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THE USE OF TOUGH2/iTOUGH2 IN SUPPORT OF THE YUCCA MOUNTAIN PROJECT: SUCCESSES AND LIMITATIONS

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ABSTRACT

The TOUGH2/iTOUGH2 family of codes is being used to analyze various processes and phenomena in the unsaturated zone at the proposed high-level nuclear waste repository at Yucca Mountain, Nevada. Various models have been developed that help quantify properties of the volcanic tuffs, water flow, seepage into drifts, and thermally driven coupled processes arising from the heat emitted by radioactive waste. These models are based on various assumptions and approximations that are generally accepted in the literature, but can give rise to different degrees of uncertainty. Some of the key approaches utilized include the continuum approximation, the van Genuchten formulation, the active fracture model, and homogeneous sublayers. These and other approximations are presented separately for the five different models considered, and the resulting levels of uncertainty are discussed.

Introduction

Many different models have been developed for the various components of the natural and engineered barrier system of the proposed high-level nuclear waste repository at Yucca Mountain, Nevada. The TOUGH2/iTOUGH2 family of codes (Pruess et al., 2000; Finsterle, 1999) is used for most of the models of the unsaturated zone (UZ) at the site.

A number of approximations and assumptions underlie the basic approaches used in these models. Some of the key concepts include the continuum approximation, the use of the van Genuchten formulation and the active fracture model, heterogeneity representation, and numerical gridding. These assumptions lead to uncertainty in model predictions, which depend upon the scale of the model, its intended use, and the reliability and completeness of the calibration data. It is difficult to precisely estimate the level of uncertainty that arises from these approximations, because data from unsaturated fractured rocks are relatively scarce. Alternative conceptual models are often employed to investigate the degree of uncertainty through comparison of predictive results for different models.

Perhaps the single most important source of uncertainty in all of the UZ models relates to the detailed flow of water through the mountain. Many different data sets suggest that the average percolation flux through the mountain is on the order of 5–10 mm/yr (Bodvarsson et al., 2000). However, questions remain regarding which fractures conduct water, the spacing of major flow paths, the importance of episodic flow, and other issues. These are fundamental questions concerning flow in unsaturated fractured rocks; without knowing answers to these questions, the precise level of uncertainty engraved in the various models is difficult to determine.

In this paper, we discuss the development of five models for different components of the UZ. In particular, we consider the calibrated-property model, the seepage model, the site-scale model, the thermal-hydrological model (TH) and the thermal-hydrological-mechanical model (THM). All of these models are calibrated using various data sets from boreholes or underground test beds. The basic characteristics of these models are given, key underlying assumptions and approximations are described, a few selected results are given, and then possible improvements are summarized. These models have been under development for many years. Some valuable “lessons learned” can be gained from this work as well as insights into fruitful paths forward to improve these types of models for Yucca Mountain and other applications.

CALIBRATED PROPERTY MODEL

The calibrated property model is developed and used for calibrating hydraulic parameters (or properties) for the Yucca Mountain UZ. It involves minimizing the difference between the model predictions and the observed data (e.g., matrix saturation and water potential data, and fracture pneumatic-pressure data) by adjusting values of the parameters, including permeability and van Genuchten (1980) parameters for both fractures and matrix, and an active-fracture-model parameter (Liu et al., 1998). The calibration is carried out using the inverse modeling code iTOUGH2 (Finsterle, 1999). As an example, Figure 1 shows a comparison of inverse modeling results to pneumatic

pressure data (collected from Borehole SD-12) for several geologic units. More detailed discussions of the calibration procedure and methodology can be found in Bodvarsson et al. (2000) and Bandurraga and Bodvarsson (1999).

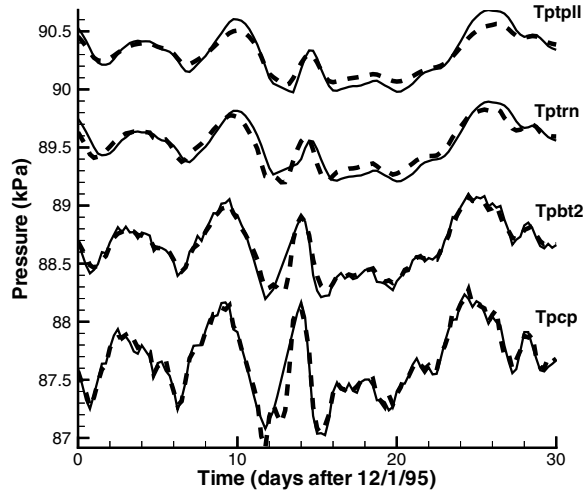


Figure 1. Pneumatic pressure matches at borehole SD-12. The solid and dashed lines correspond to measured and simulated results, respectively.

