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Field Testing and Associated Modeling of Potential High-Level Nuclear Waste Geologic Disposal Sites

Edited by G. S. Bodvarsson

December 15 and 16, 1997
Nuclear Waste Department
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Berkeley, California 94720

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc. and the Ernest Orlando Lawrence Berkeley National Laboratory, Under Contract No. DE-AC03-76SF00098.
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Yucca Mountain Field Testing

Session Chair: William Boyle DOE/YMSCO

J. Birkholzer
S.C. Blair
A. L. James
M. T. Peters
J.S.Y. Wang
An important issue for the long-term performance of underground nuclear waste repositories is the rate of seepage into the waste emplacement drifts. A prediction of the future seepage rate is particularly complicated for the potential repository site at Yucca Mountain, Nevada, as it is located in thick, partially saturated, fractured tuff formations. The long-term situation in the drifts several thousand years after waste emplacement will be characterized by a relative humidity level close to or equal to 100%, as the drifts will be sealed and unventilated, and the waste packages will have cooled. The underground tunnels will then act as capillary barriers for the unsaturated flow, ideally diverting water around them, if the capillary forces are stronger than gravity and viscous forces. Seepage into the drifts will only be possible if the hydraulic pressure in the rock close to the drift walls increases to positive values; i.e., the flow field becomes locally saturated.

In the present work, we have developed and applied a methodology to study the potential rate of seepage into underground cavities embedded in a variably saturated, heterogeneous fractured rock formation. The fractured rock mass is represented as a stochastic continuum where the fracture permeabilities vary by several orders of magnitude. Three different realizations of random fracture permeability fields are generated, with the random permeability structure based on extensive fracture mapping, borehole video analysis, and insight air permeability testing. A 3-D numerical model is used to simulate the heterogeneous steady-state flow field around the drift, with the drift geometry explicitly represented within the numerical discretization grid. A variety of flow scenarios are considered assuming present-day and future climate conditions at Yucca Mountain. The numerical study is complemented by theoretical evaluations of the drift seepage problem, using stochastic perturbation theory to develop a better understanding of the key processes involved.

We found that, for the conditions at Yucca Mountain, the heterogeneity in the flow domain is a key factor controlling the rate of seepage into drifts, because the “channelized” flow in high-permeability features promotes local ponding conditions close to the drift walls. Figure 1 shows a typical flow field in the vicinity of the drift, presenting saturation contours in three horizontal slices of the 3-D model domain for a future climate scenario of 200 mm/yr percolation flux. In the horizontal plane just above the drift (middle horizontal slide), liquid accumulates at the drift crown as the vertical gravity-driven flow is diverted around it, while in the horizontal plane below the drift a low-saturation shadow develops. In addition to this flow perturbation effect, the saturation contours reflect the heterogeneity of the model area, showing several locations where “channelized” flow accumulates creating high saturation values dependent on local permeability contrasts. In fact, at some of these locations, the saturation reaches unity, representing a local ponding condition. Obviously, the probability that local ponding occurs is highest near the stagnation point at the drift crown. Eventually, seepage into the drift occurs when a local ponding condition is encountered in a grid element adjacent to the drift wall.
Various flow scenarios have been simulated with percolation fluxes ranging from 5 mm/yr to 1000 mm/yr. Figure 2 summarizes the results of these simulation runs for the three realizations considered; it gives the total seepage flux into the drift as a function of the inflow at the top boundary of the model. The seepage flux is expressed as a percentage of the percolation flux over an area corresponding to the vertical shadow of the drift. As shown in Figure 2, seepage into drifts at Yucca Mountain is likely to start when steady-state percolation fluxes are tens of millimeters per year, the rate of seepage being strongly dependent on the assumed percolation scenario. Thus for future climate conditions with higher infiltration than the present state, drifts at Yucca Mountain will be vulnerable for water to enter. In comparison to results obtained for a homogeneous flow field, the seepage threshold fluxes are about an order of magnitude smaller, indicating the important effect of local saturation variations (local ponding). Indeed, as Figure 3 shows, the probability that local ponding conditions occur in the simulated flow fields is closely related to the potential rate of seepage into the drifts. The ponding probability given in this figure is calculated as the number of simulation grid blocks with positive or zero pressure values divided by the total number of grid blocks in the model area.

As the seepage probability is strongly dependent on details of the local heterogeneity around the drift walls, the variation between the three different realizations is significant. Particularly for small percolation fluxes where seepage locations along the drifts are sparsely distributed, the model domain size might not be sufficient to guarantee a large enough statistical sample. Ultimately, an analytical stochastic relationship would be very useful to estimate the potential rate of seepage as a function of different key parameters. As a first step in this direction, we evaluated the seepage probability from stochastic perturbation analysis by calculating the likelihood of local ponding in a heterogeneous flow field, without the presence of the drift. For the conditions found at Yucca Mountain, the results compared favorably with the numerical simulations which include the effect of the drift acting as an obstacle for the unsaturated flow (Figure 4). Sensitivities derived from these theoretical considerations indicate that, in addition to the assumed percolation scenario, the potential rate of seepage is strongly affected by the degree of heterogeneity and the mean fracture permeability.

The studies presented here were intended to be exploratory, with the specific conditions encountered at Yucca Mountain used as an example. We believe that the conceptual framework developed for the study of seepage into underground drifts at Yucca Mountain can be useful for a variety of other hydrogeologic and engineering applications. Our modeling effort was not intended as a complete stochastic analysis which would involve a Monte-Carlo type study of various random structures. In future work, we will examine a broader variety of heterogeneity fields and a larger number of realizations. Laboratory experiments and field tests on drift seepage in unsaturated heterogeneous fractured formations should be performed and used to confirm the theoretically and numerically derived conclusions from this paper.
Figure 1. Saturation contours for a percolation flux or 200 mm/yr.

Figure 2. Relative seepage rate for three realizations of random fields (Part 1, Part 2 and Part 3). Only those simulation runs are presented where seepage into the drift occurs.

Figure 3. Relative seepage rate and ponding probability for one realization (Part 1). Only those simulation runs are presented where seepage into the drift occurs.

Figure 4. Ponding probability for three realizations of random fields (Part 1, Part 2 and Part 3) compared to stochastic theory. Only those simulation runs are presented where seepage into the drift occurs.
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Estimates of Permeability Change in the Drift Scale Test Due to Thermal-Mechanical Effects

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Introduction

This paper presents results of a modeling study of changes in fracture permeability due to thermal-mechanical effects associated with the potential geological repository at Yucca Mountain. A methodology for estimating changes in permeability is developed and applied to the Drift Scale Test (DST) now being constructed in the Exploratory Studies Facility (ESF) at Yucca Mountain. Temperature, stress, and displacement of rock in the heated zone are presented along with predicted zones where slip on fractures may occur. The zones of predicted fracture slip are used as a basis for predicting where permeability may be changed. This new procedure goes beyond previous models that relate stress to strain or displacement, and provides information about rock response that is needed for design of future tests at Yucca Mountain. Our results also contribute to the understanding of coupled processes in the near-field environment of a repository.

Work Description

Our methodology is as follows: The thermal-mechanical (T-M) stress field for a cross-section of the DST is calculated at selected time intervals from the start of the DST. Input to this calculation includes the temperature field calculated using a hydrothermal model at each of the selected times. The shear stresses predicted on selected fracture planes are then used with the Mohr–Coulomb criterion to ascertain whether or not pre-existing fracture sets slip because of thermal stresses. Then, a fracture flow model that includes shear offset is used to estimate permeability changes for these fracture sets. The analysis is preliminary because it is 2-D and assumes an elastic medium whose properties do not change even when frictional slip and stress redistribution are likely to have occurred. The analysis also neglects permeability reductions as a result of increased normal stresses during heating.

Results

In broad terms three fracture sets have been identified in the ESF: set #1 is a steeply dipping set of fractures striking EW, set #2 is a steeply dipping set of fractures striking NS, and set #3 is a subhorizontal set of fractures striking EW. The axis of the heated drift is oriented EW; hence set #1 and set #3 have their strike perpendicular to the plane of our model. Thus, calculations of shear slip for vertical and horizontal fractures correspond to slip on fractures in set #1 and set #3, respectively.

To estimate regions of increased permeability for the DST we assume that permeability will double at any location where slip on fractures is predicted to occur. This assumption is based on combining the standard parallel plate relationship between flow in a fracture and the fracture aperture, with the fracture aperture distribution model of Brown. We also assume that slip on one set of fractures does not interfere with slip on any other set, and that changes in permeability predicted for one set of fractures can be
added linearly to changes in permeability predicted for the other sets. Thus, if a zone of enhanced permeability predicted for slip along a vertical set of fractures overlaps a zone of enhanced permeability predicted for a set of horizontal fractures, we predict a total permeability enhancement of 4 times for the overlapping region.

For the vertical fracture set our results show that the zone of enhanced permeability predicted to occur after one-half year of heating (i.e., heating to a temperature of ~100 °C at the drift wall) consists of two large V-shaped regions, one above and the other below the plane of the wing heaters that are deployed in the test. These areas are illustrated in Figure 1 using the light shading, and are essentially symmetric about the horizontal wing heater plane. The scale of these regions is on the order of the separation of the heated drift and the observation drift, and the width is on the order of half the drift separation (i.e., 13.5 m).

Regions of changed permeability for horizontal fractures occur between the Wing Heater plane and the Observation drift, and are centered at a distance about four meters above and below the plane of the wing heaters. These regions are illustrated with medium shading in Figure 1.

Permeability is predicted to be enhanced by 4 times in zones which occur where both fracture sets are expected to slip. These zones are also symmetric above and below the wing heater plane and comprise approximately one-fourth of the total area of permeability enhancement and are shown with the darkest shading in Figure 1.

We also predict that zones of enhanced permeability will grow with time, while maintaining the same basic shape formed after 0.5 year of heating. Zones of enhanced permeability may recede outward from the heaters as heating continues. Comparison with stress plots shows that the permeability is enhanced in areas of high thermal gradients as is expected from the formulation.

Conclusions and Discussion

We have provided a methodology that can now be used to estimate changes in permeability due to thermal-mechanical effects. Our result is quite intuitive. However, to our knowledge, no work to date has presented such a methodology for relating changes in the stress field to changes in the permeability of the rock mass. Our results are the first to show that thermal-mechanical effects on permeability may extend over significant portions of the heated region of a repository.

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Analysis of Uncertainty for 2-D Fracture Flow and Seepage Into an Excavated Drift

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Introduction

In this study we perform simulations of fracture flow by releasing a finite water pulse above an excavated niche in a 2-D vertical cross section. The amount of water that infiltrates the niche is observed through time and we analyze its sensitivity with respect to permeability, $k$ and van Genuchten's fitting parameter analogous to the inverse of air entry pressure, $1/\alpha$. Evaluation of uncertainty in the total percent infiltrate as a result of parameter uncertainty is performed using linear First-Order-Second-Moment and Monte Carlo methods. In addition, the effects of heterogeneity within the fracture continuum on flow and infiltration are observed by replacing the homogeneous fracture continuum with two randomly generated permeability and air entry pressure heterogeneous continua.

Conceptual Model

Fluid flow through a 2-D vertical cross section fracture continuum is simulated using TOUGH2, an integral finite difference simulator developed at LBNL (Pruess, 1991). In this study TOUGH2 is used to calculate an isothermal, 2-D solution to Richards Equation for unsaturated flow above and around a short excavated drift, or niche.

Simulations of fluid flow presented here are loosely based on field experiments currently being performed at Yucca Mountain, Nevada, in which a water pulse of a known volume is released above an excavated niche. In the field, movement of the water pulse is observed by collecting infiltrate through the niche ceiling. Similarly, in this numerical study, we quantify the amount of water infiltrating the niche by means of the percent infiltrate, defined as the percentage of the total liquid release volume that enters the niche. In the simulations, a water pulse of 1.4 l is released instantaneously at time zero, roughly 1 m above the niche ceiling. Within the niche, a boundary condition of 100% relative humidity is assumed such that the excavated niche acts as a capillary barrier. Table I describes the homogeneous fracture continuum parameter distributions for the two uncertain parameters. Mean values of permeability and air entry pressure are based on a 30 μm fracture aperture and cubic law. Figure 1 illustrates saturation contours within the 2-D fracture continuum surrounding the excavated niche 12 hrs after the water pulse release.

Sensitivity Analysis

Figures 2 and 3 illustrate the sensitivity of total percent infiltrate to permeability and air entry pressure. For the simulation conditions of water ponded in the release wellbore, permeability (Figure 2) affects the time frame over which infiltration occurs, but not the amount of infiltration entering the niche. Figure 3 shows percent infiltrate sensitivity to air entry pressure; as air entry pressure increases, percent infiltrate drops and as $1/\alpha$ decreases, more water infiltrates the niche. Air entry pressure significantly affects the percent infiltrate but only mildly alters the time frame over which infiltration occurs.
Uncertainty Analysis

Uncertainty analysis is performed using ITOUGH2 (Finsterle, 1997), an inverse modeling code written to interface with the TOUGH2 family of codes. In this study, ITOUGH2 provides estimates of uncertainty in the amount of water that enters the niche as a result of parameter uncertainty by linear First-Order-SecondMoment (FOSM) and Monte Carlo methods. Linear FOSM analysis assumes that uncertainty in any observable system response (e.g., percent infiltrate) can be approximated as a linear function of all uncertain system parameters (e.g., $k$ and $1/\alpha$). Generally, this method will not provide acceptable estimates of uncertainty for non-linear system behavior. A Monte Carlo analysis of uncertainty in the total percent infiltrate is performed for comparison purposes and is regarded as a more accurate but computationally costly estimation method. One hundred Monte Carlo simulations are executed, drawing randomly generated values of permeability and air entry pressure from lognormal distributions described in Table 1.

Figure 4 illustrates the results of both FOSM and Monte Carlo uncertainty analyses for parameter set 1. Horizontal lines bound the area that describes physically plausible values of percent infiltrate, from 0% to 100%. The 100 Monte Carlo simulations are presented as dashed lines. Results of the FOSM analysis are indicated on either side of the mean total infiltrate of 78%. Monte Carlo results produce percent infiltrate values ranging over 38%. The FOSM analysis fails to estimate transient uncertainties, often exceeding the boundaries of what is physically plausible. Figure 5 shows the analysis repeated for a domain of higher permeability and lower capillarity described in Table 2. This system allows a greater mean percent infiltrate (88%) while reducing uncertainty to 24%. The reduction of uncertainty in the percent infiltrate with a higher mean percent infiltrate shows the sensitivity of the uncertainty analysis to the mean.

We repeated the uncertainty analysis, this time introducing two randomly generated permeability fields. Each field was created with a vertically dominant structure (vertical correlation length of 3.0 m; horizontal correlation length of 0.2 m). Correspondingly heterogeneous air entry pressure fields were created using the J-Leverett function (Bear, 1972) to relate $k$ and $1/\alpha$. Uncertainty analyses resulted in mean percent infiltrates (and Monte Carlo ranges) of 88% (23%) and 92% (14%) for the two fields, respectively. Due to the sensitivity of the uncertainty in percent infiltrate to the mean, it is difficult to separate the effects of heterogeneity on uncertainty.

Conclusions

The amount of water to infiltrate the niche is very sensitive to van Genuchten’s air entry pressure. Under these simulated conditions, (i.e., ponding conditions in the borehole) permeability affects only the time frame over which infiltrate occurs and does not affect the total percent infiltrate. Linear FOSM analysis does not produce an acceptable estimate of the uncertainty in the amount of water to infiltrate the niche. The effect of heterogeneity on the uncertainty in percent infiltrate is not resolved due to the sensitivity of uncertainty to the mean percent infiltrate.

Acknowledgments

This work was supported by the Director, Office of Civilian Radioactive Waste Management, through a Memorandum Phase Order EA9013MCSX between TRW Environmental Safety Systems, Inc. and E.O. Lawrence Berkeley National Laboratory through U.S. Department of Energy Contract No. DE-AC0376SF0098.

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keley National Laboratory, Univ. of Calif., Berkeley, 1997.


Figure 1. Contours of liquid saturation within the 2-D fracture continuum surrounding the excavated niche 12 hrs after the water pulse release.

Figure 2. Sensitivity of total percent infiltrate to permeability.

Figure 3. Sensitivity of total percent infiltrate to air entry pressure.
Figure 4. FOSM and Monte Carlo uncertainty analyses for Parameter Set 1. The mean percent infiltrate is 78%. Uncertainty in steady-state percent infiltrate is 38%.

Table 1: Parameter Set 1 (based on a 30μm fracture aperture and cubic law).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>mean μ</th>
<th>standard division σ</th>
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<tr>
<td>log k (m²)</td>
<td>-14.58</td>
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<td></td>
<td>(2.6 millidarcies)</td>
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<tr>
<td>log 1/α (Pa)</td>
<td>3.66 (2818 Pa)</td>
<td>0.166</td>
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Table 2: Parameter Set 2 (Higher permeability, lower capillarity).

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</thead>
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<tr>
<td></td>
<td>(11 millidarcies)</td>
<td></td>
</tr>
<tr>
<td>log 1/α (Pa)</td>
<td>3.45 (2818 Pa)</td>
<td>0.166</td>
</tr>
</tbody>
</table>
The Drift Scale Heater Test at Yucca Mountain, Nevada

Mark T. Peters\textsuperscript{1}, William J. Boyle\textsuperscript{2}, Robin N. Datta\textsuperscript{1}, Ned Z. Elkins\textsuperscript{3}, Robert N. Yasek\textsuperscript{2}, Ralph A. Wagner\textsuperscript{1}, Douglas J. Weaver\textsuperscript{3}

The Drift Scale Heater Test (DST) is an integral part of the program of testing and studies being conducted by the U.S. Department of Energy to evaluate the suitability of Yucca Mountain, Nevada as a site of a deep geologic repository for the permanent disposal of spent nuclear fuel and high-level nuclear waste. The DST is a large-scale, in situ thermal test to be conducted over nearly a decade in the Exploratory Studies Facility at Yucca Mountain (Figure 1).

The overall objective of the DST is to acquire a more in-depth understanding of the physical processes that will occur in the rock surrounding the emplaced waste. There are four principal processes of concern: thermal, mechanical, hydrological, and chemical. These processes will be intensified because of the decay heat from the emplaced waste and their interaction or coupling. An understanding of these coupled processes is essential for the assessment of the long-term (over thousands of years) performance of the repository.

The DST consists of a 47.5m long, 5m diameter drift to be heated by 9 canister heaters, 1.7m diameter and 4.6m long, placed on the floor of the drift (Figures 1 and 2). Each canister heater can generate a maximum of 15kW. The drift cross-section and the canister heaters are approximately the sizes of drifts and waste packages being considered for the repository. To simulate the heat that would come from adjacent drifts in the repository and thus, to provide better test boundary conditions, 25 rod heaters, referred to as wing heaters, are inserted into horizontal boreholes on each sidewall of the drift (Figure 2). The 10m long wing heaters have inner and outer segments that can generate 1145W and 1719W, respectively. The heater outputs can be varied over a range of 10 to 100% of the designed capacity. The heated length of the drift will be isolated by a thermal bulkhead. An Observation Drift, parallel to the Heated Drift, and a Connecting Drift are constructed along the periphery of the test block (Figures 1 and 2). Approximately 3300 meters of boreholes are drilled from these three drifts into the test block (Figure 3). Approximately 3500 measuring devices of various types are installed in these boreholes.

As the rock is heated and subsequently cooled, temperature will be measured by resistance temperature devices (RTDs) and thermocouples; displacements in the rock will be measured by multiple point borehole extensometers and convergence meters; moisture content of the rock will be monitored by neutron logging, ground penetrating radar (GPR), and electric resistivity tomography (ERT); relative humidity, temperature, and pressure will be measured in sections of boreholes isolated by inflated packers; changes in rock mass permeability will be measured by conducting air-injection tests in these isolated borehole chambers; REKA probes will measure thermal conductivity and thermal diffusivity; samples of water and gas will be collected by water absorbing pads and gas sampling ports in SEAMIST liners installed in boreholes; microseismic emissions, if any, will be monitored; a remotely operated video and infrared camera system will image periodically along the
The Drift Scale Heater Test at Yucca Mountain, Nevada

The entire length of the Heated Drift. The 12.5m length at the far (west) end of the Heated Drift includes a ground support system composed of a cast-in-place concrete liner. Response of the concrete liner/rock system to the heat will be monitored by strain gages and convergence meters.

An approximately 6000 channel automated data collection system will record measurements on an hourly basis, which will generate an estimated 40 gigabytes of data over the life of the test. Other measurements, such as ERT, neutron logging, GPR, and microseismic monitoring, will be recorded using independent data acquisition systems.

During the heating phase of the DST, planned to last for four years, the drift wall temperature is planned to reach 200°C and will be maintained there for a sufficient period to ensure hydrological and chemical processes are properly observed. Over 10,000 cubic meters of rock will be heated to above 100°C, while over 200,000 cubic meters of rock is expected to be heated above ambient temperatures. Approximately 800 cubic meters of water in the rock is expected to be mobilized by the heat.

Based on laboratory studies, prior in situ thermal testing, observations of natural geothermal phenomena, and knowledge of other physical processes, scientists have developed conceptual models of the various near field processes. These models were the basis for scoping calculations to assist in the design of the test configuration and instrumentation plans. A suite of characterization measurements have been made to determine various properties of the rock in the test block. Employing these block-specific rock parameter values in the existing conceptual models, predictive analyses of the Drift Scale Test were performed to forecast the measurements to be made at various points in time during the test. Periodic comparative analyses of the predicted and observed measurements are expected to provide insights into the heat-driven near field phenomena, leading to refinement of the conceptual models. The refined models will be used to predict the measurements during subsequent periods of the test. This predictive-corrective process is expected to converge into near field process models for use in the assessment of repository performance, the level of confidence in which will be acceptably high.

