properties or flow processes exist, even though the physical distance between the holes is small.

CONCLUSIONS

The modeling performed in this study allowed water content profiles to be reasonably matched using larger infiltration rates than have previously been utilized at Yucca Mountain. Results indicate that water content or saturation profiles alone are not sufficient to validate infiltration rates. Additional criteria which are indicative of the time history of the fluid will be required for model validation, such as geochemical tracer and/or temperature data.

The choice of conceptual model may be the most sensitive component in a validation study, especially in areas like Yucca Mountain where focused recharge and non-equilibrium conditions with respect to flow and temperature are occurring. The most sensitive parameters for this model of Yucca Mountain unsaturated flow are the fracture and matrix unsaturated conductivity curves and water retention characteristics. These determine the degree of wetting in the model elements for a given infiltration rate. Unfortunately these are probably the least understood of the hydrologic properties measured thus far at the Yucca Mountain site.

The water content profiles we have simulated using this fracture model are not extremely sensitive to infiltration magnitudes or functional shape of the infiltration signal. Values below about 1 mm/yr cause simulations that appear too dry and those above 10 mm/yr appear too wet. But, varying the infiltration magnitudes in the range of 1 to 10 mm/yr serves mainly to fine tune certain aspects of the modeled profile rather than cause large scale changes in the profile shape or magnitudes. The lack of fit between the water content data and the fracture model, as well as 1 and 2-dimensional matrix models, was not large enough to eliminate either conceptual model.

At the time scales we are able to examine using this model, fracture coating has little impact on modeled water content and at 10,000-50,000 years, depending on the degree of flow inhibition between fracture and matrix, a near steady state flow condition is achieved.

Calibration should be performed against measured parameters, such as water content, as opposed to calculated properties, such as saturation, where feasible. Errors in measurement of porosity and water content are combined in the saturation calculation causing relatively large uncertainty in the saturation values.

It is recommended that the following data be collected in order to narrow the range of infiltration estimates for Yucca Mountain:

1) Runoff and infiltration data, especially in areas of focusing.
2) Information illuminating the time history of fluid infiltration such as isotope chemistry and temperature.
3) Data on fracture properties including unsaturated water retention and conductivity properties.

From the standpoint of performance assessment for a nuclear waste storage facility the flux rate and flow velocities are the crucial parameters in the unsaturated zone flow. These will determine the fastest path to the accessible environments and the dosage that may result. From this point of view a fracture flow model, such as that presented here, represents a more conservative characterization of the flow system. The higher velocities and flux rates this model predicts compared to the 1-dimensional matrix models provide a more likely upper bound to the flux rate that a repository at this site may experience. Given the lack of discriminating data to eliminate any of the prominent conceptual models, the most conservative, with respect to safety should be emphasized. More work needs to be done collecting fracture information and testing fracture models before accurate performance assessment can be done.

REFERENCES

1. SPENGLER, R.W., and M.P. CHORNACK, "Stratigraphic and structural characteristics of volcanic rocks in core hole USW C-4, Yucca Mountain, Nevada, Nye County, Nevada," USGS Open-File Report 84-789 (1984).

2. NITAO, J.J., "V-TOUGH An enhanced version of the TOUGH code for the thermal and hydrologic simulation of large scale problems in nuclear waste isolation," Rep. UCID-21954, Lawrence Livermore National Lab (1989).

3. PRUESS, K., "Tough user's guide", Sandia National Laboratories and Division of Waste Management Office of Nuclear Material Safety and Safeguards, NUREG/CR-4645, U.S. Nuclear Regulatory Commission (1987).

4. SPAULDING, G. W., "Vegetation and climates of the last 45,000 years in the vicinity of the Nevada Test Site, South-Central Nevada", USGS Open-File Report 83-535, (1983).

5. NIEBER, J.L., MUNIR, H., and Friedel, M. "A finite element model of unsaturated flow using simplex elements", US Bureau of Mines (1993).

6. THOMA, STEVEN G., DAVID P. GALLEGOS, and DOUGLAS M. SMITH, "Impact of fracture coatings on fracture/matrix flow interactions in unsaturated, porous media," Water Resources Research, Vol. 28, No. 5, (1992).

7. WANG, J.S.Y., and T.N. NARASIMHAN, "Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium," Water Resources Research, Vol. 21, No. 12, (1985).

8. HARRILL, J.R., GATES, J.S., and THOMAS, J.M., "Major ground-water flow systems in the great basin region of Nevada, Utah, and adjacent states," USGS Atlas HA-674-C, (1988).

9. HOKETT, S.L., G.F. COCHRAN, and S.D. SMITH, "Shallow vadose zone response to a simulated pluvial climate at a field site near Yucca Mountain, Nevada," Special Issue of Radioactive Waste Management and the Nuclear Fuel Cycle on the Yucca Mountain Project, (1991).

10. NIEBER, J.L., TOSOMEEN, C.A.S., and B.N. WILSON, "A stochastic-mechanistic model of depression focused recharge," Second USA/CIS (formerly USSR) Conference on Environmental Geology and Hydrology, Washington D.C., (1993).