The calibrated property model has been successfully used to develop property sets that are consistent with the relevant field observations. This consistency is an important prerequisite for predicting future flow and transport conditions at the Yucca Mountain site. Model calibration can also handle scaling issues in a straightforward manner, because the calibration can provide parameter values at scales suitable for a large-scale model. Measurements at small scales are available from Yucca Mountain for several rock properties (such as matrix and fracture permeabilities), but these cannot be directly used in a large-scale model because of the scaling issue. The model calibration indicates that matrix and fracture permeabilities generally need to be increased from their average values measured at small scales to match the observed data (Liu and Ahlers, 2003). This is consistent with the current thinking that effective permeability increases with the spatial scale (e.g., Neuman, 1994).

A considerable degree of uncertainty exists in the calibrated property sets, resulting from uncertainties in the conceptual model and in numerical approaches as well as limitation data limitation. The calibrated property model is based on the continuum (dual-permeability) approach that conceptualizes a fracture network as a continuum. While the continuum ap-

proach is commonly used for dealing with large-scale flow and transport problems (National Research Council, 1996), and has been shown to reasonably approximate important flow and transport processes observed from a number of field tests in Yucca Mountain (Finsterle, 2000; Liu et al., 2003a), its usefulness for capturing complex discrete-flow behavior in unsaturated fractured rock needs to be further verified. For example, Liu et al. (2002) suggest that the average spacing of active flow paths (in unsaturated fracture networks) within a layered system generally increases with depth. This is supported by simulation results of a large-scale fracture-network model with a realistic fracture density (Zhang et al., 2003). This is not considered by the current continuum approach.

The calibrated property model uses the van Genuchten (1980) relationships—developed specially for porous media—for describing unsaturated flow in fractures. This application can be questioned. The constitutive-relationship model has a large effect on the corresponding simulation results. Liu and Bodvarsson (2001) reported that van Genuchten relationships underestimate fracture relative permeability for a large range of water saturations, and argued that an improved relationship model is needed for fractures. More studies along the line of Liu and Bodvarsson (2001) are needed to completely resolve the issue.

The calibrated property model uses the active fracture model (AFM) of Liu et al. (1998) to deal with fingering flow and transport in unsaturated fractures. The active fracture model has been theoretically shown to be consistent with fractal flow patterns (common in different unsaturated systems), and simulation results based on the model can represent field observations from different sources reasonably well (Liu et al., 2003b). However, the active fracture model needs to be evaluated in more detail because of the complexity of unsaturated flow in fractures (Liu et al., 2003b). For simplicity, the calibrated property model assumes a uniform property distribution within a geological layer. While this treatment is generally supported by a recent study involving multiscale heterogeneity (Zhou et al., 2003), the effects of small-scale heterogeneity within a unit on flow and transport processes are not fully understood.

Data limitation is a major source of uncertainty in the calibrated property sets. Like many practical problems, we have relatively limited data compared with the number of parameters that need to be calibrated. As a result, the calibrated property values are non-unique. Furthermore, data directly related to solute transport processes in the Yucca Mountain UZ are

especially limited. Therefore, parameters important to the solute transport process, such as the effective matrix-diffusion coefficient, are not calibrated in the current calibrated property model.

DRIFT SEEPAGE MODEL

Background

Seepage of liquid water into waste emplacement drifts affects the long-term safety of the repository system. The number of waste packages contacted by water, the dissolution and mobilization of radionuclides, and the release and migration of radionuclides to the accessible environment all depend on the rate, chemical composition, and spatial and temporal distribution of water seeping into the emplacement drifts. Seepage also affects the conditions below the drift, specifically the saturation distribution in the matrix and the fractures, which in turn affects diffusive releases at the interface between the drift and natural environment, as well as the potential for fast advective transport of radionuclides through the fracture network.