The work was sponsored by the U.S. Department of Energy, Yucca Mountain Site Characterization Office under contract number DE-AC01-91RW00134 with TRW Environmental Safety Systems, Inc.

Figure 1.
The Drift Scale Heater Test at Yucca Mountain, Nevada

Figure 2

Reference Only (approximate scale)

Observation Drift
Connecting Drift
Wing Heater (typ.)
Floor Heater (typ.)
Heated Drift

LEGEND: Boreholes

Wing Heaters
Heated Drift Boreholes
Observation Drift Boreholes

Figure 3

Reference Only (approximate scale)
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Flow Tests to Quantify Seepage into Drifts

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The rate of water seepage into repository waste emplacement drifts is important for predicting the performance of engineered and natural barriers. For a pulse of water to seep into a drift, it needs to overcome the capillary force in the fractured tuff rock mass in order to drip into the mined opening. With low percolation flux, a seepage flow threshold may exist for the drift to stay in a dry condition. Two 9-meter-long niches (short alcoves) were excavated along the main drift of the Exploratory Studies Facility (ESF) at Yucca Mountain in 1997 to test the seepage processes and to monitor the flow paths. The preliminary results of the first set of active seepage flow tests and the flow paths characterized in the niche sites are presented here.

The tests are conducted in multiple stages before, during, and after niche excavation. Before niche excavations, three 10-meter-long horizontal boreholes were drilled at Niche 3566 (3566 meters from the ESF North Portal) and seven boreholes were drilled at Niche 3650. The boreholes were drilled from the ESF main drift in three levels into the wall, with the upper level boreholes above the future niche space (Figure 1). At each site, cross-hole pneumatic tests were conducted with boreholes instrumented with packers to map out the permeability field with a spatial resolution of 0.3 m (1 ft). An example of the permeability distribution along the upper middle (UM) borehole at Niche 3650 is illustrated in Figure 2. The permeability distributions were used to determine the flow paths selected for liquid release tests.

Dye-spiked pulses of water were injected at selected borehole intervals with the same pneumatic test packer assemblies. For the injection interval, one port was used for flow injection and the other port was used for return flow to breed off excess water. Of the five pre-niche liquid release tests conducted along the UM borehole, return flows were observed in three test intervals. During the niche excavation, the dye migration patterns were observed along discrete fractures and through the fracture network below the injection boreholes, with the maximum tracer penetration depth of 2.6 meters. The majority of injected dyes were excavated out of the niche space. The flow patterns from the upper borehole injections were observed on the niche Drift Seepage Test and Niche Moisture Study ceiling. Since the niche was excavated dry, other damp features without dyes were also observed in the niches. The most prominent feature observed so far was located at the end of Niche 3566, the niche between the Sundance Fault and its first reactivated cooling joint.

After niche excavation, the cross-hole pneumatic tests were repeated in the remaining boreholes. Most of the flow paths near the niche excavation are more permeable than the pre-niche conditions, as illustrated in Figure 2. Post-excavation seepage tests were conducted in the UM borehole in the same five intervals tested before the niche excavation. Only one return flow from the borehole was observed in the post-niche tests. With a fluid collection system installed below the ceiling, the total volume of
flow seeped into the niche can be measured. The test results of the percentage of injected water dripping into the niche are illustrated in Figure 3. One of the five tests did not induce dripping into the niche. Another test induced flow to reach the ceiling and migrate along the mined surfaces, but the water did not drip into the niche.

The test interval from 4.9 to 5.2 m (16 to 17 ft) with the highest permeability value along the UM borehole did not induce the highest percentage of seepage into the niche in this set of liquid-release tests. Fractures with high permeability may contain large void space and in turn require large liquid volume or high flow rate to induce a locally saturated condition at the fracture outlet on the niche ceiling. These preliminary test results have been used in two-dimensional and three-dimensional models to simulate the fractures and rock continuum above and surrounding the niche. The driftscale models calibrated against the on-going field test results should lead to credible inputs to the total system performance assessment for the Yucca Mountain site.

Figure 1. End view of boreholes on the wall of ESF Main Drift before the niche at CS 3560 was excavated.
Yucca Mountain Laboratory Testing

Session Chair: William Boyle DOE/YMSCO

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Numerical Simulation of an Experiment in a Block of Variably Saturated, Fractured Tuff

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Abstract

Numerical models of water movement through variably saturated, fractured tuff have undergone little testing against experimental data collected from relatively well-controlled and characterized experiments. This report used the results of a multistage experiment involving a block of fractured, welded tuff and associated core samples to investigate if those results could be explained using models and concepts currently used to simulate water movement in variably saturated, fractured tuff at Yucca Mountain, Nevada, the potential location of a high-level nuclear-waste repository. Aspects of the experiment were modeled with varying degrees of success.

Imbibition experiments performed on cores of various lengths and diameters were adequately described by models using independently measured permeabilities and moisture characteristic curves, provided that permeability reductions resulting from the presence of entrapped air were considered. Entrapped gas limited maximum water saturations during imbibition to approximately 0.70 to 0.80 of the fillable porosity values determined by vacuum saturation.

A numerical simulator developed for application to fluid flow problems in fracture networks was used to analyze the results of air-injection tests conducted within the tuff block through 1.25-centimeter diameter boreholes. These analyses produced estimates of transmissivity for selected fractures within the block. Transmissivities of other fractures were assigned on the basis of visual similarity to one of the tested fractures. The calibrated model explained 53 percent of the observed pressure variance at the monitoring boreholes (with the results for 6 outliers omitted) and 97 percent of the overall pressure variance (including monitoring and injection boreholes) in the subset of air-injection tests examined.

Attempts to model moisture redistribution from a saturated sand pack overlying the block resulted in many insights into the factors affecting this process. Single-fracture models predicted that fractures whose permeability and capillary characteristics most closely matched that of the overlying sand would be most important to water uptake by the block. For large-aperture fractures, water uptake at early time was limited by the intrinsic permeability of the sand and, at later times, by the small relative permeability of the fracture. In the case of small-aperture fractures, water uptake was limited by the small intrinsic permeability of the fractures themselves. For large-aperture fractures, simulated sandpack matric potentials declined to near constant values as a result of capillary barrier effects at the sand-rock interface, indicating that similar declines in matric potential observed during the experiment may have been influenced by such processes. A two-fracture model indicated that capillary barrier effects associated with large-aperture fractures could hydraulically isolate portions of the block from the actively flowing fractures, resulting in a decrease in water uptake relative to the corresponding single-fracture models. Although these simulations pro-
vided considerable insight, none could simultaneously match all of the data for this period, which included measured matric potentials in both the overlying sand pack and rock matrix and estimated cumulative drainage from the sand at 100 days.

The through-flow tests provided an opportunity to compare model-based estimates of flux based on indirect indicators, such as intrinsic permeability and matric potential, with direct measurements of flux collected over a range of matric potentials. The steady fluxes predicted by using a fractured network model were generally in very close agreement with measured fluxes, thereby lending support to the validity of the measurements themselves, the analytical methods that were used to make those estimates, and the processes that were hypothesized as causing the decline in measured flow rates.
Fast Flow in Unsaturated Fractures: Identification and Laboratory Quantification of Fracture Surface Processes

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Introduction

Important segments of the hydrologic cycle in arid and semi-arid regions remain incompletely understood. This includes processes by which water percolates through thick regions of unsaturated fractured rock. Rapid migration of solutes through some portions of deep vadose zones have been observed in several different locations. Such findings clearly show preferential flow along a fraction of potentially conductive fracture pathways, and disequilibrium between fractures and the rock matrix. Most conceptual models for flow and transport in unsaturated fractured rock require essentially saturated conditions along fast flow pathways, although evidence supportive of this criterion is often lacking. In this study, we show that common representations of unsaturated flow in fractured low-permeability rock omit two potentially important processes which support fast flow along essentially unsaturated fractures.

Most conceptual models of unsaturated-saturated flow in fractured porous media assume that the hydraulic properties of the system are accounted for solely by matrix properties and fracture aperture distributions. Some models also include hydraulic properties of fracture coatings in a limited manner to account for flow between fractures and matrix rock. In this study, we show that all of these previous conceptualizations ignore two potentially important pathways for unsaturated fracture flow, and therefore provide incomplete explanations of fast unsaturated flow. As our starting point, we hypothesize that (i) at near-zero metric potentials individual fracture surfaces can support film flow, and (ii) the fracture surface zone flow can in some cases conduct water rapidly along the fracture plane.

Previous researchers have proposed that the distribution of water in partially saturated fractures is determined solely by aperture-capillarity relations. Such models predict that over a fairly wide range of fracture saturations, water occurs in isolated regions of minimum aperture. Thus, in these models, high fracture saturations are required in order to generate fast flow. In view of a growing body of evidence that fast flow occurs through deep, unsaturated fractured rock, and the common lack of evidence for high local fracture saturations, the aperture-based models seemed incomplete. In recent work, we demonstrated that gravity-driven film flow could support fast unsaturated flow along individual fracture surfaces at near-zero metric potentials. Results from the earlier study showed that aperture-based models of unsaturated flow in fractures are inadequate, especially in regions of larger aperture and in very low matrix permeability rock. We also qualitatively showed that fracture surface roughness is important in supporting fast film flow. As part of our new research effort, more quantitative analyses of surface roughness influences on film flow are being conducted. Some of these results on simple surfaces are presented here.

While many studies have already investigated the influence of fracture coatings on fracture matrix interactions, none have considered the possibility that fracture coatings might provide a fast flow pathway along the fracture plane.
More generally, this possibility includes both high permeability fracture coatings and fracture surface regions with increased permeability due to interconnected secondary fractures or other permeability-enhancing alterations.

**Testing Mechanisms**

What we refer to as "film flow" on natural fracture surfaces is actually dominated by water flowing along a series of roughly parallel surface depressions. Fracture surfaces are irregular, thus film flow occurs along tortuous surface pathways of variable local hydraulic resistance. Dye tracer tests conducted in our earlier study showed film flow occurs preferentially down natural rough fracture surfaces rather than down artificially smoothed rock surfaces. To begin to understand basic mechanisms underlying film flow on rough surfaces, it is worth examining geometrically simpler systems first. Studies of porous media hydraulics have relied very heavily on capillary bundle models. In rough surface film statics and flow, regular corrugated surfaces provide geometric simplicity useful for identifying some important basic mechanisms. We have conducted experiments on various smooth and corrugated ceramic surfaces in order to quantitatively relate film flow to the geometry of well-defined simple surfaces of ceramic blocks. These blocks were tested at various unit gradient fluxes in an apparatus similar to that used in our earlier work.

Fracture surface zone flow was tested through various imbibition experiments. These were conducted on two different tuff samples. The first was a rhyolitic tuff with a cooling joint fracture surface (Mono County, CA). This sample contained a set of secondary fractures which propagated a short distance into the rock matrix. The second sample is a Paintbrush Tuff (Topopah Spring, welded, Yucca Mtn., NV), with a fracture coating. Fast flow in fracture surface zones have been characterized through various imbibition experiments. These include various methods of wetting by free water, by tension plate, and by "point" sources under tension.

**Results and Discussion**

The series of unit gradient steady-state flux experiments on the ceramic block samples at various values of metric head determined effective hydraulic conductivity versus metric head relations. At metric potentials close to zero, this effective K can include the influence of film flow. The effective K for the flat surface ceramic remained essentially constant until metric head values were within 10 mm of zero. Slight increases in effective K were measured within this narrow range. A ceramic block with V-channels aligned with the downwards flow exhibited film flow at metric head values within 30 mm of zero, with up to 4 orders of magnitude increase in effective hydraulic conductivity. This corresponds to film transmissivities which become as large as $2 \times 10^{-6}$ m$^2$ s$^{-1}$. Higher channel densities (numbers of surface channels per unit length) result in (i) broadening the metric potential range over which film flow is significant and (ii) increasing of the transmissivity in the lower energy region of film flow. In the higher energy (metric potential) range of film, higher channel densities can result in decreased surface transmissivities due to associated decreases in channel depth. The tortuosity of natural surface channels also decreases surface transmissivities. It should be noted that in general, the metric potentials range over which film flow is significant becomes broader in systems with lower matrix K.

Imbibition (sorptivity) experiments which examine the influence of fracture coatings are typically conducted with flow normal to the natural fracture surface. One-dimensional imbibition experiments conducted normal to fracture surfaces lend themselves to simple interpretation. Our experiments on a Topopah Spring Tuff revealed that the sorptivity of its fracture coating is 5.5 times greater than that of its matrix. Since permeability is correlated to the 4th power of sorptivity, the permeability of this fracture surface coating is about 900 times greater than that of the underlying matrix. Such high surface zone
permeabilities can support fast flow along unsaturated fractures, especially when they occur along preferential flow paths through very low permeability rock. Steady-state flow experiments are in progress to better quantify fracture surface zone hydraulic properties.

Conclusions

The previously developed film flow model was supported through experiments on ceramic blocks with well-defined surface geometries. Aperture-based models can not generally explain fast flow in partially-saturated fractures because they neglect the basic process which controls flow through unsaturated segments, film flow. Secondary microfractures and some fracture coatings can provide relatively high transmissivity zones which also allow fast flow along unsaturated fractures, regardless of the aperture distribution. Both film flow and fracture surface zone flow will also occur in near-zero metric potential environments of “very large apertures” such as caverns and excavated drifts.

Acknowledgments

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Yucca Mountain Exploratory Studies Facility Thermal Tests

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Yucca Mountain is being evaluated as a potential repository site for nuclear waste disposal in the USA. Included in the site characterization program are thermal tests being carried out in the potential repository formation of Topopah Springs welded tuff in the Exploratory Studies Facility. The in situ thermal test program consists of the Single Heater Test (SHT) and the Drift Scale Test (DST). The SHT was initiated in August, 1996. It has completed the heating cycle of 9 months and the cooling phase is being monitored. While the SHT has one 4 kW heating element of 5 m in a borehole, the much larger Drift Scale Test has a heated length of 47.5 m, heated width of 28 m, and a power capacity of 300 kW. The planned start date for the DST is December 1997 with a heating period of four years.

The primary objective of the SHT and DST is to develop a more in-depth understanding of the in situ coupled thermal, mechanical, hydrological, and chemical processes in the nearfield rock. These coupled processes are monitored by a multitude of sensors installed in numerous instrumental boreholes to measure the temperature, gas pressure, humidity, mechanical displacement, and stresses of the rock mass in response to the heat generated. In addition to the passive monitoring data, active testing by crosshole radar tomography, neutron logging, electric resistivity tomography and interference pressure response to air injection are carried out to probe the redistribution of moisture in the rock block from boiling, vaporization, and condensation. Confidence in our ability to predict the performance of a nuclear waste repository will depend on how well the thermal test data can be interpreted by the coupled process models. Pretest ambient characterization has been carried out in the SHT, and is being performed in the DST, to define the initial conditions of the local rock mass to be incorporated in conceptual models for numerical simulations of both the SHT and DST. The scientific responsibility of fielding and interpreting the tests are shared among several National Laboratories: Sandia National Laboratories, Lawrence Livermore National Laboratory, and Lawrence Berkeley National Laboratory. Based on our (Berkeley) interpretation of the passive monitoring data and the active testing results for the SHT, the thermal-hydrological responses seem to be well understood and well represented by our coupled process conceptual and numerical model. Data indicate that spatial heterogeneity of rock properties is important for understanding the test results. Other possible causes of discrepancies between simulations and measurements, and lessons learned for the upcoming DST, are discussed.
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Evaluation of Inconsistencies Between Laboratory-Determined Moisture Retention Characteristics and Matrix Sorptivity

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Laboratory measurements of physical and hydrologic properties of surface outcrop samples collected at Yucca Mountain, Nevada were conducted by Flint et al. (1996). Physical properties measured were bulk density, particle density, and porosity. Hydrologic properties measured were hydraulic conductivity, sorptivity (determined from measurements of imbibition), and moisture retention. Of the hundreds of samples analyzed, the full suite of moisture retention, hydraulic conductivity, and sorptivity measurements was performed on only 19 samples. In the present study, laboratory-measured properties of these 19 samples are used in analytical and numerical models to predict sorptivity; modeled sorptivities are then compared to the actual sorptivity observed during imbibition experiments.

Because sorptivity is a function of combined physical and hydrologic properties, the imbibition experiments conducted by Flint et al. (1996) provide a convenient means to determine whether models that use laboratory-determined rock properties as input parameters produce results that are consistent with observations. Moisture retention characteristics used in these models are in terms of the van Genuchten (1980) parameters \( \alpha, m, \) and \( n, \) and residual moisture content \( \theta_r. \)

The analytical model used is that of Par Lange et al. (1975) which provides an estimate of sorptivity \( (S) \) expressed as

\[
S^2 = \int_{\theta_i}^{\theta_s} \left( \theta + \theta_i - 2\theta_i \right) D_m d\theta
\]

where \( \theta_s \) and \( \theta_i \) are saturated and initial matrix water contents, respectively; and \( D_m \) is matrix diffusivity which can be expressed in terms of effective saturation \( [S_e = (\theta-\theta_r)/(\theta_s-\theta_r)] \), hydraulic conductivity \( (K_{sat}) \), and moisture retention properties

\[
D_m = \frac{K_{sat}(1-m)}{\alpha m (\theta_s-\theta_i)} \frac{S_e^{0.5} \left[ 1 - (1 - S_e^{1/m})^m \right]^2}{(S_e^{-1/m} - 1)^m S_e^{1+1/m}}
\]

Numerical predictions of sorptivity were obtained by use of the unsaturated mass and energy transport model, METRA, used to simulate the conditions of the imbibition experiments of Flint et al. (1996). Imbibition was simulated using one-dimensional, twenty-element models, with input parameters based on laboratory-measured physical and hydrologic properties. For each sample modeled, total imbibition was plotted against the square-root of time to determine sorptivity (Phillip, 1957).

For both the analytical and numerical modeling approaches, initial effective saturation was assumed to be one percent, and \( \theta_s \) was assumed to equal total porosity. These assumptions were tested on a limited number of samples.

Results from numerical and analytical models are generally in agreement with each other. With the exception of two samples with very low permeability \( (K_{sat} < 10^{-12} \text{ m/s}) \), both models consistently over-predict imbibition rates. Ratios of modeled to observed sorptivity exhibit strong correlation to saturated hydraulic conductivity.
These ratios range from 0.25 to 55 for the analytical model, and from 0.33 to 47 for the numerical model.

Discrepancies between modeled and observed sorptivity could be due to several factors, including: (i) assumptions about initial saturation and $\theta_s$; (ii) air trapped within the rock matrix during imbibition experiments causing reduced permeability; and (iii) the effects of hysteresis on moisture retention characteristics.

Varying model inputs for initial saturation over a range of 0.001 to 0.1, and saturated moisture content over a range of 0.90 to $\theta_s$ did not significantly change results.

If a significant amount of air is trapped in rock matrix by surrounding water during an imbibition experiment, the effect is a reduction in effective hydraulic conductivity. Assuming the model parameters $m$, $\theta_s$, and $\theta_i$ and $\theta_i$ are reasonably accurate, it can be shown from equations (1) and (2) that

$$S^2 \propto \frac{K_{sat}}{\alpha}$$

(3)

and, taking the derivative of $S$ with respect to $K_{sat}$,

$$\frac{\partial S}{\partial K_{sat}} \propto \left[K_{sat} \alpha \right]^{-0.5}$$

(4)

Thus, for small errors in the value of $K_{sat}$ used in the models, the difference $(S_{modeled} - S_{observed})$ should show a correlation to $[K_{sat} \alpha]^{-0.5}$. However, no such relationship exists (in fact, the relationship is inverse). This suggests that differences are not due to error in estimation of saturated hydraulic conductivity, and thus, probably not due to trapped air during imbibition.

Because moisture retention characteristics are determined in the laboratory using an oven drying process, and imbibition is a wetting process, an argument could be made that laboratory-determined $\alpha$ parameters are not appropriate for modeling imbibition. The difference between moisture retention characteristics observed during wetting and drying processes, called hysteresis, generally results in a higher value of $\alpha$ for wetting cycles than for drying cycles. If hysteresis is at work, then based on the relationship

$$\frac{\partial S}{\partial \alpha} \propto K_{sat}^{0.5} \alpha^{-1.5}$$

(5)

the difference $(S_{modeled} - S_{observed})$ should show correlation to the value $K_{sat}^{0.5} \alpha^{1.5}$. Indeed, such a relationship is observed with a correlation coefficient ($r^2$) of 0.91. This suggests discrepancies between modeled and observed sorptivities may be due, at least in part, to hysteresis. If this is the case, a correction factor to convert the $\alpha$ value obtained from a drying process to a value appropriate for wetting processes can be obtained from the relationship

$$\left[\frac{S_{modeled}}{S_{observed}}\right]^2 = \frac{\alpha_{wet}}{\alpha_{dry}}$$

(6)

For the samples considered in this study, these adjustment factors ranged from 0.1 to 3,100 (using the analytical model), and resulted in model predictions that are consistent with observations.