General Approach

Seepage from unsaturated fractured rock is a complex multiscale process that depends on (1) the local distribution of percolation flux, (2) the capillary barrier effect in the boundary layer around the opening, (3) microscale phenomena such as evaporation, film flow, drop formation, and drop detachment, and (4) the thermodynamic environment in the opening (relative humidity, ventilation regime, etc.).

Developing a comprehensive, physically based seepage model that covers all scales discussed above is very challenging and would require a large amount of characterization data that are difficult to measure in the field. Model conceptualization deals with the question of which characteristics and processes should be modeled explicitly and on what scale, and which effects can be captured through the estimation of site-specific, process-relevant, scale-dependent, and model-related effective parameters. The approach chosen is based on a process model of seepage in combination with effective parameters determined from *in situ* seepage experiments. The approach is limited, in that detailed predictions of drip frequency and seepage location are not made. Instead, calculated seepage rates are averaged in time and over a drift section of a certain length (the length of a waste package), i.e., they refer to the temporal and spatial scale of interest for a long-term assessment of seepage into waste emplacement drifts.

Seepage Field Testing

Approximately 100 *in situ* seepage tests were conducted at various locations within test tunnels at Yucca Mountain. Water was released from borehole intervals located above a drift, and seepage was collected as it dripped into the opening. These seepage-rate data contain information about all aspects of the seepage process. Air-injection tests were performed to characterize the heterogeneity of the test bed. Because evaporation may affect the observed seepage rates, relative humidity and temperature were also monitored. Details about the field testing can be found in Wang et al. (1999). The test design was improved based on sensitivity and uncertainty analyses of data from preliminary tests. Specifically, test duration, release rates, and evaporation control were modified to yield sufficient data suitable for analysis by inverse modeling.

Conceptual and Numerical Model

The seepage-rate data collected during the liquid-release tests are used to develop and calibrate a numerical process model. Water flow and seepage from the tuff formation at Yucca Mountain occurs predominantly through the fracture network. In a network of randomly oriented fractures, flow diversion around the drift occurs primarily *within* the fracture plane (see Figure 2), a process that is appropriately captured by a 3-D, heterogeneous fracture continuum model (Finsterle, 2000).

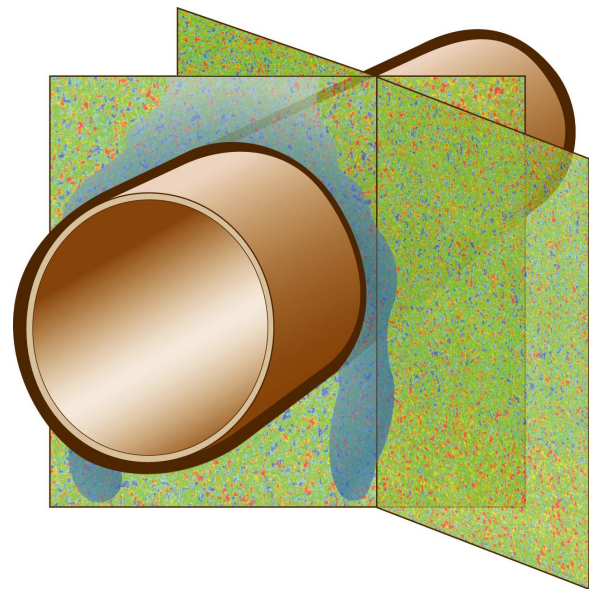


Figure 2. Schematic showing two fractures intersecting a drift. A fracture continuum model considers flow diversion occurring within multiple fracture planes that are randomly oriented to the drift axis.

The spatial structure of the air-permeability data was analyzed, with the resulting geostatistical parameters used to generate multiple realizations of a spatially correlated permeability field. These conditioned on the permeabilities measured in the borehole intervals. Permeability fields were then mapped onto a numerical grid of the drift section of interest (see Figure 3). Evaporation from the drift surface is accounted for by specifying a time-dependent water-potential boundary condition based on Kelvin's equation, in which the thickness of the diffusive boundary layer was determined from evaporation experiments at the seepage test location (Ghezzehei et al., 2003).