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Session 3
FTAM Workshop, December 15 & 16, 1997

WIPP and Other Sites

Session Chair: Ned Elkins, M&O/LANL

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Hydrochemical Constraints on Flow and Transport Models of Yucca Mountain, Nevada

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Two and three-dimensional dual permeability flow and transport models of the unsaturated zone at Yucca Mountain are used to integrate geochemical and hydrologic databases with the structural and mineralogical conceptualizations of the mountain. The combination of these databases serves two important purposes:

(1) it provides the most relevant information for understanding the past and present hydrologic response of the Yucca Mountain system to climatic changes, and (2) it serves to assess the validity of predictive radionuclide transport models, as the movement of naturally occurring solutes is closely related to the potential migration of radionuclides. In this work, the chemistry of pore waters and perched waters is used to place bounds on the response of the hydrologic system to past and present climate scenarios. Two end-member behaviors are analyzed, represented by a "fast pathway" fracture flow model, and a transient-fracture/matrix interaction model respectively. The "fast pathway" fracture flow model predicts short travel times to the water table, as the unsaturated zone strata are essentially bypassed by fracture flow. It also results in modern ages for the perched waters at Yucca Mountain. In terms of chloride concentrations, it requires that the rock matrix of overlying strata be bypassed by infiltrating meteoric waters. Alternatively, the transient-fracture/matrix interaction model, predicts longer residence times for infiltrating meteoric waters due to lateral diversion- and perching- components. This model explains simultaneously the inversion in apparent ages between pore waters and perched water in the unsaturated zone, and the low chloride content of perched waters relative to the pore waters of overlying (i.e., PTn and TSw) and underlying strata (CHn). The apparent disequilibrium in pore water and perched water contents is also consistent with the transient model. This model also suggests that stable isotope data and apparent \(^{14}\text{C}\) and \(^{36}\text{Cl}/\text{Cl}\) ages from Yucca Mountain perched water bodies, can be interpreted as resulting from a mixture of late Pleistocene/early Holocene water with modern waters. The existence of these mixed ancient/modern perched water bodies therefore implies that an additional retardation mechanism exists above the Calico Hills formation. The ubiquitous young \(^{14}\text{C}\) ages in the Calico Hills formation pore waters beneath the perched water bodies and in other areas, also imply that a lateral component of flow occurs in the vihic Calico Hills and that this formation is not bypassed.
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Effects of Gas and Brine Flow on Repository Behavior in the 1996 Performance Assessment for the Waste Isolation Pilot Plant

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In the 1996 performance assessment (PA) for the Waste Isolation Pilot Plant (WIPP) the code BRAGFLO was used to solve the system of non-linear PDE representing two phase flow (gas and brine flow) in the repository over a 10,000 year period. A suite of sampled parameters was used as input for several unique scenarios. Brine and gas flow patterns were examined from BRAGFLO results for the scenario in which a borehole punctures a waste panel and brine pocket at 1000 years, referred herein as the E1' Scenario. Sensitivity analysis indicate microbial degradation, borehole permeabilities and, to a lesser extent, metal corrosion rates and Castile reservoir pressures and compressibilities are the more significant sampled variables impacting repository behavior, for an E1 scenario throughout the modeled period. To understand how these properties and processes affect repository behavior, overlay plots for gas and brine fluxes crossing boundaries of discretely modeled regions of the repository are given for realizations assigned high or low borehole permeabilities, coupled with or without microbial degradation, and assigned either high or low metal corrosion rates. A detailed examination of these plots showed an interplay between gas and brine flow and flow direction exists within the borehole and excavated areas. This interplay is primarily controlled by the processes that dominate gas flow out of the excavated area via the borehole, and is secondarily controlled by gas production and the ability of replenishing brine, necessary for metal corrosion, to enter the repository.

General flow patterns for realizations with low borehole permeability coupled with no microbial, high iron corrosion rates, and plentiful brine supplies (either from the Castile reservoir, or UDRZ and anhydrite/marker bed drainage), as typified in Simulation 4 given in the following figures, were;

- Borehole flow is characterized by a long stretch of gas flow upward, which can last from the time of intrusion to the end of the modeled period. Brine flow down the borehole is minimal.
- Saturations and flow within the UDRZ is dominated by gas flow in a down-dip direction, towards the borehole. Minimum brine flow is seen in the UDRZ.
- Little brine flows between the lower and upper waste panel via the panel seals.
- The dominant fluid in the LDRZ is brine and flow is down-dip, from the north portion of
the repository to the area below the north half of the lower waste panel; from here it is deflected upward through the waste panel floor where it can be used for iron corrosion.

General flow patterns for realizations with similar input parameters values as above but assigned high borehole permeability, as typified in Simulation 27 given the following set of figures, were;

- Flow direction in the borehole alternates between gas flow upward and brine flow down.

- Saturations and flow within the UDRZ alternates between gas flow down-dip and brine flow up-dip.

- A large component of brine flows within the lower waste panel through the panel seals to the upper waste panel.

- The dominant fluid in the LDRZ is brine and flow is up-dip, passing under the panel seals. This up-dip flowing brine converges with down-dip flowing brine midway under the floor of the upper waste panel. From here brine is deflected upward through the upper waste panel floor where it can be used for iron corrosion.

The following three figures illustrate the differences between dependent variables within the upper and lower waste panels with respect to borehole fluid flow for two representative simulations within the sampled set. Figure 1 is as a set of overlay plots for Simulation 4 of the sampled set which typifies some of the dependent variables for those simulations assigned a relatively low borehole permeability. Figure 2 is as a set of overlay plots for Simulation 27 of the sampled set which typifies the same dependent variables as given in Figure 1, but representative of simulations assigned a relatively high borehole permeability. Figure 3 shows the differences for borehole fluid flow for the two simulations.
Figure 1. Realization 4 - Pressure Changes for the Upper and Lower Waste Panels with Respect to Gas Saturation, and the Fraction of Metal Not Yet Corroded.

Figure 2. Realization 27 - Pressure Changes for the Upper and Lower Waste Panels with Respect to Gas Saturation, and the Fraction of Metal Not Yet Corroded.
Figure 3. Overlay Plots Comparing Gas and Brine Flow Within the Borehole for Both Simulation 4 and 27.
Discrete-Feature Model for a Repository in Fracture Crystalline Rock

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Introduction

Groundwater flow in sparsely fractured granitic rock is understood to be dominantly via mechanical discontinuities that exist on a wide range of scales (Olsson et al., 1992), including simple and compound fractures (10-2 to 102 m), site-scale fault zones (101 to 103 m), and regional fault zones (103 to 105 m). On any particular scale these discontinuities tend to interconnect in an irregular fashion, so that groundwater flow and contaminant transport occur via a complex network of hydraulically transmissive features. For such rock, the concept of an equivalent porous continuum defined by a permeability tensor may not be valid (Long et al., 1982), and anomalously fast solute transport may occur through otherwise low-permeability rock (Abelin et al., 1987).

Here we describe an application of a multi-scale, 3-D, discrete-feature (DF) model to predict groundwater flow and radionuclide transport in fractured granitic rock. This model was developed as part of the Swedish Nuclear Power Inspectorate's recently completed SITE-94 study (SKI, 1996), which is a site-specific performance-assessment study for a high-level, radioactive-waste repository located hypothetically at the site of the Åspö Hard Rock Laboratory (HRL) in Sweden. To represent the initial stage of site licensing in Sweden, the study is restricted to data from surface-based investigations performed prior to underground work at the HRL.

Discrete-Feature Model for the SITE-94 Project

The DF model for SITE-94 (Figure 1) integrates hydrologic and structural geological data for discrete hydrologic features on scales ranging from detailed-scale (1 m to 50 m) fractures to semiregional-scale (up to 5 km) fault zones. The smallest-scale discontinuities are represented as a stochastic, discrete-fracture network (DFN) in the vicinity of the hypothetical repository.

Within each identified lithologic/structural domain, a DFN submodel is derived by statistical analysis of borehole and outcrop data. The validity of each submodel is tested by simulating constant-pressure injection tests within stochastic realizations, and statistically comparing the distributions of effective transmissivity and flow dimension to those for the suite of actual injection tests. Larger-scale fault zones structures are represented in the DF model as piecewise-planar, transmissive features with deterministic geometry. Their hydrologic properties are estimated by calibration with respect to undisturbed heads and drawdowns during a series of large-scale pumping tests.

Groundwater flow through the network of features is modeled by the Galerkin finite-element method. The mesh is defined on the entire network comprising the large-scale, deterministic features and each of multiple realizations of the stochastic, discrete-fracture network. Specified-head, specified-infiltration, and specified-net-flux boundary conditions are applied at
intersections between the network and physical boundaries such as the ground surface, boreholes, waste deposition holes, and repository tunnels. Solute transport is modeled by advective-dispersive particle tracking. The integrated DF model has been tested by simulating drawdowns and solute arrival during a long-term pumping test and radially-convergent tracer experiment, with satisfactory results.

**Application to Performance Assessment**

The SITE-94 DF model has been used to evaluate spatial variability and uncertainty in the hydrologic parameters governing geologic-barrier performance for the hypothetical repository. A total of 42 calculation cases have been analyzed, representing combinations of 25 distinct variations which address nonquantifiable sources of uncertainty such as changes in the interpreted hydrogeologic conceptual model for the site, as well as ordinary parametric uncertainty. For each calculation case, realization, and canister location, key hydrologic parameters are estimated including: (1) the groundwater flux passing through each canister location, and (2) the Peclet number and the ratio \( F = a_r L / u \) for each canister location that discharges solute to the surface environment, where \( a_r \) is the wetted surface per unit pore water volume along the discharge path, \( L \) is the path length, and \( u \) is the net advective velocity. Scoping calculations for SITE-94 (SKI, 1996) indicate that the peak radiation dose to the biosphere (for a given radionuclide source term and fixed geochemical conditions) is essentially characterized by \( F \) and \( P_e \), with \( F \) being by far the more important. Low \( F \) implies a relatively low potential for retardation of radionuclides by sorption and matrix diffusion, and thus a higher dose to the biosphere in the event of a canister failure.

**Main Findings Regarding Uncertainty in Geologic-Barrier Performance**

Among the many aspects of uncertainty that have been evaluated for the Áspö site, the most significant influences on geologic-barrier performance (as measured in terms of \( F \)) relate to (1) the connectivity of the fracture network around the repository, which depends on lithologic variability, and which controls the percentage of canisters that connect to the far-field network, and (2) the possibility of local correlations.
between transmissivity and transport properties within the large-scale features. When an empirical correlation between local porosity and transmissivity (based on a compilation of data from in-situ experiments in single fractures) is assumed to hold within each large-scale feature, the result is a significant increase in the spatial variability of $F$ relative to the case in which a uniform feature porosity is assumed. A third significant source of uncertainty in geologic-barrier performance is found to arise from spatial variability of transmissivity within these features.

**Calibration Methodology for Future Applications**

To address the major sources of residual uncertainty in geologic-barrier performance for an eventual actual repository, it is anticipated that more intensive hydrologic and tracer testing programs will be needed, on varying spatial and temporal scales. In order to extract as much information as possible from such tests, we anticipate that efficient methods will be needed for calibrating DF models with respect to both multi-well hydrologic tests and tracer tests. To achieve these aims, we are implementing a general stochastic/deterministic algorithm based on a Laplace-Transform Galerkin (LTG) formulation of the DF network problem.

For transient flow in response to hydrologic interference tests, the LTG finite-element equations after imposing boundary conditions are:

$$A^*(s)h^*(s) = \tilde{q}^*(s) + B^*h^*(0)$$

(1)

where $A^*(s)$ and $B^*$ are known functions of the discretization and the local transmissivities and storativities, $h^*(i)$ is the vector of unknown heads to be solved for, $q^*(t)$ is the vector of known fluxes, and bars denote Laplace transforms. Sensitivity coefficients for measured head and flux with respect to a parameter vector $\Pi$ are obtained by solving an equation of identical form, except that the unknown $\tilde{h}(s)$ is replaced by $\partial h(s)/(\partial \Pi)$ and the right-hand-side is replaced by a sum of other known terms. Thus decomposition of the matrices $A^*(s)$ need be performed only once to solve for both head and the sensitivity coefficients.

For the case of solute transport in a tracer test under steady-flow conditions, the LTG equations are exactly analogous to (1) except that the coefficients in $A^*(s)$ and $B^*$ are related to advective velocities, dispersion, and mass transfer, the unknown vector $h^*(i)$ is replaced by concentration, and $q^*(t)$ is replaced by a mass flux vector. The remainder of the calibration problem is specified by choosing the objective functions to be minimized (e.g. sums of the squared residuals for head, flux, and solute breakthrough curves at the points where measurements are available) and by specifying a relationship between the vector of calibration parameters and the local hydrologic and transport parameters, e.g. identities in the case of blocked calibration, or kriging weights in the case of the pilot-point method (RamaRao et al., 1995).

**Conclusions**

The discrete-feature approach has been applied to model site-scale flow and transport for a hypothetical repository located at an actual site in Sweden. The model provides a synthesis of both structural and hydrologic data, and compares satisfactorily with a long-term pumping and tracer test that was used as a validation case. Practical application of the model in SITE-94 has shown it to provide a flexible method for evaluating the consequences of a broad variety of sources of uncertainty, while retaining the discrete nature of connections between individual radionuclide sources and the hydrologic network, for a realistic repository layout. Current research is aimed at extending the method to provide for efficient calibration with respect to
tracer tests as well as multi-well hydrologic interference tests.

References


Hydraulic Characterization Activities in Support of the shaft-Seals Fluid-Flow Modeling Integration into the WIPP EPA Compliance Certification Application

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Background for Investigation

The Waste Isolation Pilot Plant (WIPP) is a planned geologic repository for permanent disposal of transuranic waste generated by the U.S. Department of Energy. Disposal regions consist of panels and drifts mined from the bedded salt of the Salado Formation at a depth of approximately 650 m below the surface. This lithology is part of the 225 million year old Delaware Basin, and is geographically located in southeastern New Mexico. Four shafts service the facility needs for air intake, exhaust, waste handling, and salt handling. As the science advisor for the project, Sandia National Laboratories developed the WIPP shaft sealing system design. This design is a fundamental component of the application process for facility licensing, and has been found acceptable by stakeholders and regulatory agencies. The seal system design is founded on results obtained from laboratory and field experiments, numerical modeling, and engineering judgment. This paper describes a field test program to characterize the fluid flow properties in the WIPP shafts at representative seal locations. This work was conducted by Duke Engineering and Services under contract to Sandia National Laboratories in support of the seal system design.

Salt formations offer several advantages for waste disposal. Among these are very low permeability, presence of minimal amounts of pore fluid, and the ability of the host rock to “creep” into any excavation, thereby encapsulating the stored material. During this creep process deviatoric stresses may be sufficiently high such that microscopic fractures form. These can eventually coalesce into macroscopic openings in the salt. Although this process is reversed such that healing of the host rock is achieved over time, a potential flow path forms through the “disturbed rock zone” (DRZ) at the time an excavation is created. This path remains until the salt returns to a state of low deviatoric stress. The DRZ is characterized as a region of increased porosity and permeability for purposes of flow calculations. The increased porosity may also be concomitant with a zone of decreased pore fluid saturation. For the Salado the pore fluid is brine. Low permeability and partial saturation with respect to brine are two factors which lead to difficulty in design of test programs, and in the interpretation of field data obtained using traditional methods of formation characterization. Adequate characterization of the Salado DRZ surrounding the WIPP shafts was needed to quantify the impact of any flow which might occur through this zone. This information was critical to demonstration of the efficacy of the seal system design. This paper describes a field test approach which utilized multiple techniques to characterize the DRZ around the WIPP shafts.

Shaft DRZ Characterization Test Program

All testing was accomplished through fluid injection into boreholes (10.2 cm diameter) drilled into the wall of the air intake shaft at WIPP. A total of six holes were tested at two elevations in the shaft. The lower elevation was located at a depth of approximately 629 m, near the repository horizon, and the upper elevation...
was located approximately 100 m below the interface between the Salado formation and overlying lithologies, or about 346 m below ground surface. The boreholes were drilled immediately preceding test conduct, such that additional disturbance to the host rock was minimized (Dale and Hurtado, 1996). Three objectives were defined for the test program. These were: 1) locate the radial extent of the partially-desaturated zone; 2) bound the radial extent of enhanced permeability in the DRZ; and 3) establish a basis for calculating DRZ permeability as a function of radial distance form the shaft wall.

The first objective was accomplished through gas injection into an isolated test interval. Test conduct included a constant-pressure injection phase followed by monitoring of pressure decay in the test interval. Details on this testing method at WIPP may be found in Stormont, (1990). Injection pressure was kept low (on the order of 0.14 MPa) to ensure minimal brine displacement during testing. Data obtained from gas injection tests was interpreted using the well-test simulator GTFM (Pickens et al., 1987) to estimate the formation permeability to gas. Gas flow testing was conducted systematically at intervals located at 0.1 to 3m from the shaft wall. Equipment capabilities of the gas testing system extends to a permeability on the order of $10^{-23}$ m$^2$. The undisturbed (i.e., undamaged due to excavation effects) salt permeability ranges from $10^{-21}$ to $10^{-24}$ m$^2$ and is impermeable to gas when injection pressures are below several MPa. Intervals estimated to have a gas permeability on the order of $10^{-23}$ m$^2$ were assumed to be either undisturbed or saturated with respect to brine. This is due to the assumption that pore space in the salt which is filled with brine will present an impermeable barrier to gas migration at the injection pressure. Pore space which is partially filled with brine will also be manifested as a zone of reduced permeability to gas. Gas testing was terminated when equipment limitations were met, and brine testing was initiated.

The second objective was accomplished through constant-pressure injection and pressure pulse testing using brine, as described in Beauheim, et al. (1993) and Dale and Hurtado (1996). The first interval tested with brine started just beyond the radial point at which gas flow testing had ceased on the basis of the criterion mentioned previously. Two intervals per borehole were tested.

Estimated permeabilities to gas and brine are depicted in Figures 1 and 2. It is important to recognize that the permeability to gas values are estimates, due to uncertainty in the brine saturation state of the formation during test conduct. These estimates, combined with laboratory testing and mechanical process models (RISD, 1996) were used to develop a mathematical model for DRZ permeability as a function of radial extent from the shaft wall, thus meeting the third objective of the DRZ characterization program. This model significantly enhanced predictive simulation capability for the WIPP shaft seals program.

Summary and Conclusions

The field test program described in this paper was developed to meet the specific needs of the WIPP shaft seal system design program. The principal objective of the program was to assess the permeability of the DRZ surrounding WIPP shafts. Uncertainty in the brine saturation state of the DRZ led to implementation of both gas and brine flow testing techniques. These data were formulated into a mathematical model describing the permeability of DRZ surrounding WIPP shafts. As a result, the efficacy of the shaft seal system design was quantitatively demonstrated.

References


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Figure 1. Estimated permeabilities at 346 m below ground surface.

Figure 2. Estimated permeabilities at 629 m below ground surface.
Measurement and Modeling of Two-dimensional Unsaturated Zone Water Fluxes near Buried Radioactive Waste at the Idaho National Engineering and Environmental Laboratory

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Pronounced layering within the 200-m thick unsaturated zone near a waste disposal area at the Idaho National Engineering and Environmental Laboratory causes extreme anisotropy favoring lateral flow. The upper 5 m of the unsaturated zone is primarily a silt loam soil, with layering that has been altered significantly in the landfill. Annual snowmelts cause large infiltrations of brief duration. Nearby (within 2 km) artificial infiltration ponds are used to dispose of surface water in unusually wet years. The episodic timing and geographic nonuniformity of these events greatly enhances the possibility of substantial contaminant-carrying fluxes.

We have assessed the value of several standard unsaturated hydrologic investigational techniques for characterizing the waste-disposal site, the effect of landfill-construction disturbance, and the effect of layering on two-dimensional unsaturated flow. We measured hydraulic and other properties of the unsaturated medium in the laboratory on core samples and on bulk soil, as well as in the field. We performed measurements by identical procedures on a simulated waste trench and on nearby undisturbed soil. The techniques included high-resolution water-retention measurements with submersible pressure outflow cells, and a field instantaneous profile experiment involving 24 hours of flood infiltration followed by redistribution. We simulated two-dimensional infiltration and redistribution of water using the Richards'-equation-based VS2DT model, incorporating measured properties of nine layers down to 4 m depth. The field observations provide direct comparisons to the modeled results, and permit evaluations of the relative usefulness of the various techniques.

Landfill construction by excavating and replacing soil as practiced at the INEEL has a great effect on the behavior of unsaturated flow, as evidenced by how the unsaturated zone responds to the artificial 24-hour flood. During the flood, there is rapid wetting throughout a 2-m thickness of profile in the undisturbed soil, but a sharp, slower moving wetting front in the simulated waste trench. Water flow is impeded at 2 m depth in the undisturbed medium, but not in the waste trench. Both preferential flow in macropores and flow retardation due to layering are important in the undisturbed medium.

Either core-sample measurements or field instantaneous-profile measurements can give unsaturated hydraulic properties, and the results show good agreement between core-sample and field measurements. In the case studied, however, a physical simulation of an event such as a flood shows the behavior of the unsaturated system better than do the individual property measurements. The measured hydraulic conductivity and water retention data, applied in a basic numerical Darcy- and Richards-based model (VS2DT) did not accurately predict the unsaturated-zone response to the flood. The numerical model is a poorer approximation in the undisturbed than in the disturbed medium. Preferential flow is underestimated in the modeling, suggesting that the implicit inclusion through the measured properties of the media is inadequate. Two-dimensional modeling, which can account for lateral flow, is in closer agreement with the...
measurements than one-dimensional modeling, but still underestimates downward fluxes in the undisturbed and overestimates them in the disturbed medium.