Model Calibration

The numerical model is automatically calibrated against late-time seepage-rate data from liquid-release tests using iTOUGH2 (Finsterle, 1999). Early-time seepage data are discarded because they are affected by storage effects and the properties of a few fractures connecting the injection interval with the drift opening. These fractures are not necessarily representative of the fracture network engaged in flow diversion around the entire opening under steady-state conditions. Late-time data are more representative of near-steady conditions and are less influenced by storage effects, i.e., they better reflect average conditions on the scale of interest.

Detailed sensitivity analyses and synthetic inversions were performed to identify the calibration parameters most important for seepage. The capillary-strength parameter $1/\alpha$, which enters the van Genuchten capillary-pressure function, is estimated as an effective, seepage-relevant, model-related parameter.

Figure 3 shows the simulated propagation of the liquid plume from the injection interval towards and around the underground opening. The calculated saturation distribution at the end of the test shows that significant diversion of injected liquid around the niche has occurred. Despite the fact that a continuum model is being used, seepage occurs at only a few discrete locations, consistent with qualitative observations of drip locations.

Figure 4 shows the match of the calculated seepage rates (red line) to the observed data (blue symbols), along with the measured and modeled release rates (gray and black lines) and the relative-humidity data (green line). The model correctly replicates the initial, 34-day-long no-seepage period. The increase in release rate induces seepage, the magnitude of which is well reproduced by the calibrated seepage model.

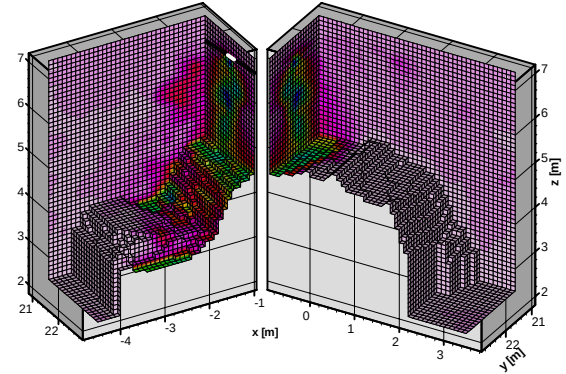


Figure 3. Simulated saturation distribution at the end of liquid-release testing in a niche.

Fluctuations in the seepage-rate data can be correlated to changes in relative humidity, which drives evaporation. The favorable match provides confidence that the conceptual model appropriately represents the key processes and their interactions, including (1) unsaturated flow using a continuum representation of fracture flow based on Richards' equation, (2) seepage into the opening, accounting for the capillary barrier effect, and (3) vaporization of water from the drift surface. The rather complex system behavior, which includes expansion and shrinkage of the liquid plume along the drift surface, signifies the importance of handling unsaturated flow, seepage, and evaporation in a fully coupled manner.

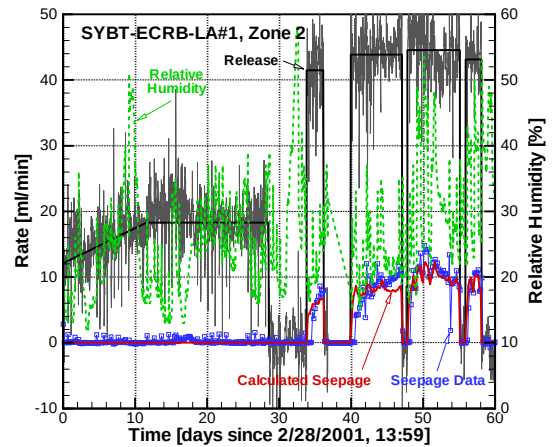


Figure 4. Comparison between measured and calculated seepage rates for the liquid-release test. Blue symbols represent measured data; the red line is the calculated seepage rate. Measured release rates are shown in dark gray; the black solid line shows the injection rate used in the model. Relative-humidity data are shown as a green line.

Seepage-rate data from multiple test events, using different liquid-release rates, were inverted simultaneously. Inversions were repeated for multiple realizations of the underlying stochastic permeability field to capture the uncertainty induced by local heterogeneity. Seepage-relevant capillary-strength values were estimated for each location. An average capillary-strength parameter is calculated from the estimates at the different test locations within a given unit.

The ability of the calibrated model to make seepage predictions is tested by comparing model-calculated rates to measured seepage rates from liquid-release tests at locations not used for model calibration. The uncertainty in the calculated seepage rates is evaluated by means of Monte Carlo simulations, in which the uncertainty in the capillary-strength parameter and that from small-scale heterogeneity is propagated through the prediction model. The measured seepage rates lie within the uncertainty band of the model predictions on a appropriate significance level, providing confidence that the calibrated model is suitable for predicting seepage into waste emplacement drifts.

Concluding Remarks about Seepage Modeling

The two key elements of the seepage modeling approach are (1) the use of a physically based, numerical process model as the basis for predicting seepage into large underground openings, and (2) the calibration of this model against data from *in situ* liquid-release experiments. This approach is considered appropriate for the following reasons:

- Hydrological process modeling is the preferred means for predicting seepage, because (1) the key process relevant to seepage is directly modeled based on established physical laws, (2) only a few assumptions need to be made, (3) the approach has the potential to simulate conditions that cannot be observed in the field, (4) numerical models are flexible enough to accommodate the nonideal initial and boundary conditions as they occur during seepage experiments.
- Seepage experiments provide calibration data that reflect the process of interest. Measured data automatically reflect the factors and features pertinent to seepage. The effective parameters are capable of reproducing observed seepage data and are thus likely to yield reasonable seepage predictions.

- The experiments test the capillary barrier effect on the scale of interest, i.e., no upscaling is required. The water reaching the drift is partly diverted around the opening, engaging the relevant portion of the fracture network on the appropriate scale.

Analyses and model predictions suggest that seepage into waste emplacement drifts only occurs for high local percolation fluxes and unfavorable combinations of seepage-relevant parameters (i.e., low permeability and weak capillarity).

The close interaction between numerical test design, field experimentation, and data analysis using iTOUGH2 lead to a defensible and consistent approach to solving the seepage problem. Additional experimental and numerical work (including an effort to obtain a complete water mass balance during a liquid-release test) will further the confidence in the predictive capabilities of the calibrated seepage model.

3-D SITE-SCALE MODEL

Basic Model and Major Data Sets Used

The need for quantitative investigation of water and gas flow, heat transfer, and radionuclide transport at Yucca Mountain has motivated a continual effort to develop site-scale flow and transport models in the last two decades. As a result, a number of large site-scale models have been developed and used to characterize unsaturated zone (UZ) flow and transport processes, these by designing the repository and assessing the system's performance (e.g., Wu et al., 2002). Since the middle 1980s, site-scale UZ models have evolved from 2-D moisture flow models (e.g., Rulon et al., 1986) to complicated 3-D models, incorporating site geological and hydrological complexities (Wittwer et. al., 1995) as well as additional physical processes, such as gas and heat flow, and perched-water body formation (e.g., Wu et al., 1999).

The more recent Yucca Mountain site-scale models (e.g., Wu et al., 2002) are able to incorporate a wide variety of field data, and take into account the coupled processes of flow and transport in highly heterogeneous, unsaturated fractured porous rock. Various scenarios of current and future climatic conditions and their effects on the UZ are evaluated to aid in the assessment of the proposed repository's system performance using different conceptual models of unsaturated flow. These large-scale UZ models have been calibrated against field-measured data of moisture content, the existence of perched water, pneumatic pressures, temperatures, and geochemical iso-

topes. These data have proved to be useful in estimating the hydrological conditions of the Yucca Mountain site.

Alternative Conceptual and Numerical Approaches

Subsurface flow and transport processes in the UZ occur in a heterogeneous system of layered, anisotropic, fractured volcanic rock. Our knowledge of such processes has been aided by continuous efforts of data collection and analysis as well as modeling studies. Figure 5 illustrates a typical geologic profile along vertical east-west transects as well as the conceptual model that characterizes the potential lateral flow in the PTn unit and the effects of faults and perched water on the UZ system.