The destruction of layers and macropores has significant hydrologic influence. These two elements have opposing effects: layers can retard downward flow, and macropores can increase infiltration during a flood. The net result, however, may be that landfill construction increases the likelihood of water moving to the water table because the natural layering, which could hold water high in the root zone for removal by evapotranspiration, no longer exists.
Time-dependent Changes in the *In Situ* Hydrologic Properties of a Shear Zone

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Abstract

Subsequent to the initial impoundment of the Bad Creek Reservoir in northwest South Carolina in January 1991, lake level fluctuations (up to 33 m/day) caused delayed (98 hours) correlative water level changes in an observation well (OW3). The amplitude of the water level changes in OW3 was ~ 1/5 of that in the reservoir. Assuming 1D diffusion of pore pressure, in the shear zone between the reservoir and OW3, these values of delay and amplitude ratio of the water levels, yield an estimate of 103 cm$^2$/s for hydraulic diffusivity and a permeability of ~ 0.1 millidarcy. In subsequent years (1992-96) the delay reduced to 72 hours and $\Delta W/\Delta L$ increased to ~ 1/4. These observations suggest ~ 40% increase in the intrinsic permeability of the shear zone. We interpret these changes to be due to the flushing of fines in the shear zone due to the pumping action of the lake level fluctuations.

Both the delay and amplitude of the water levels in OW3 showed frequency dependence, the longer periods being transmitted more efficiently (higher $\Delta W/\Delta L$) but with longer delays than the shorter period fluctuations.

Introduction

The Bad Creek Reservoir in northwestern South Carolina is the location of reservoir induced seismicity studies. In conjunction with the construction of the dams and intake tunnels, six southeast dipping shear zones were discovered (Figures 1a and b). Observation wells OW1 - OW3 were drilled to intercept shear zones F, E and C respectively. OW3 is ~ 100 m deep and is located 335 m SE of the reservoir and is connected to it by a 1 m wide shear zone.

Initial impoundment of the reservoir in January - March 1991 was followed by correlative water level rises in the three observation wells. The water level in OW3 increased from 2,093 ft. (ASL) to a mean value of 2,128 ft. in 1992. It fluctuated about this mean value in response to fluctuations in the Bad Creek Reservoir (lake) with a delay of 98 hours ($\Delta t$). We have continued to monitor OW3 and the results of monitoring have been used to infer the temporal hydrologic properties of the 1 m wide shear zone C and are the subject of this paper.

Figure 2 shows the water level in OW3 plotted on an enlarged scale and compared with that in the lake. The lake level has been shifted 98 hours. The water level in OW3 mimics that in the lake in both the long period and in the short period changes.

The amplitude ratio of the water level changes in OW3 ($\Delta W$) and in the lake ($\Delta L$). ($R = \Delta W/\Delta L$) was calculated by comparing the hourly water level values ($\Delta L$ shifted 98 hours) and also by comparing the largest amplitude changes. $R$ was found to be 0.19.

Calculation of Hydraulic Diffusivity and Permeability- The transmission of fluid pressure from the lake to OW3, at a distance $r$, through the shear zone was by diffusion. Based on the assumption of 1D fluid pressure diffusion,
the ratio $R$ is a measure of the pressure changes, i.e.,

$$R = \frac{\Delta W}{\Delta L} = \frac{P(r, t + \Delta t)/P(o, t)}{1 - \text{erf}(r/2 \sqrt{C \Delta t})}$$

(1)

where $P(o, t)$ and $P(r, t + \Delta t)$ are the pressures in the shear zone at the bottom of the lake, at a time $t$, and at $OW3$, at a time $(t + \Delta t)$. $C$ is the hydraulic diffusivity ($\text{cm}^2/\text{s}$) of the shear zone. Knowing $r$, $R$, and $\Delta t$, $C$ can be calculated from equation 1. By assuming reasonable values of the fluid viscosity, porosity and effective compressibility of fluid and assuming them to be constant, the in situ permeability value of the shear zone can be calculated.

**Temporal Variation of Hydrologic Properties** - Using the assumptions described above $C$ and $k$ were estimated for the shear zone. The results are shown in Table 1. After an initial delay of 98 hours in 1992, $\Delta t$ reduced to 72 hours and there was a small increase in the ratio $\Delta W/\Delta L$. These values suggest $\sim 40\%$ increase in $k$. We ascribe this increase to the flushing of fines in the shear zone.

**Frequency Analyses** - Spectral analyses of the water levels in the lake and $OW3$ (1992) showed five peaks corresponding to periods of 28, 17, 12, 7 and 1 days (Figure 3). In 1995-1996, similar peaks were obtained. $\Delta t$ and $R$ were found to be frequency dependent. $R$ followed the relationship $R = 0.5 \exp(-1.29 \times 10^6 f)$ where the frequency $f$ is in hertz. This observation suggests that longer period fluid pressure changes (related to the lake levels) were transmitted more efficiently (larger $R$) but with longer delays ($\Delta t$). Shorter period lake level fluctuations were attenuated.

**Conclusions**

By monitoring water level changes in the lake and in $OW3$ (connected to the lake by 1 m wide shear zone), it was possible to estimate the permeability of the shear zone. The permeability $\sim 0.1 \text{mdarcy}$ in 1992 increased by $\sim 40\%$ in the next few years, possibly due to the flushing of fines in the shear zone by the pumping of lake levels. The longer period fluid pressure changes in the lake were transmitted more efficiently than the short period fluctuations.
Table 1: RESULTS

<table>
<thead>
<tr>
<th>Period</th>
<th>AW/AL</th>
<th>At (hours)</th>
<th>C(×10³ cm²/s)</th>
<th>k (mdarcy)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6/92-8/92</td>
<td>0.19</td>
<td>98</td>
<td>1.0</td>
<td>0.10</td>
</tr>
<tr>
<td>8/94-1/95</td>
<td>0.18 to 0.25</td>
<td>72</td>
<td>1.18-1.63</td>
<td>0.11-0.15</td>
</tr>
<tr>
<td></td>
<td>~0.22</td>
<td></td>
<td>1.44</td>
<td>0.13</td>
</tr>
<tr>
<td>7/95-9/95</td>
<td>0.23</td>
<td>72</td>
<td>1.50</td>
<td>0.14</td>
</tr>
</tbody>
</table>

Figure 1a. Location of shear zones to observation wells, and Bad Creek Reservoir in northwestern South Carolina.

Figure 1b. NW-SE cross section to show the location of OW3.

Figure 2. Water level in OW3 (enlarged scale) compared with the lake level (shifted 98 hours).
Figure 3. Normalized amplitude spectra of water levels in the lake and OW3. The peaks A-E correspond to periods of 28, 17, 12, 7 and 1 days.
Yucca Mountain Hydrochemistry

Session Chair: Ned Elkins, M&O/LANL

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Hydrologic Inferences from Strontium Isotopes in Port Water From the Unsaturated Zone at Yucca Mountain, Nevada

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Calcite is ubiquitous at Yucca Mountain, occurring in the soils and as fracture and cavity coatings within the volcanic tuff section. Strontium is a trace element in calcite, generally at the tens to hundreds of ppm level. Because calcite contains very little rubidium and the half-life of the $^{87}$Rb parent is billions of years, the $^{87}$Sr/$^{86}$Sr ratios of the calcite record the ratio in the water from which the calcite precipitated. Dissolution and reprecipitation does not alter these compositions so that, in the absence of other sources of strontium, one would expect the strontium ratios along a flow path to preserve variations inherited from strontium in the soil zone.

Strontium isotope compositions of calcites from various settings in the Yucca Mountain region have contributed to our understanding of the unsaturated zone (UZ), especially in distinguishing unsaturated zone calcite from saturated zone calcite. Different populations of calcite have been compared, either to group them together or distinguish them from each other in terms of their strontium isotope compositions. Ground water and perched water have also been analyzed; this paper presents strontium isotope data obtained on pore water.

Although pore water can be squeezed from the nonwelded tuffs at Yucca Mountain, the volumes recovered from reasonable lengths of drill core are small. We have used dry-drilled core samples that have dried during storage, as repositories of pore water salts that can be carefully leached with deionized water for analysis of strontium isotope ratios. Crushed core is sieved to obtain a coarse sand (30-60 mesh) fraction that is then leached for less than an hour with deionized water to redissolve the pore-water salts. This water sample is then centrifuged and filtered; strontium is separated by standard techniques for analysis by thermal ionization mass spectrometry (TIMS). Strontium isotope ratios are reported as differences from modern seawater in parts per thousand.

The first samples tested were cuttings from borehole USW UZ-14. These samples were used primarily to determine the best experimental procedure. Most of these samples were leached with water, and then leached again with weak hydrochloric acid (HCl). From these results, we determined that leaching times of less than an hour were adequate to dissolve pore-water salts and that longer times may leach strontium from the rock or secondary minerals. The HCl leaches dissolve calcite with a strontium isotope composition similar to the pore water. The close comparison of $\delta^{87}$Sr from water-leached pore-water salts and that of water squeezed in adjacent core in this borehole indicates that the extraction method is valid. Strontium isotope compositions in the host volcanic rocks are distinct, indicating that pore water has not reached equilibrium with the tuffs.

Once we were satisfied with the experimental technique, we sampled whole core from USW SD-7, excluding core containing macroscopic calcite coatings. The pore water strontium data obtained from USW SD-7 are remarkable in their systematic variation with depth and their distinction from whole rock compositions. At the top of the core, the $\delta^{87}$Sr in the pore water is 3.6,
matching the δ⁸⁷Sr found in surface coatings of calcite at the drill pad. Delta-⁸⁷Sr increases with depth; this increase is especially evident within the nonwelded units of the Paintbrush Tuff (PTn) and is only slightly discernible in the underlying welded Topopah Spring Tuff (TSw).

Although the data preclude local equilibrium between pore-water and rock, the rock data can predict the strontium isotope composition of the pore water if recalculated as a down-hole cumulative value weighted according to strontium content of the rock samples and the associated depth interval. An additional weighting factor that takes into account the higher reactivity of the PTn provides a close match to observed pore-water strontium values throughout most of the TSw. Deviations of the pore water δ⁸⁷Sr from the predicted values are likely due to the presence of clays or zeolites which may contain a long-lived record of pore-water strontium compositions and could have been partially leached in the laboratory.

Our working model assumes that strontium is added to infiltrating water by dissolution of calcite in the soil zone. During times of increased surface vegetation, soil waters are more acidic and volcanic detritus in the soil zone can contribute radiogenic strontium into infiltrating water, thus increasing the ⁸⁷Sr/⁸⁶Sr ratio in the thick calcretes formed during these times. There are two separate populations of soil carbonate that can contribute strontium to infiltrating water; one is dominated by eolian carbonate with a δ⁸⁷Sr = 3.6 and the other is dominated by calcretes in thick alluvial soils with δ⁸⁷Sr = 4.5. Although the eolian signal, represented by soil A/B horizons and calcite coatings on bedrock surfaces, exists throughout the Yucca Mountain region, the strontium signal from calcretes may dominate the strontium contributed to infiltration where they are present. Water infiltrating into welded tuff (Tiva Canyon Tuff or Topopah Spring Tuff) tends to retain the strontium isotope composition of the overlying soil. However, the pore water data indicate that water infiltrating into or percolating through nonwelded tuff (PTn) reacts readily and acquires a strontium isotope signature reflecting interaction with this unit. The strontium isotope composition of the volcanic rocks changes systematically over millions of years due to the decay of ⁸⁷Rb. As a result, pore waters interacting with these rocks would have δ⁸⁷Sr values that decrease linearly with age. Delta-⁸⁷Sr of pore waters in the TSw unit are predicted to change from a modern value of 4.9 to about 0.4 at the time of TSw emplacement (12.7 Ma). The observation that δ⁸⁷Sr varies with microstratigraphic position within thick calcite coatings that occur in the TSw and the match between these ratios and the predicted values strongly suggests that the calcite coatings derive their strontium from the same source as the pore waters; in other words, both pore water and the fracture water leading to calcite deposition within the TSw derive strontium from water-rock interaction in the overlying section, dominantly in the nonwelded units. This model indicates that pore waters in the PTn are redistributed between pore and fracture water that subsequently percolates through the TSw.
Evaluation of the chemistry of pore waters, perched waters and saturated zone ground waters from the Yucca Mountain area leads to the conclusion that there are basically two types of waters. The first type is found in pore waters extracted from hydrologic units above the Calico Hills Tuff. The second type occurs as perched waters and as saturated zone ground waters. Pore waters in the Calico Hill Tuff appear to be a mixture of the two types of water. The first water type is strongly influenced by soil zone processes including evapotranspiration and the precipitation of pedogenic minerals such as silica, calcite and gypsum. Once these waters percolate out of the soil zone, their compositions appear to be minimally affected by rock/water interactions in the unsaturated zone except possibly for ion exchange reactions. The ionic strength of these waters is primarily a function of the time interval between infiltration events of sufficient magnitude to cause soil waters to percolate into the unsaturated zone. These waters are generally saturated with opal-CT and show only limited evidence for ion exchange reactions. The pH of these waters is buffered by elevated carbon dioxide partial pressures in the unsaturated zone which currently exceed the partial pressure of carbon dioxide in the atmosphere. The oxidation/reduction potential of these waters are likely in the oxidizing range (400-500mv) due to the presence of atmospheric levels of oxygen in the unsaturated zone gas phase.

The second type of water shows relatively minor influence from soil zone reactions but is strongly influenced by water/rock interactions in the unsaturated zone. These interactions consist primarily of dissolution reactions and ion exchange reactions. Hydrolysis reactions involving aluminosilicates appear to be of secondary importance. The dissolution reactions are driven by the fact that the newly infiltrated unsaturated zone waters are significantly undersaturated with silica and the aluminosilicate phases in the rocks. Because silica is by far the most abundant component in the rocks (70-80 wt.%), dissolution of a silica phase or volcanic glass is likely the dominant dissolution reaction. The dominant ion exchange reaction involves the exchange of sodium ions in solid phases such as feldspar and volcanic glass with hydrogen ions in the solution phase. The dissociation of carbonic acid is the primary source of hydrogen ions for these reactions and results in increased bicarbonate concentrations in the solution phase. The pH of these waters is a function of the partial pressure of carbon dioxide in the water/rock system. In systems open to the unsaturated zone gas phase, the pH of water will remain in the range of 7.0-8.0. Systems that become closed for some reason may have lower or higher pH values depending on whether or not additional sources of hydrogen ions exist within the system. The Eh of these waters will range from oxidizing to reducing depending on whether they have access to atmospheric oxygen or reducing agents, respectively.
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Use of Air-Flow and Rock-Gas Chemistry Data From Boreholes Open in the Unsaturated Zone to Estimate Permeability and Effective Air-Filled Porosity

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SUMMARY:

Yucca Mountain, the proposed site for a high-level radioactive waste repository, is under intense study to evaluate the potential for liquid and gas transport, based on estimates of the hydraulic and pneumatic properties of the unsaturated host rock. Many numerical simulations have been performed to identify these properties, but these generally have been handicapped by a lack of measured fluxes of gas and/or water flow. Long-term measurement of air flow from well UZ6s that arises from barometric, thermostyphon, and windpumping effects provide data that can be used to identify the permeability to air and the air-filled porosity of the fractured densely welded tuffs in the vicinity of wells UZ6s and UZ6 at Yucca Mountain crest.

Two sets of data on variation of flow with time were collected from well UZ6s, which taps the full thickness of the Tiva Canyon tuffs at the crest of Yucca Mountain. These data include records of hourly average flow collected during 4,732 hours from December 1988 to August 1989 and 15-minute average data collected for a total of 6,141 hours from June 1993 to March 1994. Flow velocity magnitude data were collected using a hot-wire anemometer, and magnitude and direction were obtained using a propeller anemometer. These data were corrected for frictional well losses and were adjusted for wind effects, which could not be modeled. Wind corrections were made based on the results of regression analysis of the residual flow that is not explained by temperature-induced density differences or by barometric pressure fluctuations. Results of the regression analyses are somewhat questionable. Although wind clearly causes greater flow from well UZ6s, the increased flows appear to be better explained by linear regression with wind speed than with the theoretically more justifiable wind speed squared. The regression-based linear relationship between wind speed and flow had to be used for the flow corrections, as the implied offset of the wind-speed squared regression could not be modeled.

Flows corrected for well-loss and wild effects were used in the simulation model Modflow p to determine the transport properties of the tuffs comprising Yucca Mountain. Steady-state simulations based on the density contrast induced by temperature differences between the atmosphere and rock gas provided a means of matching the measured profile of flow with depth. Results of this calibration indicated that the most permeable of the Tiva Canyon tuffs have a permeability of about 3,500 Darcies, but that the Tiva Canyon caprock has a permeability of no more than about 5 Darcies.

Numerous suites of gas-chemistry data based on samples collected from various wells at the crest of the mountain indicate that much of the flow from well UZ6s is derived from cross-formational flow from the Topopah Spring tuffs through well UZ6, which is open through the bottom 90 m of the Tiva Canyon and the full thickness of the Topopah Spring. The feasibility of testing this finding by releasing trace gas into well UZ6 when it was exhausting into the Tiva Canyon tuffs and monitoring for trace-gas arrival...
in well UZ6s was tested by simulation. The calibrated steady-state model was used to simulate wintertime gas transport from the node locations representing well UZ6 to those representing well UZ6s, based on particle tracking. The simulated travel time of about 5 days, based on the laboratory-determined air-filled porosity of 0.05, was well matched by the results of the subsequent tracer test, which indicated a peak concentration arrival time of 5.8 days.

Transient simulations performed to match short-term barometrically induced flows have been much less successful. Simulations based on the laboratory-determined air-filled porosity provide a poor match to these short-term fluctuations. Inverse simulation indicates that an implausibly large value for air-filled porosity of 0.38 would be required to mimic measured fluctuations. A hypothesis that the implied need for a larger potential storage reservoir could be met by incorporation into the model of the underlying Topopah Spring formation and a short circuit through well UZ6 was tested. Results of these efforts were also disappointing, as the model still required implausibly large air-filled porosity of the Topopah Spring and/or the Tiva Canyon to mimic short-term flow variations.

Our inability to simulate short-term flow variations based on any reasonable sets of pneumatic properties indicates that some as-yet unidentified physical process must be incorporated in the model. Our current hypothesis, not yet tested, is that the soils and weathering of the rock outcrops has resulted in the near-surface permeability being lower than that of the unweathered rock, requiring that the mountain be modeled as having a low-permeability "skin".
Secondary Mineral Evidence of Large-Scale Water Table Fluctuations at Yucca Mountain, Nye County, Nevada

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At Yucca Mountain, which is currently under consideration as a potential permanent underground repository for high-level radioactive wastes, the present-day water table is 500 to 700 m deep (Luckey et al., 1996). This thick unsaturated zone (UZ) is part of the natural barrier system and is regarded as a positive attribute of the potential site.

The USGS has studied the stable isotopes and petrography of secondary calcite and silica minerals that coat open spaces in the UZ and form irregular veins and masses in the saturated zone (SZ) (Szabo and Kyser, 1990; Whelan et al., 1994). These studies have revealed a thick barren zone in which secondary mineral occurrences are rare. This barren zone extends from about 100 m above to more than 300 m below the present water table (fig. 1). Shallow groundwater beneath Yucca Mountain is undersaturated with respect to calcite (Benson and McKinley, 1985) and have the potential to dissolve calcite along active flowpaths in this interval. The rare occurrences of secondary calcite in this barren interval appear to have formed at times when the water table was much lower than at present.

Strontium isotope studies of secondary calcite within Yucca Mountain (Marshall et al., 1993), and regional analysis of ground water discharge deposits indicate that water table elevations were higher in the past (Quade et al., 1995). Discharge deposits at paleospring sites in southern Crater Flat, 15 to 20 km southwest of Yucca Mountain, indicate at least a 100 m rise in the water table during the late Pleistocene (Paces et al., 1997). Past water table rises beneath Yucca Mountain of ~100 m are likely and a possible explanation for the paucity of secondary minerals within the lower UZ, although Ca depletion in the zeolitic tuffs through cation exchange may produce calcite undersaturation of percolating waters. Only drillhole USW G-2 contains significant amounts of calcite within the lower 100 m of the UZ.

Figure 1. Stable C and O isotopic compositions of calcite, plotted with respect to the water table, from boreholes collared on the crest or eastern flank of Yucca Mountain. Fields discussed in text are outlined and labeled.
Drusy coatings of free-growing calcite and silica phases formed in the UZ from surface percolation fluxes moving down fracture footwalls and, locally, collecting on the floors of lithophysal cavities. Most UZ calcite $\delta^{13}C$ values, which are generally between -9 and +2‰, indicate derivation of solutes from the overlying soils during infiltration (fig. 1). Local occurrences of early calcite from UZ exposures in drill core and the Exploratory Studies Facility have anomalously heavy $\delta^{13}C$ values (as high as 9‰) that are inconsistent with soil organic matter as the sole carbon source.

Textures and compositions of calcite occurrences from deep in the SZ are distinctly different from those in the UZ. Deep SZ calcite occurs as tightly intergrown crystal masses that filled existing open spaces, replaced phenocrysts, and formed pore-filling cements. This SZ mineralization appears to have formed from moderate temperature alteration of the tuff (Broxton et al., 1987) by Paleozoic ground waters that introduced calcite with $\delta^{13}C$ values of $0\pm2‰$ (Whelan et al., 1994). Timing of alteration is consistent with the formation of the Timber Mountain caldera (Bish and Aronson, 1993).