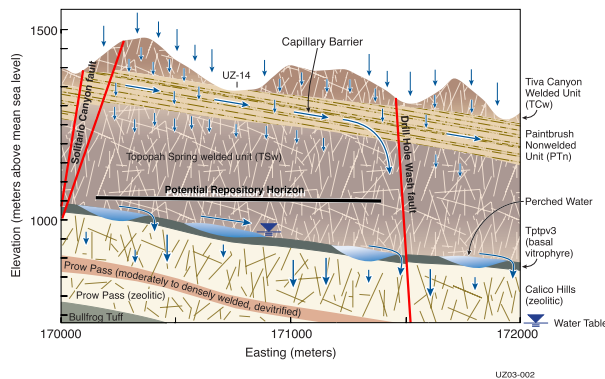


Figure 5. Schematic showing the conceptualized flow processes and effects of capillary barriers, major faults, and perched water zones within a typical east-west cross section of the UZ flow model domain.

As illustrated by Figure 5, the fundamental conceptual models for UZ flow processes are:

- Top boundary is subject to spatially varying, but steady-state net infiltration.
- Surface transient infiltration rapidly penetrates TCw through highly permeable fractures.
- Once entering the PTn, percolation transitions into matrix-dominated flow. There may exist capillary barriers, causing lateral diversion. Downward-moving transient pulses arising from episodic surface infiltration are effectively damped and homogenized by PTn (temporally and spatially), such that flux at the bottom of PTn is approximately at steady state.
- Flow becomes fracture-dominated again in TSw.

- Perched-water zones exist below the proposed repository horizon along the bottom of TSw and top of CHn, and may change vertical flow paths.

In addition, field data indicate that the formation at Yucca Mountain is more heterogeneous vertically than horizontally, with layer-wise representations providing a reasonable approximation of the complex geologic system. Therefore, site-scale models have used the following hydrogeological conceptualizations: (1) The hydrogeological units/layers are internally homogeneous, and the material properties of each unit are continuous throughout each layer, unless interrupted by faults; (2) ambient water flow in the system is in a steady-state condition; and (3) faults are represented by vertical or inclined rock columns having finite width.

How to handle fracture and matrix flow and interactions under multiphase, multicomponent, isothermal, or nonisothermal conditions has been a key issue for simulating fluid and heat flow in the unsaturated fractured rock of Yucca Mountain. Currently, most site-scale models are based on the dual-continuum method to handle fracture-matrix interactions. This is because the dual-continuum method appears to provide an appropriate representation of flow and transport processes within the UZ at Yucca Mountain. This approach is computationally much less demanding and requires fewer data than the discrete-fracture-modeling approach. The traditional dual-permeability concept is modified using the active fracture model (Liu et al., 1998) to represent the fingering effects of flow through fractures, and to limit flow into the matrix system.

Several alternative modeling approaches, such as discrete fracture or weeps-type models, have been investigated for their applicability. However, these modeling methods are subject to high uncertainties in fracture distribution data within the mountain, and extensive computational burden for a site-scale model that cannot be solved currently or in the near future. On the other hand, the Equivalent Continuum Method (ECM) (although the most computationally efficient among the modeling possibilities), may not capture important rapid-transient interactions in flow and transport between fractures and matrix.

Major Limitations/Uncertainties and Possible Impact

The accuracy and reliability of site-scale model predictions are critically dependent on the accuracy of estimated model properties, other types of input data, and hydrogeological conceptual models. These site-

scale models are limited mainly by the current understanding of the mountain system, including the geological and conceptual models, the volume-averaged modeling approach, and the available field and laboratory data.

Past site investigations have shown that large variabilities exist in flow and transport parameters over the spatial and temporal scales of the mountain. Even though considerable progress has been made in this area, uncertainty associated with the site-scale model input parameters will continue to be a key issue for future studies. The major uncertainties in the model parameters are: (1) accuracy in estimated current, past, and future net-infiltration rates over the mountain; (2) quantitative descriptions of heterogeneity of welded and nonwelded tuffs, their flow properties, and detailed spatial distributions within the mountain, especially below the proposed repository; (3) fracture properties in zeolitic units and faults from field studies; (4) evidence of lateral diversion caused by zeolites in the CHn units and within the PTn units; and (5) transport properties (e.g., adsorption or K_d coefficients in different rock types, matrix molecular diffusion coefficients in different units for different radionuclides, dispersivities in fracture and matrix systems).

Another important limitation or approximation with current site-scale models is the use of large-scale volume averaging. For example, a typical mesh size of a site-scale model is ($\Delta x \times \Delta y \times \Delta z \approx$) $100 \text{ m} \times 100 \text{ m} \times 10 \text{ m}$, so that each element may contain hundreds and thousands of fractures. Detailed flow behavior through these fractures is averaged out rather than precisely captured.