Secondary mineral occurrences formed in the UZ and the SZ are distinguished by the following characteristics:

1. **Textures/mineralogy** - UZ calcite occurs as free-growing crystals, with patchy chalcedony or drusy quartz in the early stage and with opal in the later stages. Alteration-event calcite, locally with banded chalcedony and quartz, formed interlocking crystal mosaics that filled SZ open spaces.

2. **UV fluorescence/phosphorescence** - Early UZ calcite does not fluoresce or phosphoresce nor does later calcite found at depth in the UZ; late UZ calcite fluoresces and phosphoresces bright white in occurrences from the near surface. Alteration-event calcite fluoresces bright orange but does not phosphoresce.

3. **Cathodoluminescence** - Calcite from the UZ generally does not luminesce but locally contains thin, irregular growth bands that luminesce faintly to moderately orange. Alteration-event calcite invariably luminesces a fiery bright orange.

4. **Fluid inclusions** - Calcite from the UZ has fluid inclusions that are typically single-phase, either all-liquid or all-vapor, indicative of entrapment in a UZ setting (Roedder et al., 1994). Alteration-event calcite contains dominantly two-phase inclusions indicative of moderate-temperature (94 to 239°C), SZ mineral growth (Bish and Aronson, 1993).

5. **Strontium isotopes** - $^{87}Sr/^{86}Sr$ ratios of calcite samples display slightly overlapping ranges of 0.7096 to 0.7127 in the UZ and 0.7086 to 0.7098 in the SZ, and do not clearly differentiate between the UZ and SZ (Marshall et al., 1993).

Anomalous barren zone calcite occurrences from the upper SZ are outlined on figure 1. These anomalous occurrences range in depth from about 140 to about 300 m below the present water table and generally resemble UZ calcite because they: (1) are free-growing; (2) do not fluoresce or phosphoresce; (3) locally display orange growth banding but are largely nonluminescent; and (4), based on preliminary fluid inclusion observations, formed below $\sim50°C$ in a vadose setting. Finally, (5) the $^{87}Sr/^{86}Sr$ ratios of the calcite from these anomalous occurrences range from 0.7094 to 0.7104; although not definitive, these ratios are similar to the bulk rock compositions of the host rocks and could form during UZ conditions.

Based on these observations, the anomalous secondary mineral occurrences from the upper SZ appear to have formed under UZ conditions — lower water table elevations in the past is the most straightforward mechanism to explain an UZ setting at these depths. Other explanations involve movement of the tuff sequence relative
to a more or less static water table position. For instance, past rates of tectonic uplift are unclear, as is the rate of isostatic crustal depression following eruption of the tuff sequence. Conceivably, such processes could have raised the tuff sequence with respect to a static water table.

The $\delta^{13}C$ values of the anomalous occurrences range widely from almost -10‰ to nearly +5‰. This range is comparable to the entire range of secondary calcite $\delta^{13}C$ values recorded by the more than 9 M.y. mineralization history of the UZ. The range of $\delta^{13}C$ values in this anomalous interval, therefore, may be evidence of more than one period of significantly lowered water table elevation.

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Isotopic Data for Pore Water Extracted from Unsaturated-Zone Cores at Yucca Mountain, Nevada

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Isotopic compositions of unsaturated-zone (UZ) ground water ($\delta^{18}$O, $\delta$D, $\delta^{13}$C and $^{14}$C) at Yucca Mountain, Nevada, the site of a potential permanent national nuclear waste repository, can be used to infer the origins of water, residence times of the water, water flux, climatic and evaporative history of water, flow paths and velocities. These data can also be used as indicators of transport properties or water-rock interaction. The lack of long-term direct measurements of infiltration requires proxy indicators of water movement through the UZ to extend the record into the past. This report will discuss $\delta$D and $\delta^{18}$O data obtained from pore water, along with the$\delta^{13}$C and $^{14}$C data of gas and water obtained from four boreholes dry-drilled through all UZ lithologic units to infer the existence of nonvertical flowpaths through the mountain and residence times of pore water.

Stable isotope compositions of pore-water samples from the USW SD-7, -9, -12 and USW UZ-14 boreholes indicated that little evaporation occurred before infiltration. Furthermore, the top two-thirds of the Topopah Spring Tuff in the SD boreholes are similar to values of similar samples from the Paintbrush nonwelded unit in borehole UZ-14 ($\delta$D > -100‰). Also these data display a trend toward more negative values as the depth increases. Borehole USW SD-9 stable isotope data are slightly scattered, but mostly are greater than -100‰. If mixing of a significant amount of the last ice-age water (more depleted in $\delta$D due to cold climate) occurred in the matrix water of the Topopah Spring Tuff, the pore water $\delta$D values would be shifted to more negative values; this was not observed. However, in the basal vitrophyre near the bottom of the Topopah Spring Tuff, the pore water $\delta$D values consistently are shifted to more negative values, implying that pore water probably contains a component of the last ice-age water. Previous study (Pei Yu, 1996) indicated that vacuum distillation of pore waters for stable isotope analysis produced unreliable results from tuffs containing zeolite minerals. However, mineralogical analyses of these cores in the basal vitrophyre indicated absence of zeolites. The stable isotope values of pore water in the Calico Hills Formation in all boreholes are greater than in the immediately overlying Topopah Spring Tuff, and are similar to the values above the basal vitrophyre. Therefore, the pore water above the vitrophyre zone in the Topopah Spring Tuff and in the Calico Hills Formation is likely to be Holocene water, but in the basal vitrophyre the pore water is likely a mixture of ice-age water with the Holocene water.

Gas-phase $^{14}$C data from borehole USW UZ-1 should be representative of borehole USW UZ-14 because these two boreholes are only 30 m apart. The $^{14}$C activities of gas-phase CO$_2$ in borehole USW UZ-14 decrease steadily from the surface to a depth of about 366 m (where $^{14}$C activity is about 20 percent modern carbon (pmc), equivalent to $^{14}$C residence time of about 13,000 years, and increase near the top of the Calico Hills Formation with some irregularly large activities of about 100 pmc for three samples. The $\delta^{13}$C values of two of these samples are about -9‰, indicating a larger component of atmospheric CO$_2$ gas possibly introduced during drilling (atmospheric CO$_2$ has $\delta^{13}$C = -7 to -8‰). The third sample has a $\delta^{13}$C value of -15.3‰. The other gas samples in the Calico Hills Formation have $^{14}$C activities which increase with depth and range from 48 to 80 pmc. The $^{14}$C activities of gas-phase CO$_2$ in borehole USW SD-12 decrease from the surface to depth similar to the trend observed in borehole USW UZ-14 with two anomalously large $^{14}$C activities:
one near the lower part of the Topopah Spring Tuff (386 m or 1,266 ft); and the other near the upper part of the Calico Hills Formation (436 m or 1,430 ft). In any case, the majority of $^{14}$C activities in gas-phase CO$_2$ in the Topopah Spring Tuff of USW SD-12 are consistent with the data in borehole USW UZ-14. However, the change in gas-phase $^{14}$C activities in the Calico Hills Formation is due to equilibration of CO$_2$ gas and the bicarbonate ion in the liquid phase which probably was transported through fractures. The modification of $^{14}$C activities in the gas phase will be greater because the liquid phase contains an order of magnitude more carbon than the gas phase (most pore spaces in the Calico Hills Formation are occupied by water which has a large concentration of bicarbonate ion, i.e. the dominant carbon-bearing species). Therefore, gas-phase $^{14}$C activities should be representative of the pore-water $^{14}$C activities.

Pore-water $^{14}$C values in the upper 91m of boreholes USW UZ-14 and USW SD-12 are in general agreement with the gas phase data, indicating equilibration between the liquid and gas phases. However, in the Calico Hills Formation of borehole USW UZ-14, some aqueous-phase $^{14}$C data are about 30 pmc younger than the gas-phase $^{14}$C data from the equivalent depth. The reason for the non-equilibrium condition in the aqueous and gaseous phases for the carbon species likely is due to core samples that were contaminated with drilling air. Gas samples were pumped for 18 hours to remove any atmospheric gas before sample collection. Thus the pumped gas samples were assumed to be equilibrated with the in-situ pore water (but not aircontaminated core water), and are similar to the pore-water $^{14}$C residence times.

In conclusion, the UZ pore-water stable-isotope values at Yucca Mountain, Nevada, are generally larger than the measured lowest value of -99.8 permil in $\delta$D except in the basal vitrophyre zone near the bottom of the Topopah Spring Tuff, indicating water of Holocene age. The $\delta$D values near the basal vitrophyre in three of four boreholes examined (USW SD-7, -9, and -12) consistently are shifted to more negative values, implying that waters were infiltrated during the colder climate of the last ice age. The $\delta$D values in the Calico Hills Formation in all three boreholes are larger than those of the basal vitrophyre zone and similar to those values above the basal vitrophyre zone, indicating post-ice age water.

The gas-phase $^{14}$C profiles show a general increase in residence time downward with depth in the Topopah Spring Tuff to 13,000 years around the vitrophyre zone. The gas-phase $^{14}$C residence times in the Calico Hills Formation below the vitrophyre zone are younger, ranging from 1,000 to 6,000 years. This time inversion is consistent with the interpretation of the $\delta$D values. This inversion could be attributed to mixing of vertically percolating pore water with younger water derived from a different flow path, such as lateral flow from the Calico Hills Formation charged through the rest or west side of Yucca Mountain.

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International Papers

Session Chair: Paul Witherspoon LBNL/UCB

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Hydogenic Experiments in Fractured Granite at the Kamaishi Mine, Japan

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Purpose

This experiment investigates groundwater flow and transport in fractures at a scale of several meters to several tens of meters. This work complements laboratory experiments on 1-m scale being carried out at PNC's ENTRY Laboratory in Tokai.

Some major goals of this experiment are:

- identify water bearing fractures and their geologic and geochemical characteristics
- understand how fractures and fracture zones form flow networks
- understand how the openings of the fractures relate to the transport velocity
- identify mechanisms controlling transport such as dispersion along flow paths.

The experimental area is located at the 550-m level of the Kamaishi Mine, approximately 350-m below the surface. The experiments are being conducted using seven, 80-m long boreholes (KH-19 to KH-24) in an area north of the KD-90 experimental drift. KD-90 is a 50-m long drift excavated in 1990 and used for studies of flow to underground openings. The region around the KD-90 drift has largely been drained of water by the mine, and the groundwater pressures are equivalent to a water column about 10 to 35 meters above the drift floor. The task 3-2 experiment was developed after high groundwater pressures (about 200m of water above the 550 level) were discovered in a borehole from the KD-90 drift (KH19).

Hydrogeologic Characterization

During drilling the Task 3-2 holes, the flow rate and pressure in the borehole were measured daily. The groundwater pressures in previously drilled holes were also monitored to detect when hydraulic connection is made with the hole being drilled. These hydraulic responses indicated the intersection of conducting fractures with the borehole. We have found that groups of monitoring intervals respond to pressure interferences together. We have named these groups, or zones, using letters from A to F.

After the holes were finished drilling, we logged each hole with a high-resolution television camera to map the fractures. We also conducted geophysical measurements using radar reflection. After the geophysical measurements, we used packers to log the location and flow rate of groundwater into the hole to a resolution of 1-m of length. When we completed the flow logs, we prepared multiple packer piezometers to isolate the major conducting zones from one another. The computer data acquisition system added these test zones to the pressure monitoring system for the next borehole. After all the piezometers were been installed, we ran pressure
interference tests by withdrawing water from selected piezometer intervals, and monitoring pressure drops in all the other intervals.

Each borehole has equipment that isolates the major conductive zones and provides access for measurements and pumping water. The boreholes have from four to ten separate intervals separated by inflatable packers. Each packer has separate flow, pressure measurement, and packer inflation lines. The borehole equipment was designed and built by Baski Inc. of Denver, Colorado, USA. Each piezometer uses fixed-end packers and stainless steel pipes such that the entire system has a constant outer diameter of about 70-mm. The piezometer fills the 76-mm boreholes as much as possible to minimize the water storage in the hole. Intervals that are selected for tracer testing have an additional instrumentation coupling. The coupling has a large diameter tube for withdrawing water, as well as a carrier with a sensor to measure the electrical conductivity and temperature of the water.

**Hydrogeologic Conceptual Model of the Task 3-2 Area**

After high pressure was found in KH-19, we made a hypothesis that there was a flow barrier separating the high pressure groundwater connected to the surface from low pressure groundwater connected to the mine. As we developed the boreholes, a more complicated picture emerged -- one of several groundwater compartments. Each compartment or zone has its own pressure. Each responds rapidly to pressure interferences within the compartment, but not to interferences from other compartments or zones.

Zone D is apparently the largest compartment with the highest pressure, about 180-200 meters of groundwater head relative to the ISO-level of the mine. Zone D was the original high-pressure zone discovered in KH-19. Zone D decreases in diffusivity from east to west. The zone occupies most of KH-19. In KM-2; it splits into two “tongues” which are separated by a section of the C zone. By KH-21, the D zone has lower diffusivity, and the zone disappears by KH-22.

Zone F is the next highest pressure zone. It occupies the deepest parts of KH-21, 23, 24, and 25 and has a groundwater head of about 140 meters.

Zone E and C are minor zones in the central part of the borehole array, but they become more important zones to the west in KH-22.

Zone B is the shallowest significant zone. It has a lower pressure than the other zones and appears to be connected to the mine through zone A. Zone B appears across the entire borehole array, except for hole KH-23, which it skips to re-appear in KH-22. The compartments are not completely isolated, as water likely flows from higher pressure regions which are well connected to the surface to lower pressure regions which are well connected to the mine.

The cause of the compartmentalization of flow at the Kamaishi Task 3-2 site is not known for certain. Hypotheses include:

- a clustering of fractures reflecting fractal spatial distributions.
- shearing or minor faulting which cuts fractures and isolates them with low permeability, clay fault gouge.
- the continuous evolution of fracture transmissivity due to tectonic reactivation and geochemical modifications of fracture fillings.

**Tracer Tests and Groundwater Chemistry**

Tracer tests define the transport properties of the fractures and the compartments. The tracer tests are focusing on two single fractures, one in
the "F" zone and one in the "E" zone. Fracture zone tracer tests are being run in the "D" zone. The tests will use a range of distances between 2 meters and 10 meters.

The tracer tests are designed to be conservative using low-concentration saline solutions. Tracers are injected using dipoles, that is, injecting traced water at one rate, and withdrawing the water from another packer section at the same or a different rate. We measure the concentrations in the injection packer interval using downhole conductivity sensors. At the withdrawal hole we measure concentrations in the downhole interval as well as using specific ion electrodes at end of the withdrawal tube. Water is automatically sampled for chemical analysis at regular intervals during the tests to check the accuracy of the ion electrodes. The tracer program will look at variations due to anisotropy, dipole strength, and reciprocity (reversing the injection and withdrawal intervals).

As to groundwater chemical composition, there is no major variation among the compartments in the Task 3-2 area, and the water is a similar, Na-HCO₃ composition to waters from the 250-m level. The task 3-2 water differs, however, from Ca-HCO₃ waters sampled nearby in the KD-89 area. These preliminary results suggest that the Task 3-2 area compartments do not isolate waters of different chemical composition.

Implications for Radioactive Waste Performance Assessment

- Compartmentalized flow systems will have lower groundwater velocities and flow rates than other systems with similar permeability and hydraulic gradient.

- It is not clear yet what makes the compartments, or how unique they are to Kamaishi, however, compartments and flow barriers are known in petroleum reservoirs and in faulted rock masses.
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Geological Characteristics of the Armenian Nuclear Power Plant’s Region and Hydrological Criteria of a Medium for Isolation of Radioactive Wastes

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The Armenian Nuclear Power Plant (ANPP) has been functioning since December 1976. After 20 years of uninterrupted operation it was stopped in 1989 after the catastrophic Spitak earthquake occurred on December 7, 1988.

The ANPP restarted operation at the fall of 1995, which is a unique event for such energy objects. At present the second unit (one of two reactors) successfully operates at approximately 300 MW.

The ANPP comprises two WER-440 reactors with a power of 420 MW, which were manufactured in the Russian Federation. During the first period of operation the ANPP power was about 850 MW.

The volume of radioactive wastes of various categories accumulated during the whole period of its operation (14 years) is estimated as follows:

a) solid wastes were 6809 tons, including 51 tons of high level ones, 1324 tons of medium level, and 5434 tons of low level;

b) liquid wastes (of medium and low levels) were 2771 m³; the medium level wastes contained mainly $^{137}\text{Cs}$, $^{90}\text{Sr}$, $^{60}\text{Co}$, $^{54}\text{Mn}$ and other radionuclides. The used fuel before stoppage of the ANPP was taken out of the country to Russia for further re-treatment. After the ANPP reopening (the fall of 1995) this fuel remained in the territory of Armenia.

All the radioactive wastes of the ANPP are temporarily stored in special containers and are preserved in the special premises in the territory of the ANPP, and the used fuel is kept in the cooling ponds of Units 1 and 2.

An urgency for solving the problem of safe and long-term burying of permanently-increasing-in-volume radioactive wastes and used fuel of the ANPP in the geological medium in the territory of the Republic of Armenia is based on the above mentioned facts. However, up to now there is neither governmental nor other program aimed at solving this very complicated problem.

The proposals on assessment of safe isolation of radioactive wastes in the geological medium in the republic’s territory, presented in this report, are very preliminary.

Geological and tectonic characteristics

The territory of Armenia occupies the north-western part of the Armenian Highland, which is included into the Tavro-Caucasian segment of the Alpine-Himalayan orogenic belt. In the contemporary structure this region is an intra-continental heterogenous orogenic-block mountainous formation. It comprises different-age structural elements (blocks) which have different geological pre-history and are merged into a united microcontinent in the result of collision during a neotectonic phase. The following structures are distinguished in this region (from the north to the south):
1. Somkhet-Karabakh-Kapan arc-island block of the Mesozoic consolidation, which was developed on the sialic Hercynian basement;

2. Armenian block of the Late Cenozoic consolidation on the Baikalian basement;

3. Sevan ophiolite suture zone, which is confined to the northern branch of the Mesothetys oceanic basin and separates these two structures;


The Late Cenozoic history of geological evolution in the collision zone between the Euro-Asian and Iranian-Arabian continental plates corresponds to collision settings. They caused an intensive Pliocene-Quaternary volcanism within the Armenian block and distinctly pronounced neotectonic and seismic-and-tectonic activities of the given territory. Fig. 1 shows a model of neotectonic activity of the region according to A. Karakhanyan (1997).

The Earth’s crust thickness in the region, according to seismic data, varies from 48 to 55 km. The sedimentary cover’s thickness does not exceed 8 km. The crust is broken by a net of faults of various orders and different spreading.

**Hydrological and hydrogeological conditions**

In geomorphological aspects the region is a highly dissected high-mountainous country situated between the rivers of Koura and Araks, the main water arteries of the Minor Caucasus, which belong to the Caspian Sea basin. The principal geomorphological units are represented by combinations of folded mountain ranges, large volcanic massifs, uplifted lava plateaus with numerous volcanic cones, narrow river valleys and gorges, and lacustrine intermontane depressions-plains. The absolute altitudes vary from 400 m to 4,090 m with about 90% of the territory being situated above 1,000 m above sea. The climate is dry continental one. A vertical zonality caused by a mountainous landscape, together with a seasonal variation of climatic conditions, such as drastic temperature changes, non-stable regime of precipitation and surface water discharge and evaporation are observed in the region. The mentioned factors specify a complexity and unstable character of the region’s hydrological regime. The region as a whole is characterized by low-water and nonhomogenous surface discharge.

In hydrogeological aspects the area is a highly uplifted drainage zone and is confined to the zone of intensive water exchange with a characteristic direction of surface and underground water discharge from the axial belt of the folded formation towards the Koura and Araks depressions. In spite of the Minor Caucasus being an arid zone in general, the subsurface of the territory of Armenia is rather water abundant.

The Pliocene-Quaternary volcanic formations (various lavas, tuffs, ignimbrites, slags, pumice sands, etc.), lacustrine-and-river and surface loose-fragmental formations play an extremely important role in supply and distribution of underground water.

In order to specify the hydrological and hydrogeological criteria aimed at solving the posed problem, the regional scheme of hydrogeological zonation of the territory of Armenia (A. V. Avetisyan, 1976) was used.

The territory of Armenia is divided into four regions according to structural-and-tectonic plan’s character, geological formation types, relief morphogenesis and physical-and-geographical conditions: I - northern and north-eastern folded and folded-block formations; II - central volcanic highland; III - southern and south-eastern folded ranges; and IV - intermontane depressions.

For the given purpose the regions I and III are most interesting. Ancient volcanogenous,
volcanogenous-sedimentary and plutonic complexes, which are basically characterized by low water permeability, low filtration parameters and low water abundance, are widely developed here. The second region formed by young volcanic formations that have high porosity and fracturing, high filtration factors, water permeability and absorption, humidity, etc., is of lesser interest. The fourth region is formed by water-abundant lacustrine-and-river (pebble beds, gravels, sands, clays, etc.) formations alternating with flows of highly porous fractured lava and pyroclastic formations. There are many horizons with artesian water and underground water line is established at the depth near the surface. These specific features exclude prospecting within this region aimed at finding promising sites for burying radioactive wastes.

Criteria for preliminary choosing of sites

Depths where radioactive wastes are to be placed are of principle importance for their safe burying. Unique constructions designed to store high level wastes (HLW) shall be situated in deep horizons (down to hundreds of meters); medium and low level wastes (M&LLW) may be isolated in shallow horizons (tens of meters from the surface) for safe and long-term storing, in accordance with the IAEA recommendations (IAEA, 1995 and 1997). In order to choose preliminarily promising sites suitable for our problem, we accept both options and further studies should be carried out in accordance with more particularly posed objectives.

Substance composition and properties of a medium planned for waste storing are of no less importance. The articles published in the collection of the Second Worldwide Review on Geological Issues in Isolation of Radioactive Wastes (Berkeley, 1996) show that in different regions of the world it is proposed to use rocks of various genesis and types for radioactive waste isolation, and there are no any strict restrictions.

Based on specific features of the geological structure of Armenia, several types of geological objects for further studies as suitable sites are considered.

A basis for preliminary choice of suitable sites was comprehensive geological and hydrogeological and structural-and-tectonic criteria for a medium. Geomorphological, physical-and-geographical, volcanic conditions, environmental situation and other factors were taken into account as well.

Positive criteria are mainly rock's water resistance (or its minimum water saturation degree), positive character of plicative structures (anticlinal folds), ancient consolidated volcanogenous-sedimentary complexes, as well as far distance from water-abundant sites and river flood-plains, active fault zones, low thickness of young (N₂³ - Q) effusive strata (with water confining base), low populated regions, etc.

The proposed sites are shown in the scheme of region’s hydrological zonation (Fig. 2). In the first region the sites are confined to the piedmonts of Goughark (1 and 3), Mourgous (2) and Somkheti (4) ranges. They are characterized by a moderately humid climate, development of the Late Cretaceous-Eocene granitoids (1) or volcanogenous-sedimentary complexes, as well as far distance from water-abundant sites and river flood-plains, active fault zones, low thickness of young (N₂³ - Q) effusive strata (with water confining base), low populated regions, etc.

In the second region five sites are distinguished. Two of them (5 and 6) are situated in the northern part within the Goukasian-Ahotsk medium-altitude volcanic plateau in the upstream of the Akhourian River basin in a zone of moderate mountainous climate. The plateau is formed by a water-permeable layer (100 to 250 m) of (N₂³ - Q) doleritic basalts, which is underlain by the Eocene water-resisting volcanites of andesitic-dacitic-ryholitic composition. The
other sites are situated in an arid continental climatic zone within the eastern (7,8) and southern (9) peripheral volcanic plateaus of Mount Aragats massif. The plateaus are formed by highly water-permeable stratum of porous fractured basaltoids and overlapping the Upper Pliocene-Quaternary tuffs with the thickness of 200 m (in the west) to 450 m (in the south). They are deposited of the Eocene volcanites (in the north-west) and the Miocene thick clayey sandy formations (2,000 m), which are a regional water confining stratum in this region. Underground water line is at the depth of 80 to 100 m.

In the third zone the proposed sites are located in its north-western part within the Vayk (11) Range, in the areas with arid hot desert climate.

In these sites the Palaogene and Palaeozoic water-unsaturated (dry) and practically water impermeable deposits (clayey carbonate formations) are developed. The last two sites are located in the southernmost part of this region within the Bargusha (12) range slopes, where the Mesozoic (Jurassic-Cretaceous) volcanogenous and volcanogenous-sedimentary weakly water permeable deposits are developed, and the Meghri Range (13) formed by the Neogene granitoids.

Proposals and recommendations

The preliminary analysis of available factual material and review of the databases allow to distinguish suitable sites very conditionally at this stages of study, and according to a number of signs to assess their prospectivity for further investigation.

It is recommended to establish a special division (team) involving corresponding experts for drafting special program and projects in comprehensive and detailed study of geological-and-hydrogeological and seismic-and-tectonic aspects in the above mentioned sites with the aim to choose most promising sites. In the area where many young volcanoes are situated it seems necessary to carry out special researches on assessment of volcanic hazard. The next stage of study should include a comprehensive field testing aimed at revealing of hydrogeological and geotechnical parameters to solve engineering-and-geological problems, as well as a computer simulation of an object. It is also proposed to draft a program for collaboration of experts from Armenia, the USA and European countries to carry out successfully the above mentioned researches aimed at solving finally this urgent problem.

References


Figure 1. Active tectonics in the central part of collision zone between the Arabian and Eurasian lithosphere plates. 1 - main strike-slip faults; 2 - main thrust faults; 3 - relative motion of lithosphere plates, microplates and blocks with respect to Eurasia; 4 - relative motion of the North-Armenian arc Blocks. TUP. MP - The Turkish lithosphere microplate, IR. MP - the Iranian lithosphere microplate; Naa - North-Armenian Arc; UA - Urmian Arc; DA - Dagestsn Arc; Active faults: DFE - Javakh extension fault; E-SF - Zhetorehensk-Sarikamish fault; P-SF - Pambak-Sevan fault; AF - Akhurian fault; Gf - Garni fault; T-CF - Tutak-Chaldran fault; B-TF - Balikgheld-Tabris fault; NAF = The North-Anatolian fault; EAF - East Anatolian fault; SF - Zagross fault; MTGC - the Main Atrust of Greater Caucasus.

Figure 2. Hydrogeological zonation of the territory of Armenia. I - northern and north-eastern folded and folded block ranges; II - central volcanic highland; III - southern and south-eastern folded ranges; IV - intermontane depressions. Circled numbers - proposed sites.
Future of Geological Formation Usage for Radioactive Waste Isolation in Western Ukraine

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Introduction

Presently there are not enough storage facilities in the Ukraine for safe disposal of radioactive wastes (RAW) and hazardous chemical wastes (HCW). Accumulation of these wastes occurred during last decades and reached immense sizes after the Chernobyl nuclear catastrophe in 1986. Low, medium and high-level RAW now sit uncovered near the Chernobyl NPP, as well as far away. RAW are formed also by other four NPPs, industrial and military objects.

HCW are produced in four basic regions:

5. Kyiv-Chernobyl region - of high RAW prevalence;
6. East-Ukrainian region, including 2 NPPs - both RAW & HCW occurrence;
7. Dnieper region (including 2 NPPs) - RAW & HCW occurrence;

According to the developed state program of radioactive waste management, the construction of a national RAW storage facility is planned. The possibility for creation of regional storage facilities also exists. The program of HCW control is still being developed. If we take into account that, potentially, the total amount of HCW is much greater than of RAW, a similar approach to the latter seems prospective.

Within the External zone, the thick mass of Neogene clay deposits occur. This zone is of primary interest. For a more detailed study, the two sites within Ciscarpathian foredeep external zone were selected. The first site is located in the region of Sadova Vishnya village. In its geological structure, the Dashavian suite is mostly interesting for RAW and HCW storage. The suite, having a total thickness of 1000 m, is composed of clays, aleurolites, tuffs and rare interbeds of sandstone. The intercalations are presently rich of organics. The last factor is beneficial, since organic matter promotes sorption of radionuclides and chemicals. In the mineral structure of clays, the hydromica and montmorillonite are dominating.

The second site is situated 40-50 kilometers north-west of Kolomyia. Prospective locations for RAW and HCW disposal is in the clayey Kosovian suite having thicknesses up to 400 meters, able collectors (salts and zeolite tuffs) and suitable geological and flow conditions (aquiclude and low filtration properties of rocks).

The aquiclude salts of Tereblya formation are of great interest for further research. The salts within the traced Danilov-Tereblya brachyanticline are believed to be favorable. These salts are of poor quality and have no industrial use, because they are enriched with clay particles. The Tereblya salt stock is the most favorable for waste burial within the brachyanticline (optimum depths: 700-1000 m).

Novoselitsa tuffs favorable for RAW disposal occur at depths exceeding 1000 meters in the zone of stagnant groundwater flow regime.
In addition, the Novoselitsa formation exhibits a considerable sorption capacity due to high zeolite content (up to 40-60%).

The Teresvinian suite is also prospective, because of high concentration of zeolites (clinoptyllolite, analcime) in tuffs and low filtration properties of rock at depths more than 500 meters.

A significant part of the Volynian-Podolian margin of the East-European platform is characterized by adverse conditions because of limited occurrence of low permeable deposits, wide occurrence of rock disintegratuerian clayey rocks which can be studied north-east of L'viv. They occur at 1000 m and greater depths, underlying low-permeable marls and chalks. They are characterized by very low permeability.

1. Lower Carboniferous, Devonian and Silurian clayey rocks can be studied north-east of Lages, with detailization of explorations. It will allow to us select some more prospective sites for: National RAW storage, regional RAW, and HCW storage.

2. Western Ukraine is one of four basic regions with significant volumes of RAW and HCW. Therefore, researches of prospective places for their isolation are expedient there.

3. Presently seven prospective sites can be selected in Transcarpathian foredeep, Ciscarpathian foredeep and Volyn-Podolian margin of the East-European platform.

4. From the geological viewpoint, the most prospective for studying are:

- Tereblynsk salt stock and Novoseltsk tuffs.

- Sudova Vyshnya site (clays).

- Vladimirets' sites been confirmed by world research experience.

5. At these preliminary stages of research it is expedient to estimate sites' prospective both for RAW and HCW disposal.

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Introduction

The evaluation of the suitability of a specific site or formation for deep geologic disposal is based on a total system performance assessment. This includes consideration of the engineered barriers, the repository near-field, the far-field (or geosphere) and the biosphere, for the particular waste form.

Obtaining the required data for the performance assessment is one of the four major objectives of the site characterization activities, namely: (1) data for performance assessment; (2) data for construction; (3) basis for the design of future exploration steps; (4) baseline information for the evaluation of environmental impact effects from underground constructions.

The role of groundwater flow modeling is to provide quantitative and qualitative input to all these four categories mentioned above. However a decision on a site’s suitability cannot be based on results of groundwater flow modeling alone.

The Geodataset(s)

With the exception of baseline monitoring data (e.g., piezometric head in observation wells, discharge and water quality in springs) none of the other data collected in the field flow directly in the performance assessment models, the database for the construction or the design of future exploration steps. The process of converting the field data and observations to the information required above is referred to as Data Synthesis (or Geo-Synthesis) (NAGRA 1997, 1994). The final product, which is also the link with the total system performance assessment are the Geo-datasets (GDS). The main strength of the methodology that Nagra has followed lies on the interdisciplinary interaction for the development of the geo-dataset and its traceability. Typical GDS entries are:

**GDS: Performance assessment**

6. Conceptual models
7. Mineralogy/Geometry of Water-Conducting Features
8. GW-Flow
9. Flowpaths
10. Reference Waters
11. Repository Gas Migration
12. Longterm Scenarios

**GDS: Construction**

13. Tunnel Layout
14. Geotechnical Parameters
15. Stress State

**GDS: Exploration**

16. Extent of host rock
17. Distribution of K
18. Layout determining features

In order to obtain from the field data the required information shown above a close interaction among the involved technical disciplines, e.g., geology, hydrogeology, hydro-chemistry and rock mechanics, is required. As part of the Data Synthesis process the following stages are...
then encountered: interpretation of primary data (i.e. data collected within the same discipline), preliminary conceptualization, interpretation and integration of secondary data (i.e. relevant results from other disciplines), improved conceptualization, numerical modeling. The last three stages can be repeated until the results are consistent with all available data.

The role of groundwater flow models

The groundwater flow models are part "site characterization" and part "performance assessment". Their primary role is to provide the necessary information to assess the suitability of the site, as defined above. The exchange with the performance assessment models that calculate radionuclide transport is mainly performed through the Geodataset.

There is a significant data reduction and abstraction involved developing the Geodataset, but if it is done in an interactive and systematic manner then the proper representation of the natural system in the PA models is ensured. As "tools" the groundwater flow models are very powerful in assisting to understand, in both a qualitative and a quantitative sense, the fluxes and flow patterns in a particular site. More importantly they are an additional incentive for inter-disciplinary interaction to develop a consistent hydrogeological conceptualization the site.

Groundwater flow models are also used to assess the effect of parameter uncertainty or the effect of different conceptualizations. It is at this mode that they are most useful for the design of future exploration programs, because they can assist in prioritizing the different exploration steps.

Probably the most difficult step to realize is the simplification of the natural system - the data abstraction and reduction required for the geodataset. From the site characterization point of view the model chain is very complex and groundwater flow is only a small part of it. Nagra's experience has been to repeat the whole process of geodataset development at least once, in order to facilitate communication and to also assess what are the critical issues. The most recent example is the Wellenberg Synthesis of the investigations of Phase I and II (Nagra 1997). The presentation will highlight the role of groundwater flow models and point out some of the lessons learned based on this particular application.

References


Complexation of Structural-Geodynamic and Hydrogeological Methods of Studying Areas to Reveal Geological Structural Perspectives for Deep Isolation of Radioactive Wastes

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Introduction

After the Chernobyl disaster on April 26, 1986, at Chernobyl NPP 4th Unit, a huge amount of radioactive wastes (RAW) appeared within so-called “Chernobyl exclusion zone” having area over 2000 sq. km. The urgent problem now is of safe isolation of these dangerous wastes.

The Chernobyl NPP is situated within the boundaries of Ukrainian crystalline shield’s (WCS) slope. For this reason it is necessary to reveal favorable geological structures, primarily, in crystalline rocks of UCS, for safe isolation of RAW. Exploration of prospective sites for this purpose have not been performed, and it seems expedient to make preliminary assessment of the UCS territory by various methods.

Generally, for obtaining such preliminary assessment of area, the results of structural-geological and petrological works are widely used. But in our case, because of very weak degree of studying, this approach would not provide reliable result. For this reason, we decided to apply a complex methodology which includes development of two models—structural-geodynamic and hydrogeological.

The region of our exploration covers the eastern part of the Korosten Plutone and its slope, reaching the Chernobyl NPP.

Basic principles of research methodology

19. Structural-geodynamical model.

In present practice only three direct methods exist of strain field reconstruction, namely the field investigations based on the large-scale fracturing tests, petroprotectical and optical polarization methods. Unfortunately, all these methods are extremely laborious and need the regular field tests, which is difficult to conduct in the areas of rock outcrops.

The methodology proposed is based on the analysis of vertical and horizontal anisotropy of gravitation and geomagnetic fields, as well as of topography.

The geodynamical characteristics are calculated by uniform matrices of the physical fields. One of the information components of these characteristics is a set of static indexes, including azimuths and axes-dip angles for intermediate strain, maximum and minimum compression-extension strains, as well as regions of prevailing extension, compression and intermediate strain. The regular areal character of distribution of parameters reflecting three-axial state of strain ellipsoid enables to create highly reliable structural-cinematic 3D model.

The objectives of cinematic analysis are: (1) based on geodynamic maps analysis, to reconstruct the forces direction and strain distribution scheme during formation of principal structures and structural parageneses of studied area; (2) based on the determined strain scheme, to predict the real location of expected tectonic dislocations, zones of rock fracturing and disintegration, and mass-stable blocks.

More than 30 transformations of each physical field were analyzed, including their first and second derivatives, histogram characteristics and correlation
coefficients between the fields. Based on these data, the structural-geodynamical maps are drawn which reflect the dynamics of territory development on the ground of paleoreconstruction of successive activity stages having formed the present-day lithosphere. The analysis of these materials enables also to create structural-geodynamical maps of the Earth’s crust sections at different depth. As a result, the classification of areas is performed into zones of extension characterized by enhanced permeability of rocks, and zones of consolidation with minimal rocks permeability. In addition, the vertically alternating zones of extension and consolidation are identified. These data correlate with results of cosmic and aerophotographs decoding.

20. Hydrogeological model

The hydrogeological model development starts from the upper hydrodynamic zone, for which the data are available on hydraulic parameters. After intercalibration of the upper model elements, the deep part of the model is developed using data about the permeability structure of the crystalline rock massif, obtained from the structural-geodynamical model. The results of analysis and the discrepancy of hydrodynamic regime modeling are used to refine the model representativity for the rocks permeability structure. This iterative process of consecutive correlation and refinement of model may be repeated many times. As a result of this technique implementation, the areas (massifs) of active and very slow water exchange are found, and the system is revealed of vertically alternating zones of enhanced filtration and weak permeability. Based on these data, the sites are pre-selected, which are prospective for subsequently more detailed works on grounding the possibility of RAW isolation in geological formations.

The use of the methodology described above is expedient at the stage of more detailed works, if the corresponding complex is provided of geophysical, hydrogeological, field and modeling investigations.

Some research results

The works performed enabled us to draw preliminary structural-geotectonic map of the region under study, which reflects the principal systems of tectonic breaks, their cinematics and morphology. The principal origins structures are revealed and development of their related structural-substance and tectonic processes determined.

In the result, two regions were selected characterized by existence of geodynamical processes of cooling, thermal shrinkage and structural-substance packing of geological medium. Analysis of neotectonic processes have also shown the geodynamical stability of selected structures. Such regions seem to be the most perspective for deep RAW burials.

The first structure is located in rapakivi granites within the eastern side of the Korosten Plutone (near Stanishovka village), 45 km south-west of Chernobyl, the second one—in the same rocks within the north-eastern part of the Korosten Plutone, 80 km west of Chernobyl.

The next stage of works includes drawing of structural-geodynamic sections and deep-in-layers maps (to depths of 1000-1500 m). Involving these maps along with hydrodynamic characteristics data into a unified database will enable us to obtain a complex 3D model for finding filtrational-migrational characteristics of separate parts of crystalline rock massif and regioning the territory under study by degree of suitability for deep RAW isolation. Such researches are now in process.
Introduction

Site characterization studies for deep disposal of nuclear wastes may include hydraulic testing at various scales to estimate the properties of the rock mass. Small-scale measurements commonly consist of brief injection tests in short double packer intervals, and large-scale measurements are typically long-duration interference pumping tests. To incorporate test data of both scales in performance assessment modeling, Swedish Nuclear Fuel and Waste Management Company (SKB) has developed HYDRASTAR, a stochastic continuum groundwater flow and transport program. HYDRASTAR uses conditional geostatistical simulation and inverse modeling to condition the model simulations on both the small-scale hydraulic conductivities and the large-scale head response. The purpose of this conditioning is to reduce bias and variability in the model simulations and improve site understanding.

Approach

HYDRASTAR is a three-dimensional finite difference groundwater flow modeling program that considers flow governed by Darcy’s Law in an equivalent porous medium. It incorporates the small-scale measured hydraulic conductivities via upscaling and direct conditional geostatistical simulation. The upscaling uses a heuristic averaging to upscale tile data to the model grid scale so that the variogram of upscaled data approximates the regularized variogram. Subsequent direct conditional simulation of interblock conductivities via the turning bands method (Journel and Huijbregts, 1978) thus creates hydraulic conductivity fields which honour the small-scale measurements and have a realistic level of variability and correlation (Norman, 1992).

Inverse modeling calibrates the conditional simulations of hydraulic conductivity to the observed heads of large-scale pumping tests. HYDRASTAR uses the pilot point inverse solution to calibrate the conditional geostatistical simulations at discrete locations (pilot points) to improve agreement between the simulated and observed heads (Eriksson and Oppelstrup, 1994). Adjoint State sensitivity analysis determines the appropriate changes in the pilot point hydraulic conductivity. The pilot point affects the hydraulic conductivities locally within the range of the variogram, and globally by influencing the mean of the field (de Marsily et al., 1984; RamaRao et al., 1996).

Illustrative Example

HYDRASTAR was applied to the Åspö Hard Rock Laboratory (HRL), a research facility owned and operated by SKB. The HRL is beneath an island in southeastern Sweden, and resides in a host rock of a fractured diorite. The SKB site characterization program included 1302 single hole injection tests in 3m double...
Three Dimensional Inverse Modeling of Multi-scale Hydraulic Test Data

Figure 1. HYDRASTAR simulated drawdowns versus observed drawdowns. Mean and one standard deviation of 30 realizations for uncalibrated (left) and calibrated (right) simulations.

packer intervals with 10 min duration. The hydraulic testing also included the second Long-term Pumping Test (LPT2), a large-scale multi-rate pumping test of 90 days duration (Wikberg et al., 1991).

The HYDRASTAR model of the HRL consisted of a 30 x 30 x 40 regular grid of 30m cubic blocks, a volume of approximately 1 km3. Model simulations used the method of superposition to calculate only the transient drawdowns, reducing the execution time and simplifying the boundary conditions (no-flow upper boundary and constant head boundaries of zero elsewhere; Hubbell et al., 1997). Large-scale fracture zones were included as simple stepwise increases in hydraulic conductivity relative to the surrounding rock mass. Geostatistical analysis of the 3m data suggested a spherical regularized variogram model with a range of 80m and sill of 2.3. 32 pilot points were scattered arbitrarily in the domain for use in the calibrated simulations.

Preliminary simulations evaluated the boundary conditions and grid extent, showing that the model was affected by the limited domain and highlighting the importance of the boundary conditions. These simulations also indicated that the model is sensitive to changes in specific storativity and kriging parameters. Comparison of the uncalibrated and calibrated drawdowns indicates that calibration tends to reduce the bias of the simulated drawdowns and decreases the variability of the simulations (Figure 1). The success of the final calibrated model simulations in representing the responses to the LPT2 supports both the site conceptual model and its representation by HYDRASTAR.

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SKB continues to develop HYDRASTAR as part of its research and development program. Several future enhancements were suggested by this study, including additional boundary condition options, improved representation of pumped boreholes and nonparametric geostatistical simulation.