Overall What Works and What Does Not

In the last decade, site-scale UZ model results have been used to simulate past, present, and future hydrogeological, geothermal, and geochemical conditions and processes within the Yucca Mountain UZ to support various TSPA-LA activities. For example, the UZ site-scale models have been successfully applied to generate 3-D steady-state flow fields for TSPA-VA (Viability Assessment), TSPA-SR (Site Recommendation) and current TSPA-LA (License Application) efforts. Site-scale UZ flow models and submodels have been shown to match various types of field data reasonably well, on the model scale, including matrix liquid saturation and water potential, perched water elevations, pneumatic data, geothermal gradients, chloride, calcite and strontium data.

However, site-scale flow models cannot be used to predict exact locations or distributions of flow paths or rates in the UZ system. For example, these models cannot determine flow rate along a particular fracture, nor can they predict perched-water zones smaller than a grid block. What the models predict is averaged results over a volume of about $100,000 \text{ m}^3$.

Future Developments

In addition to unavoidable approximation resulting from large-scale averaging, a number of additional uncertainties and limitations remain with the current site-scale models. Among them, few measurements of fracture properties for CHn units and for faults are available. These fracture and fault properties are determining factors for radionuclide transport or groundwater travel from the repository to the water table. Heterogeneity within model layers has not been incorporated into site-scale models. Application of van Genuchten relative permeability and capillary pressure functions to fractures is questionable and needs to be further investigated. Furthermore, a large number of small-scale fractures, as observed in underground tunnels, have not been taken into account in current models, and their effect on flow and transport through the UZ is poorly understood.

Thermal-Hydrological Modeling

This section describes numerical modeling of coupled thermal-hydrological (TH) processes at Yucca Mountain. During the first several hundred years following waste emplacement, the fractured rock in the drift vicinity will be heated to above-boiling temperatures, caused by the radioactive decay of the nuclear waste. Boiling of rock water will give rise to significant thermal-hydrological perturbation of the ambient state. As the pore water in the rock matrix vaporizes, the vapor moves away from the drift through the permeable fracture network, driven primarily by the pressure increase caused by boiling. In cooler regions away from the drift, the vapor condenses in the fractures, and the resulting water can drain either toward the heat source from above or away from the drift into the zone below the heat source.

Capturing the drift-scale TH behavior at Yucca Mountain in predictive models is important for performance assessment, because the amount of water seeping into emplacement drifts can be affected. The superheated rock zone that will develop close to the heat source may form an effective vaporization barrier that limits seepage into drifts (Birkholzer et al., 2003a). On the other hand, condensed water will form a zone of elevated water saturation in the fracture network. Seepage may be in-

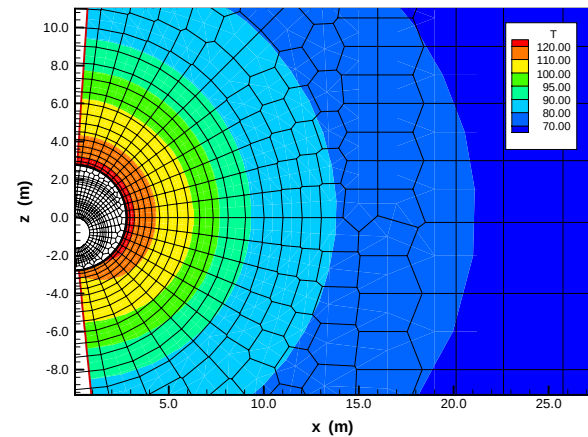
creased in case water from this zone is mobilized to flow rapidly towards the drift.

Basic Modeling Approach

The general conceptual model for flow and transport simulations in the densely fractured, unsaturated tuff at Yucca Mountain is used for all of the UZ models. A dual-continuum model comprising separate fracture and matrix components, coupled with the active fracture model to adjust the fracture-matrix interface area, is used as the basic model for predictive simulation of the coupled processes of liquid, gas, and heat movement (Birkholzer et al., 2003a). The computer code used for modeling these TH processes is the integral-finite-difference simulator TOUGH2, Module EOS4 (Pruess et al., 2000). With this code, while fluid flow is described with a multiphase extension of Darcy's law, heat flow occurs by conduction (with heat conductivity a function of saturation) and convection. Thermodynamic conditions are based on a local equilibrium model of the three phases (liquid, gas, and solid rock). The EOS4-module considers vapor-pressure lowering, allowing for the presence of liquid water at temperatures higher than the nominal boiling point.