Acknowledgments

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Three Dimensional Inverse Modeling of Multi-scale Hydraulic Test Data

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Acoustic Detection of Rock Damage

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Excavation induced damage is of significance to many types of engineering structures but no more so than in the case of repository design for waste disposal. Professor Young’s research and that of his group, formally at Queen’s University Canada and now at Keele University UK, has focused on the development of acoustic techniques for the detection and quantification of excavation induced damage. The application of earthquake seismology to this problem has provided the opportunity to study the micromechanics of damage mechanisms in situ.

Since 1987 Professor Young has been a principal investigator at Atomic Energy of Canada’s Underground Research Laboratory (URL), responsible for the development of acoustic emission techniques (AE). In the last ten years, the application of acoustic techniques to rock damage assessment has been pioneered by his group and successfully applied in several major international projects. The presentation will address the following questions by reference to selected case histories from multi-national projects:

1. Why use acoustic techniques?
2. What information can AE studies provide?
3. How does excavation method and stress contribute to damage?
4. How can AE and other acoustic techniques be used in repository design and performance monitoring?
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Yucca Mountain Modeling A

Session Chair: Russell Patterson, DOE/YMSCO

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Alternative Approaches for Modeling Unsaturated Flow and Transport in Fractured Rocks

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The vadose zone at Yucca Mountain is about 700 m thick, with a water-filled porosity averaging about 10%. For many years, the average infiltration flux was believed to be between 0.1 and 1.0 mm/year, implying that the average groundwater travel time from the surface to the water table would range from 70,000 to 700,000 years in the absence of significant fracture flow. Even without retardation, radionuclides would remain in the vadose zone for tens to hundreds of thousands of years after release from the engineered barrier system. Fracture flow seemed to be precluded by the capillary properties of the matrix: assuming local capillary equilibrium, fractures would contain almost no water until the matrix is almost completely saturated, and therefore flow and transport would be essentially confined to the matrix.

Unfortunately, this simple description of vadose zone flow and transport at Yucca Mountain has not been supported by data and observations over the last decade. It now appears that significant, perhaps dominant, vadose zone flow and transport occur in fractures at Yucca Mountain and at other sites in arid regions. At Yucca Mountain, occurrence of fracture flow in the vadose zone is supported by environmental tracer data (Bomb-pulse $^{36}$Cl and $^{99}$Tc at the repository level), chloride concentration changes from the surface through the different stratigraphic intervals, $^{14}$C age determinations, and the distribution of calcite deposits (little to none in the matrix; present in about 8% of the fractures). However, there have as yet been no direct observations of fracture flow in the Exploratory Studies Facility (ESF). This lack may reflect the expected transient, episodic nature of infiltration: on the average, only about one year in five will have sufficiently intense precipitation to generate fracture flow in the near-surface bedrock.

At Rainier Mesa, fracture flow has been observed and measured in tunnels, even though the matrix is not saturated. The stratigraphic sequence above the tunnels is similar to that of Yucca Mountain, but average precipitation is about 50% higher. Nevertheless, the observation of fracture flow in rock with less than 100% matrix saturation clearly requires a conceptual model that does not force local capillary equilibrium. This requirement is made stronger by observations of dye infiltration in a test at Fran Ridge, response of seepage to surface precipitation at the Superior Mine haulage tunnel in Arizona, and the migration in a few decades of environmental tracers from the surface to depths of 20 to 60 m through fractured chalk in the Negev Desert. The permeability of the chalk matrix is about the same as that of the welded tuffs at Yucca Mountain, and the precipitation is about the same as that of Rainier Mesa.

Realistic modeling of vadose zone flow and transport must account for the contribution of fractures, a requirement that has become increasingly important over the past decade in assessing the long-term performance of proposed nuclear
Alternative Approaches for Modeling Unsaturated Flow and Transport in Fractured Rocks

waste repositories, the potential migration of radionuclides and organic contaminants at government and industrial sites, and the design and application of remediation techniques. The concept of volume-averaging over a representative elemental volume (REV) is commonly applied to simulate flow and transport in variably saturated permeable media from pore scale to field scale. Codes based on these “macro-scale continuum concepts” include implementation of effective continuum (ECM), double porosity (DPM), dual permeability (DKM), and multiple interacting continua (MINC) models. Large computer models employing these codes typically use spatial discretization on scales of tens to hundreds of meters and attempt to incorporate “spreading” of a contaminant plume by assigning values of transverse and longitudinal dispersivity. Even in saturated systems, attempts to extrapolate spreading behavior to larger distances, using dispersivity values from observations at small distances, have not been successful. Instead of reaching some constant asymptotic value, the apparent dispersivity increases, perhaps linearly, with the scale of the problem. This suggests that the REV for transport may be the size of the system of interest.

In partially saturated systems, the volume-averaging approach also does not adequately account for episodic flow and transport along localized “fast pathways” and perched-water zones. Field data indicate that travel over large vertical distances through thick vadose zones does not damp out flow transients caused by rapid changes in infiltration flux, and some fraction of infiltrating water can reach depths of hundreds of meters in a few decades. This has inspired the development of alternatives to the conventional large-scale volume-averaging approach, all of which attempt to incorporate, with varying degrees of rigor, the effects of small-scale heterogeneity on large-scale phenomena such as localized seepage along preferential pathways through partially saturated porous rock.

Explicit, process-level models, such as multiphase versions of Darcy's law, can adequately represent system behavior if they are applied on the proper scale. However, preferential pathways are typically controlled by orders-of-magnitude variability in flow properties on a scale of 1 m or less. Explicit resolution of spatial variability on this scale is possible for studies of individual seeps or for a small collection of interacting seeps, but is computationally impractical for site-scale analysis. The current practice of large-scale volume averaging simplifies the computational problem at the cost of averaging out the essential features of flow and transport in heterogeneous media, including rapid travel of some fraction of the percolating fluid, bypassing of much of the pore volume, and transient response to surface events. Indeed, if significant percentages of flow are localized in preferential pathways, much of the system volume would not participate in these flows, and volume averages may be completely meaningless.

Opinions in the technical community are divided about whether this kind of flow behavior may be adequately represented by means of macro-scale continuum concepts. Some researchers believe this can be accomplished by appropriate adjustments in model parameters and constitutive relations, while others hold that entirely different approaches need to be employed. A consensus on these issues is not likely to emerge at any time soon. However, most researchers would probably agree that, at the present time, the applicability and validity of macro-scale continuum concepts for describing unsaturated zone flow at Yucca Mountain have not been established. All of the macro-scale conceptualizations entail approximations and simplifications whose applicability needs to be carefully investigated. This is being done by comparison of model calculations with site observations and data and by developing alternative modeling approaches that do not invoke the same approximations.
Several alternative approaches appear capable of resolving spatial and temporal variability and describing localized and episodic flow features. There are tremendous differences in the level of detail represented; these translate into qualitatively and quantitatively different data needs. These approaches also differ in their ability to represent those features of the flow system that are most relevant to nuclear-waste isolation. From the standpoint of site viability and suitability, the most important issues are the groundwater travel time (GWTT) distribution and the magnitude and spatial variability of water flux. GWTT has first-order impacts on solute transport and potential radionuclide transport velocity distribution through the unsaturated zone (UZ). The temporal and spatial distribution of liquid water flux into the emplacement drifts will have a major impact on waste package design and package lifetime and will determine the rate of release of radionuclides from failed waste packages.

In attempting to resolve these issues, we recommend pursuing two alternative modeling approaches:

21. Mechanistic process models for flow and transport should be developed that represent much more spatial detail than is possible with the current generation of volume-averaged approaches. The detailed process models will be considerably more complex than the large-scale, volume-averaged approaches, but they could conceivably be substantiated by further observations and field experimentation at the Yucca Mountain site; they also may provide a conceptual basis on which the approximate validity of macroscale approaches may be tested.

22. We also recommend that, as an alternative to detailed process models, much simpler phenomenological models be developed (e.g., weeps-type transfer function and transit time approaches). These kinds of models are attractive in our view because of their conceptual simplicity, transparency, and robustness. They can directly address the crucial issues for site suitability and repository performance (groundwater travel times, spatial variability of flux), while requiring a minimum of assumptions whose validity may be difficult to establish.

We also note that these two approaches are complementary. It is unlikely that we will ever have the degree of spatial resolution of physical properties needed for a rigorous application of mechanistic process models at even the scale of a single drift. Even with direct measurements of seepage, we will not have small-scale measurements between a drift and the ground surface, measurements that would be required for highly resolved, rigorous mechanistic models. However, we can put in reasonable spatial distributions of properties, perform calculations with the mechanistic model, and then fit the results with the simpler phenomenological models to investigate how the small number of parameters in the latter models vary with the assumed spatial statistics.

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Effects of Faulted Stratigraphy on Saturated Zone Flow Beneath Yucca Mountain, Nevada

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Introduction

We have developed a sub-site-scale-saturated zone (S4Z) model for the saturated zone (SZ) at Yucca Mountain, Nevada. The model was constructed in part to investigate the effects of the complex three-dimensional hydrogeologic structure on SZ flow. In this presentation, we (i) summarize model development highlighting the geologic realism captured in the model, and (ii) present simulation results that show the significance of the faulted stratigraphic structure on SZ flow and resulting macrodispersion.

Modeling Approach

The S4Z model is a 3-dimensional integral finite difference model developed for use with TOUGH2. The model covers an area of approximately 100 km2 as shown in Figure 1. There are 23 model layers and approximately 50,000 gridblocks. The finely discretized region near the center of the domain corresponds to the area near the C-hole field test complex. The northernmost model area corresponds to the location of the large hydraulic gradient. The water table defines the top of the model. The bottom of the model is defined by the base of the Lithic Ridge Tuff, a thick confining unit.

One of the primary objectives in the development of S4Z was the inclusion of realistic geologic structure. Gridblocks preserve the thickness, orientation, dip, and lateral continuity of strata, as defined in a 3-dimensional geologic model of Yucca Mountain, ISM2.0. Displacement by faults is also explicitly considered. Figure 2 shows the vertical layering scheme in S4Z, and the corresponding cross section through ISM2.0. Note the preservation of geologic unit displacement and variation in layer thickness, elevation, and intersection of different units at the water table. Although discrepancies exist, for example due to the assumption of vertical faults in S4Z, the overall character of the faulted and dipping stratigraphic layers is preserved.

S4Z geologic units are subdivided to account for the vertical variation of rock properties evidenced by rock welding characteristics and results of vertical flow surveys in boreholes. Transmissivity values were obtained from analysis of pumping tests. Water table elevations and results from C-hole pumping tests are used for model calibration. We use hydrochemical data as a qualitative check on conceptual models and flow results.

Results

SZ flow geometry is greatly influenced by fault properties, whether faults are high permeability fault zones, low permeability fault zones, or faults with displacement only. The following simulation highlights new insights of flow behavior that result from displacement-only faults. The simulation considers the injection of a passive tracer into the Bullfrog Tuff which
intersects the water table below the potential repository. The simulation models flow in the low-gradient area immediately downgradient of the potential repository. Constant head boundaries are applied at the locations of the 731 m water table contour (Figure D, and on the east side of the model, which is parallel to water table contours.

Figure 1. Numerical grid of the $S^4Z$ Model. Dots mark location of saturated zone boreholes. Heavy lines represent fault traces. Dashed line is 731 meter water table elevation contour. Coordinates are Nevada state plane coordinates.

Figure 3 shows the tracer distribution within the central Bullfrog unit five years after initiation of tracer injection. The black dots mark the locations of tracer injection. A high pore velocity results from the small fracture porosities used ($\phi = 2 \times 10^{-4}$). Because steady-state fluid travel time is inversely proportional to porosity, the simulation results shown also represent the tracer plume approximately 50 yrs after injection for a porosity of $2 \times 10^{-3}$ or 500 years for porosity of $2 \times 10^{-2}$. The assignment of porosities clearly has a very large effect on flow calculations. Rather than focusing on the particular time scale, we emphasize here the mechanical macrodispersion that results from the complex flow geometry.

Figure 3a shows that both plumes are diverted southward along strike of the Bow Ridge and Midway Valley faults. These faults offset the Bullfrog unit and effectively create a lower permeability obstruction in these areas. The displacement at the Paintbrush Canyon fault completely abuts the Bullfrog against the Tram Tuff in the area near C-holes. A flow-barrier effect results from the abutment because the Tram Tuff is assigned a permeability 1000 times less than the Bullfrog Tuff. Particle tracking has shown that the plume does not continue to disperse, but rather converges into a single channel downstream. This behavior is not considered using simple dispersion models, and was not anticipated. Furthermore, the simulation showed that fluid at depth migrates in directions different from those inferred by simple water table gradient interpretations.

Figure 3b shows the plume distribution at the water table. Rather than observing a dispersed tracer distribution at the water table downgradient from the source, we observe isolated areas of high concentration, upgradient-source fluid. The simulation results of flow in a 2-D cross-section in the same area highlight the processes that lead to this distribution. Figure 3c shows how the plume descends within the high permeability and dipping Bullfrog Tuff. The abutment of different permeability units at the Paintbrush Canyon fault causes flow bifurcation and hence vertical upwelling. Mixing and vertical hydraulic gradients result, even without a fluid source from the Paleozoic formations. This simulation dramatically illustrates how hydrogeologic structure controls macrodispersion, and illustrates the need to properly account for this structure in SZ flow and transport simulations.
Conclusions

We have developed a sub-site-scale integral finite difference flow model called S^4Z for Yucca Mountain. S^4Z is consistent with the geological model of ISM2.07 and is discretized to handle fault offset explicitly. Numerical simulations of the flow downstream from the region directly below the potential repository show that the high permeability Bullfrog Tuff may act as the primary conduit for repository source water, and because all geologic units are offset by faults, flow is diverted and bifurcated laterally and vertically downstream. This gives rise to unforeseen and complicated flow geometries that greatly contribute to macrodispersion. In addition, these complex flow patterns are consistent with geochemical data that show evidence for vertical mixing as well as flow stagnation.1

Acknowledgment

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U. S. Department of Energy, through Memorandum Purchase Order EA9013MCSX between TRW Environmental Safety Systems Incorporated and Ernest Orlando Lawrence Berkeley National Laboratory, under Contract No. DE-AC03-76SF00098. Technical reviews by Tim Kneafsey and Yvonne Tsang are greatly appreciated.

References

Effects of Faulted Stratigraphy on Saturated Zone Flow Beneath Yucca Mountain, Nevada


Development and calibration of a preliminary three-dimensional model of the saturated zone at Yucca Mountain, Nevada, the potential location for a high-level nuclear-waste repository, is presented. The development of the model advances the technology of interfacing: (1) complex three-dimensional hydrogeologic framework modeling; (2) fully three-dimensional, unstructured, finite-element mesh generation; and (3) ground-water flow simulation.

The three-dimensional hydrogeologic framework model is developed using geologic maps, geologic cross sections, and well data that are converted to structure contour maps. The structure contour maps are stacked to form a three-dimensional solid using a 1,500 meters by 1,500 meters horizontal sampling area, and a variable vertical thickness. The framework model consists of different hydrogeologic units covering a 1,350 square-kilometer rectangular area, 45 kilometers long and 30 kilometers wide.

The framework-model data are used as direct input to an automated mesh generator, which is designed to discretize irregular three-dimensional solids using tetrahedral elements, and to assign unit identifiers from the hydrogeologic framework model to the nodes within the mesh. The mesh generator facilitates the addition of nodes to the finite-element mesh that correspond to the three-dimensional locations of the midpoints of either the water column for uncased boreholes or the screened or packed-off interval within the borehole. These nodes then are used as observation points for hydraulic head during model calibration. The resulting mesh consists of 9,279 nodes and 51,461 tetrahedral elements representing 16 different hydrogeologic units.

The ground-water flow capabilities of a ground-water flow and heat transport simulator with variable saturation are used with the resulting finite-element mesh to simulate ground-water flow. Calibration of the model is facilitated using an automated parameter-estimation routine, which minimizes the difference between 94 observed and simulated values of hydraulic head, by adjusting selected permeability and flow parameters. Optimal permeability estimates for the sixteen hydrologically units lie between high and low values for the same units reported in the literature. Simulated hydraulic-head values agree well with observed values, the majority of which have residuals of less than 5 meters.
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Synthesis of Environmental Tracer Data and Numerical Simulations to Test Models of Flow and Transport at Yucca Mountain

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We examine the role of studies coupling environmental isotope analyses with numerical flow and transport modeling for identifying governing processes in the unsaturated zone as well as constraining the property sets used to model them. These studies also serve to evaluate alternative conceptual models explaining field and laboratory measurements, often from a variety of independent data collection activities. The numerical flow and transport model FEHM is used to simulate multiphase transport processes in fractured, porous media with a dual-permeability formulation. The primary data we focus on are porewater chloride and the $^{36}\text{Cl}/\text{Cl}$ ratios measured from samples collected in the Exploratory Studies Facility (ESF), an 8-km tunnel excavated beneath Yucca Mountain, Nevada through the horizon of the potential high level radioactive waste repository. These data provide evidence for percolation rates and travel times of water from the surface to depths of several hundred meters. A strong correlation between structural features and apparent fast paths is supported with these data. Away from structural features, apparent travel times of thousands to tens of thousands of years imply that percolation flux transients on the time scale of precipitation events are damped out. If this is the case, then predictive simulations for repository design and repository performance assessment which must consider the next ten thousand years may not need to resolve short time scales. The alternative conceptual model which suggests ubiquitous fast flow through the entire system, including the nonwelded volcanic tuff between the surface and the potential repository, is examined with respect to other geochemical data sets, various hydrologic parameter sets, surface infiltration estimates, and transport simulations used the most recent material property sets available.
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The saturated zone beneath Yucca Mountain is an important component of potential radionuclide transport to the accessible environment. It holds promise of attenuating radionuclides released from the unsaturated repository zone through the processes of dilution and retardation. The saturated zone must be understood and modeled at a variety of scales. Regional scale models, on the order of hundreds of kilometers, provide the large scale water balance but typically have only a few distinct hydrogeologic units. Site-scale models, on the order of tens of kilometers, have the resolution necessary to represent large-scale heterogeneities like hydrogeologic units. Sub-site scale models, on the order of kilometers, are able to resolve the hydrogeologic units with even more detail. Models at different scales should have consistent fluxes at model boundaries. Travel time calculations are presented for several important radionuclides using a coupled sub-site-scale and site-scale computational model. Special attention is given the numerical grid issue of proper representation of the hydrogeologic units. Travel times are affected by the temporal characteristics and concentration of radionuclide release, retardation coefficient magnitude and distribution, fracture-matrix interaction, and porosity and permeability distribution. Retardation coefficients are affected in turn by the mineralogical property distribution. To simulate radionuclide transport with sorption, the mineralogical distribution is mapped onto the computational grid and the sorption coefficient is assigned spatially based on the mineralogic distribution. The sensitivity to parameters and processes affecting radionuclide transport are discussed.
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Session 7

FTAM Workshop, December 15 & 16, 1997

Yucca Mountain Modeling B

Session Chair: Russel Patterson, DOE/AMDCE

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A Site Scale Model for Modeling Unsaturated Zone Processes at Yucca Mountain, Nevada

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The U. S. Department of Energy (DOE) is currently investigating the feasibility of using the unsaturated zone at Yucca Mountain, Nevada, as the site for the permanent geologic disposal of high-level nuclear waste. The site has been extensively studied for more than 15 years, and many types of data have been collected. These data have been used to develop conceptual and numerical process models of Yucca Mountain to simulate ambient conditions and perform predictive studies of physical and chemical changes in the mountain due to climate-related, thermal, and geochemical perturbations.

The primary objectives of the unsaturated-zone (UZ) flow model developed at the Lawrence Berkeley National Laboratory (LBNL) are the following:

(a) to integrate the available data from the unsaturated zone into a single comprehensive three-dimensional model,

(b) to quantify the flow of moisture, heat, and gas through the unsaturated zone,

(c) to evaluate the effects of repository loading on moisture, heat, and gas flow within the mountain, and

(d) to provide Performance Assessment and Repository Design with a defensible and credible model of all relevant unsaturated-zone processes.

The 3-D site-scale UZ flow model provides estimates for important parameters and processes such as:

23. the spatial and temporal values of percolation flux at the potential repository horizon,
24. the components of fracture and matrix flow within and below the potential repository horizon, and
25. the probable flow pathways from the potential repository to the water table.

The UZ flow model also provides important input to various other Yucca Mountain process models, such as ambient and thermal drift-scale models, the mountain-scale thermohydrological model, and the UZ transport model.

Overview of Key Conceptual Issues

UZ flow simulations are performed with numerical grids that represent the conceptual model of the unsaturated zone at Yucca Mountain. The conceptual model develops a framework, based on evaluation of collected data, to explain unsaturated-zone flow processes such as liquid, heat, and gas flow. Important components of the conceptual model are highlighted below and are illustrated in Figure 1.

HYDROGEOELOGIC SETTING

Yucca Mountain lies in a tectonically complex, arid environment, comprised of heteroge-
neous layers of anisotropic, fractured volcanic rocks. Figure 2 shows the 3-D geological model of Yucca Mountain, with the location of the UZ flow model boundary and potential repository area provided as reference points. These variably welded tuffs display highly contrasting hydrologic characteristics (porosities, fracture densities, permeabilities, etc.). Alteration of volcanic glass into clays and zeolites is common in the non-welded units, especially near the water table, and greatly impacts matrix saturations, permeabilites, and groundwater flowpaths and travel times. Lateral diversion occurs below the repository horizon above the low-permeability zeolitic material, often resulting in the formation of perched water, as observed in several boreholes in the potential repository area.

**INfiltration**

Infiltration to the repository is spatially and temporally variable due to the nature of precipitation, near-surface geology, and variations in soil cover and topography. Estimated average infiltration rates over the UZ model area range from about 1-15 mm/yr. Lower infiltration rates are assumed where significant thicknesses of alluvium overlie volcanic bedrock because of the high storage capacity in the alluvium (leading to near-surface evaporation). Higher infiltration rates are believed to occur on ridgetops and sideslopes where outcrops are exposed and fracture flow can be directly initiated into the bedrock. Current infiltration conceptual models are based on shallow borehole measurements and are verified by evaluation of geothermal profiles and geochemical data.

**Percolation Flux**

One of the most important hydrological parameters that can be investigated through the use of the UZ flow model is percolation flux at the level of the potential repository, as it quantifies the amount of water available to contact the waste canisters. Geochemical and isotopic data suggest that percolation flux is greater in highly-fractured, welded rocks because fracture networks allow water to bypass the low-porosity matrix. Conversely, percolation flux is believed to be dampened in the relatively unfractured, high-porosity non-welded rocks, as indicated by pneumatic data and chlorine-36 concentrations. Furthermore, capillary barriers may exist between welded and nonwelded units above the potential repository horizon creating lateral diversion and moisture redistribution, thus limiting the amount of water available to reach the repository horizon. Analyses of temperature and heat flow data with the UZ model suggest that the percolation flux across the repository area is on the order of 5 to 10 mm/yr. Faults may also have a large impact on percolation flux by providing fast pathways for infiltration, allowing moisture to travel to great depths at Yucca Mountain without significant attenuation in the nonwelded units.

**Fracture Flow & Fracture-Matrix Interaction**

Fracture flow accounts for the majority of the mass flux in the welded units (and thus in the repository unit) at Yucca Mountain because the low-permeability matrix allows only a few mm/yr of flow. It is likely that most of the perched water bodies are fed by vertical flow through fractures based on the relatively young ages of the water (on the order of 2000-6000 years) and the extremely slow travel times of water through the matrix. Isotopic concentrations suggest that limited mixing of matrix pore waters and perched water bodies occurs, thus prompting a reduction in the fracture-matrix interaction coefficient used in the dual-permeability formulation of the UZ model.

**Summary of UZ Modeling Studies and Results**

Incorporating extensive data that are available from numerous studies of Yucca Mountain, the UZ flow model captures the important flow processes that occur in the unsaturated zone,
such as: moisture flow, capillary pressure effects, gas flow, convective and conductive heat transfer, evaporation and condensation, moisture and gas flow travel times, and transport of conservative and reactive species in the mountain. Figure 3 shows the major components of the UZ flow model.

The UZ model uses USGS matrix property data that describe the important hydrogeologic layers at Yucca Mountain to develop rock parameters sets for each model layer. A detailed fracture property model has been developed by LBNL using pneumatic data, fracture data from boreholes, and detailed fracture data from the ESF. This model yields results for fracture permeabilities, porosities, effective spacing, and derived van Genuchten parameters.

Much effort has been devoted to calibration of the UZ flow model. The model is calibrated against water potential and liquid saturation data using various infiltration maps and conceptual models for fracture-matrix interaction, pneumatic data, borehole temperature data and thermal properties, perched water data, and environmental isotopes, including chlorine-36, total chlorides, strontium and carbon-14. Figure 4 is an example of a calibrated saturation distribution over the UZ model domain.

FLOW ABOVE THE POTENTIAL REPOSITORY

Net infiltration into the bedrock at the land surface is episodic, and significant pulses are thought to occur only every few years. After traveling relatively rapidly through fractures in the upper welded tuff (TCw), the pulses are attenuated by the high storage capacity of the Paintbrush non-welded unit (PTn). As a result, flow reaching the underlying welded repository unit is fairly uniformly distributed. However, some proportion of percolation flux travels along structural fast pathways, such as major faults that cut through the entire thickness of the PTn.

PERCOEATION FLUX AT THE POTENTIAL REPOSITORY HORIZON

Since the repository horizon, located in the Topopah Spring welded tuff (TSw), contains a dense network of fractures with permeabilities several orders of magnitude greater than matrix permeabilities, moisture flux through this unit is predominately through fractures. From total chloride, strontium, and carbon-14 analyses, in addition to temperature studies, percolation flux through the TSw ranges from 1-10 mm/yr. Figure 5 is a result of percolation flux studies using the UZ flow model.

FLOW PATTERNS BELOW THE REPOSITORY

Zeolitic rocks affect flow patterns below the potential repository, resulting in the formation of perched water, and potentially retarding radionuclide migration to the water table. Laterally diverted flow above zeolites may encounter a fault or extensive fracture system that can re-initiate predominantly vertical flow to the water table. Though characterization of flow below the repository is essential, available data are limited as to the spatial distribution and fracture characteristics of zeolitic horizons. Future work will hopefully shed light on these important issues.

All aspects of the UZ site-scale flow model are described in detail, and all appropriate references are cited, in the LBNL report entitled, “The Site-Scale Unsaturated Zone Model of Yucca Mountain, Nevada, for the Viability Assessment,” G. S. Bodvarsson, T. M. Bandurraga, and Y. S. Wu, eds. (1997), LBNL-40376, UC-814.
A Site Scale Model for Modeling Unsaturated Zone Processes at Yucca Mountain, Nevada

Figure 1. Schematic cross section through Yucca Mountain Showing various model data and processes.

Figure 2. 3D geological framework (Calyton et al. 1997).

Figure 3. Major components of the UZ Site Scale Flow Model.

Figure 4. Chair cut display of liquid saturation in the UZ model domain.

Figure 5. Simulated percolation flux through Yucca Mountain.
Introduction and Background

A multi-scale thermal-hydrological (T-H) model-abstraction methodology has been developed that integrates the results from 1-, 2-, and 3-D drift-scale models and a 3-D mountain-scale model (Fig. 1) to provide a full description of the T-H variables (Table 1) affecting the performance of the engineered barrier system (EBS). This information is required by Total Systems Performance Assessment for the Viability Assessment (TSPA-VA) to assess waste-package (WP) corrosion, waste-form dissolution, and radionuclide transport in the EBS. The T-H variables (Table 1) are provided to TSPA-VA as a function of

- Location in the repository area, including the influence of the local stratigraphy and percolation flux,
- WP type, such as civilian spent nuclear fuel (CSNF) versus defense high-level waste (DHLW), WP age and burnup, WP spacing, and WP sequencing,
- Design options such as the line-load design or backfill.

The influence of the following model assumptions and boundary conditions can be assessed:

- Infiltration-flux distributions, including the influence of climate change,
- Conceptual models of fracture-matrix interaction, such as the effective continuum model (ECM) and dual permeability model (DKM),
- Heat-flow assumptions at the water table, such as a fixed-temperature assumption versus explicitly representing heat flow in the saturated zone (SZ).

This model abstraction methodology uses complementary T-H and thermal-conduction (T) models at various scales and conceptualizations, including the following:

26. Smeared-heat-source, mountain-scale T model (Fig. 1 d) that incorporates,

- Geometry, hydrostratigraphy, and boundary conditions of the site-scale unsaturated zone (UZ) model (Bodvarsson and Bandurraga, 1996; Bodvarsson et al., 1997),
- Geometry of the reference 85-MTU/acre repository design,
- Heat flow in the SZ, including the influence of regional groundwater flow.

27. Drift-scale T and T-H models (Fig. 1a, b, c) that incorporate

- Local hydrostratigraphy and boundary conditions of the site-scale UZ model,
• Local infiltration flux from an infiltration map, including the TSPA-VA base-case and long term-average (LTA) maps and multiples of those two maps [For this study, as well as for the T-H calculations supporting TSPA-VA, infiltration flux is assumed to be equal to percolation flux because lateral diversion above the repository appears to be minor (Wu, 1997).],

• DKM approximation (with the ECM as an alternative conceptual model)

• Complementary 1-D SDT models, 2-D LDTH models, and 3-D DDT models (Figs. la, b, e) that are regularly spaced throughout the repository area in either a 3xS or a Sx7 grid. For each grid location, parallel SDT and LDTH-model calculations are conducted for AMLs of 85, 56.67, and 42.5 MTU/acre (the lower 2 AMLs are required to represent cooler areas in the repository such as edge locations), resulting in 6 model calculations per grid location; thus, 90 drift-scale model calculations are required for the 3x5 grid (210 calculations for the Sx7 grid). The abstracted-model results in this study were determined with the 3xS grid (with 15 drift-scale model locations). For TSPA-VA, the Sx7 grid (with 35 locations) is used to provide a more finely resolved representation of the infiltration-flux distribution in the repository area. Besides the SDT and LDTH models, at least 1 DDT-model calculation is required by the T-H model-abstraction methodology; additional DDT-model calculations can be included to capture the wide range of potential WP-type/sequence scenarios that may arise during emplacement.

• Alternative hydrological-parameter sets, including (1) the TSPA-VA 7/97 base-case set, (2) the 11/97 “T-H” set calibrated to temperatures measured in the Single-Heater Test, and (3) an imbibition-test set that is calibrated on the basis of laboratory measurements of matrix imbibition sorptivity (Flint et al., 1996),

• Reference point-load design, as well as alternatives such as the line-load design and backfill.

Discussion of Abstracted-Model Results

Three key T-H concerns for EBS performance assessment are (1) the magnitude and distribution of decay-heat-mobilized liquid-phase flux and the influence of that flux on seepage into emplacement drifts, (2) the spatial and temporal extent of rock dryout and relative humidity RH reduction, and (3) the influence of rock dryout and convective heat-flow (e.g., the heat-pipe effect) on temperatures in the near field and in the EBS (and on WPs). Rock dryout is the result of the balance between (a) the rate of vaporization and vapor transport away from emplacement drifts and (b) the rate of return liquid-phase flow to the dryout zone. Two mechanisms influence the rate of rewetting:

• Gravity-driven percolation and condensate flux in fractures

• Capillary-driven

=> matrix imbibition, as quantified by the matrix wetting diffusivity \( D_{imb} \) (Buscheck et al., 1997a; 1997b)

=> wicking in fractures, as quantified by \( 1/\alpha_f \), where \( \alpha_f \) is the van Genuchten alpha parameter for fractures, which is equivalent to the air-entry (or bubble-point) pressure.

Therefore, two of the key factors governing dryout (the infiltration-flux distribution and \( D_{imb} \) in the host-rock units) are the focus of this study. Table 2 gives \( D_{imb} \) for the host-rock model units (Bodvarsson and Bandurraga, 1996) for the hydrological-property sets considered in this
Table 1. Thermal-hydrological (T-H) variables that are determined by the T-H model-abstraction methodology are indicated with an "x." The T-H variables provided to TSPA-VA are indicated by a bold X. The T-H variables include temperature T, relative humidity RH, gas-phase air-mass fraction Xair,gas, liquid-phase saturation Sliq, and liquid-phase flux qliq.

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<th>Location</th>
<th>T</th>
<th>RH</th>
<th>Xair,gas</th>
<th>Sliq</th>
<th>qliq</th>
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<tr>
<td>Rock above drift wall</td>
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<td>x</td>
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<td>X</td>
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<tr>
<td>Rock at drift wall</td>
<td>X</td>
<td>X</td>
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<tr>
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For the TSPA-VA 7/97 base-case set, which has been used in the majority of the T-H model calculations conducted for TSPA-VA, the upper to middle host-rock units (tsw33—tsw35) have about the same value of Dimb, while the lower two units (tsw36 and tsw37) have much larger values. Accordingly, it is found that near-field rock dryout (and RH reduction on WPs) in the central to eastern regions of the repository persists considerably longer than it does in the western region of the repository. Rock dryout and RH reduction persists longest in the north to northeastern region of the repository, where the lowest infiltration fluxes occur, while regions that underlie the summit of Yucca Mountain, where the highest infiltration fluxes occur (Bodvarsson et al., 1997), have relatively shorter duration dryout and RH reduction.

For the 11/97 "T-H" parameter set that was calibrated using temperatures measured during the SingleHeater Test (Birkholzer, 1997; Buscheck et al., 1997b), Dimb in the tsw36 is much lower than in the 7/97 base-case set (Table 2); consequently, dryout is more persistent, particularly at the western repository edge. The sensitivity of rewetting time on Dimb is greater in areas with low infiltration flux and less for high infiltration flux. The corresponding increase in the duration of reduced RH on WPs is seen by comparing Figs. 2b and e with 2a and d. Also notice that the "hot" 21-POOR WPs remain dry longer than the "cold" WPs. For the imbibition-test parameter set, which was calibrated using measurements of matrix-imbibition sorptivity (Flint et al., 1996), Dimb is considerably lower than in the other two sets. Consequently, the duration of reduced RH on WPs is longer (compare Figs. 2c and f with Figs. 2b and e).

Figure 3 indicates the magnitude of infiltration flux strongly affects dryout and rewetting for the flux range considered in this study (repository-area-averaged infiltration fluxes of 1.4, 7, and 35 mm/yr). A factor of 5 change in infiltration flux results in a factor of 2 change in mean rewetting time (to RH= 85%) for WPs. Note again that "hot" WPs are dry considerably longer than "cold" WPs.

References

Influence of Imbibition and Infiltration Flux on Near-Field Thermal-Hydrological Conditions at Yucca Mountain.

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Table 2. The value of matrix wetting diffusivity $D_{mb}$ for the host-rock units is given for various DKM hydrological-parameter sets; the value of $D_{mb}$ is determined for an assumed $S_{uq}$ of 90%. The majority of repository horizon lies in the tsw35 (lower lithophysal TSw) unit; the eastern edge of the repository lies in or close to the tsw34 (middle nonlithophysal TSw) unit, while the western edge lies in or close to the tsw36 (lower nonlithophysal TSw) unit. Because the tsw33 (middle lithophysal TSw) unit and tsw37 (the basal vitrophyre) unit lie close to the eastern and western edges of the repository, respectively, the value of $D_{mb}$ for those units also influences near-field rock dryout.

Model of Yucca Mountain, Nevada. Lawrence Berkeley National Laboratory, Berkeley, CA.


Figure 1. Schematic of conceptual models used by the T-H model-abstraction methodology, including (a) smeared-heat-source, drift-scale T (SDT) model, (b) line-heat-source, drift-scale T-H (LDTH) model, (c) discrete-heat-source, drift-scale, T (DDT) model, and (d) smeared-heat-source, mountain-scale (SMT) model.
Figure 2. Histogram of the time for the waste package (WP) surface to attain relative humidity $RH = 85\%$. Histograms are given for (a,b,c) a "hot" design-basis-fuel (DBF) 21-PWR CSNF WP and (d,e,f) a "cold" 21-PWR CSNF WP. Distributions were determined for the TSPA-VA base-case infiltration map and various hydrological-parameter sets, including (a,d) the 6/97 TSPA-VA base case, (b,e) the 11/97 "T-H" set calibrated using the single-heater test, and (c,f) a parameter set in which the matrix-wetting diffusivity $D_{mb}$ is constrained using imbibition-test data (Flint et al, 1996).

Figure 3. Histogram of the time for the waste package (WP) surface to attain relative humidity $RH = 85\%$. Histograms are given for (a,b,c) a "hot" design-basis-fuel (DBF) 21-PWR CSNF WP and (d,e,f) a "cold" 21-PWR CSNF WP. Distributions were determined for the TSPA-VA 7/97 base-case hydrological-parameter sets and 0.2, 1, and 5 times the TSPA-VA base-case infiltration map.
Arid Unsaturated Zones as Groundwater Contamination Barriers for Radioactive Waste Disposal

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Evidence for rapid transmission of radioactive contaminants into groundwater through the overlying unsaturated zone in arid areas (e.g., Nativ, 1991; Gee et al., 1994; Nativ et al., 1995; Striegl et al., 1996; Fabryka-Martin et al., 1996; Conaway et al., 1997) contrasts with evidence of little or no downward movement of moisture including lack of change in moisture content below depths of a few meters and upward water-potential gradients (Fischer, 1992); upward decrease in water vapor density in response to thermal gradients, and decrease in CO2 vapor pressure, interpreted to indicate upward vapor movement from the water table (Prudic and Striegl, 1994); concentration of chloride in the upper 10 m, interpreted to indicate no downward movement of precipitation below ~10 m for 16-33 ka (Andraski and Prudic, 1997); and stable isotope distribution of deuterium and oxygen-18, interpreted as consistent with upward movement of moisture throughout the unsaturated zone (Prudic et al., 1997). In some places, evidence for both downward movement and the long-term absence of downward movement of moisture is found in the same sample sites. For example, elevated 3H, inferred to have moved laterally and downward by saturated flow (Striegl et al., 1996) occurs within the zone of high chloride concentration (Prudic, 1994) near the Beatty, Nevada low-level radioactive waste (LLRW) site.

This conflicting evidence appears to be in part the result of limited sampling in geologically complex environments, lack of understanding of the geologic history of study sites, lack of sitespecific data, and limited understanding of the mechanisms of moisture movement in the unsaturated zone. Thus, at the Beatty, Nevada site, among the best-studied sites, interpretations of water-content and water-potential variability are based on measurements made at only three closely spaced locations, and the water-potential data were selectively chosen on the assumption of site homogeneity; interpretation of the chloride data as indicating no downward movement of precipitation below ~10 m for 16-33 ka assumes stability of the Amargosa River floodplain on which the sample sites (four) are located for that period of time, which is not supported by recent flood history of the Amargosa R. (Anderson et al., 1997) and is further contradicted by presence of 3H within the chloride zone. Prudic et al. (1997) interpret δD values in groundwater and the unsaturated zone at the Beatty site as consistent with upward movement of moisture from the water table. This conclusion is derived by postulating that the δD of the groundwater differs from that of modern recharge on the basis of only 6 sampled precipitation events in 18 months at a locality 35 km distant; these isotope data are better interpreted on the basis of long-term measurements of deuterium in regional precipitation, which support modern recharge.

Apparent contradictions among data sets can be reconciled if pathways for contaminant movement are distributed on scales both larger and smaller than sampling intervals. Such preferred pathways, including fractures in both consolidated and unconsolidated materials, are being called on with increasing frequency to explain the fact of deep unsaturated zone contamination in contrast to model predictions (e.g., Striegl et al., 1996; Fabryka-Martin et al., 1996; Conaway et al., 1997).

Attempts have been made by proponents of controversial projects, such as the proposed Ward Valley, CA LLRW site, to vitiate evidence of rapid leakage
of radionuclides from similar arid sites (Beatty, NV) by asserting that contamination of groundwater is the result of sabotage, or that the problems were caused solely by disposal of liquid wastes, which for unexplained reasons migrated rapidly through the unsaturated zone whereas much larger volumes of natural precipitation are unable to migrate deeper than a few meters. In view of the fact that rapid migration of contaminants in the unsaturated zone has occurred in the absence of liquid waste disposal [e.g., Richland, WA (Kearney, 1987) and Yucca Mountain (Fabryka-Martin et al., 1996) sites], attention is more appropriately focused on the general lack of understanding of rates and mechanisms of contaminant transport in the unsaturated zone.

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A Modeling Study of Perched Water Phenomena in the Vadose Zone

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The presence of perched water bodies in the vicinity of the potential repository at Yucca Mountain has many implications, and it may provide insight into moisture movement, flow pathways, or surface infiltration history of the mountain. The first implication is that percolation flux does not travel vertically through the unsaturated zone to the water table, but has been trapped, blocked or diverted laterally. As a result, nonuniform recharge rates are expected at the water table. Another concern is that perched zones may divert water around low-permeability zeolitic lenses underlying the potential repository horizon. By-passing of these units, which are thought to have substantial capacity to retard radionuclide transport, could have important implications for the capability of the geologic system to mitigate radionuclide releases to the environment.

We have conducted a series of 3-D modeling simulations to investigate the perched water occurrences at the Yucca Mountain site, using a numerical code and available perched water data from six boreholes. A spatially varying surface infiltration map (Flint et al., 1996) is used to describe areally distributed net infiltration at the model land surface. Perched water data observed in the field were used to calibrate the model in terms of matrix and fracture permeabilities, capillary functions, and relative permeabilities of gas within the perched zones. Calibrated parameter values were within the range of field and laboratory measurements. The steady-state simulation results are in agreement with the observed perched water data in terms of water saturation and perched water locations. Furthermore, the results of a transient numerical pumping test conducted, using a 3-D submodel, matched water level data observed during field pumping tests.

Perched-water has been intersected in a number of boreholes (UZ-14, NAG-7a, SD-9, and G-2), at Yucca Mountain (Striffler et al.; 1996). Perched water was also found at borehole SD-7 (Czarnecki; 1995), (Personal Communication, Soeder; USGS, 1995), and wet core was recovered from borehole SD-12 (Patterson; 1996). The observed perched data are listed in Table 1.

Perched water may occur where percolation flux exceeds the capacity of the geologic media to transmit flux in unsaturated zones. The conceptual model of water movement in the vicinity of investigating the perched water zones indicates that: 1) no large-scale connected fractures intersect the underlying low-permeability units, and 2) both vertical and horizontal permeabilities within the perched water zone must be small when compared with measurements outside these zones.

This modeling study indicates that the key factors necessary to create a perched-water zone using a numerical model are: (1) a water perching geologic structure with low permeability zones or a capillary barrier underlain and surrounding, (2) weak capillary forces under high saturation condition within and near perched-water zones, and (3) sufficient water infiltration rates.
A Modeling Study of Perched Water Phenomena in the Vadose Zone

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<th>Boreholes</th>
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