The main features of the predictive TH model include: (1) a large-scale model grid honoring the stratigraphic conditions at Yucca Mountain, (2) specific grid refinement in the vicinity of waste emplacement drifts, honoring the future repository and drift geometry, (3) hydrological properties based on inverse modeling of ambient flow at Yucca Mountain, (4) thermal properties based on site-specific measurements, (5) small-scale heterogeneity in the drift vicinity, based on air-permeability measurements, (6) time-varying infiltration conditions to account for climate changes, and (7) time-varying thermal load to account for radioactive decay. Predictive simulations are conducted for a period of several thousand years after emplacement. Example results are given in Figure 6 for the drift-scale conditions at 100 years after waste emplacement. At this time, the rock temperatures in the drift vicinity will be above 120°C, leading to significant boiling in the rock. A several meter wide dryout zone will develop close to the drifts, followed by a condensation zone where water flow in the fractures is much larger than at the ambient state. The observed flux variability stems from the heterogeneity in fracture permeabilities.

Rock Temperature and Numerical Grid



Fracture Saturation and Liquid-Flux Vectors

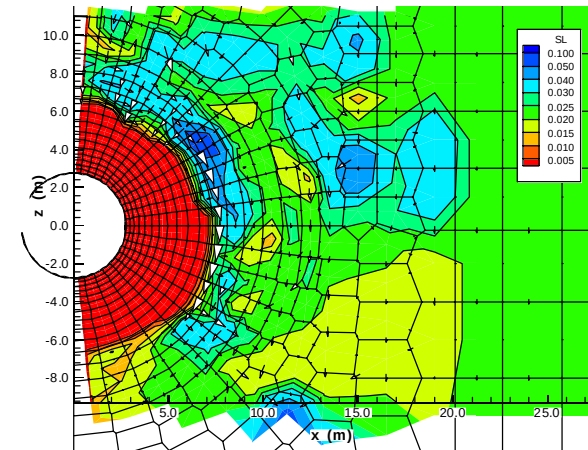


Figure 6. Close-up view of drift vicinity with circular drift opening in the center. The simulated rock temperatures, fracture saturations and liquid flux vectors are displayed at 100 years after waste emplacement.

Lessons Learned: Computational Issues

TOUGH2 and other comparable numerical codes have been reasonably successful in modeling the highly dynamic, complex TH processes occurring in fractured. Long-term simulations over time periods of several thousand years are possible, despite the fact that the highly transient nature of the processes requires small time steps. Including the effect of vapor-pressure lowering in the simulation usually has a positive effect on both the accuracy of the results and the convergence of the simulations. However, the type of characteristic relationship used to describe the capillary pressure/saturation dependence requires specific attention in this case, because boiling of rock water may drive the saturation level below residual

saturation. Typical capillary pressure relationships such as van Genuchten's function (van Genuchten, 1980) are not defined for this specific case, because they approach unreasonable values or are not defined for saturations at and below residual saturation. It is important to adjust the characteristic functions to maintain physically meaningful values at all liquid saturations (Pruess, 1997). This can be done, for example, by capping the chosen function at a defined maximum capillary pressure or by using a different function for low saturation values.

Lessons Learned: Conceptual Model

The conceptual model chosen for the predictive TH simulations has been extensively tested by comparison against the measured response in three *in situ* heater tests of different scales and geometries conducted at Yucca Mountain (Tsang and Birkholzer, 1999; Birkholzer and Tsang, 2000; Mukhopadhyay and Tsang, 2002). These tests generally involve: (1) continuous measurement of temperature, pressure, and relative humidity at various locations; (2) periodical geophysical measurements of matrix saturation; (3) periodical air permeability measurements in packed-off borehole sections; and (4) periodical withdrawal of liquid water in packed-off boreholes if necessary.

As demonstrated in the publications cited above, the agreement between model results and these measured data is generally good and leads us to believe that TH processes are well captured in the model. Uncertainty remains, however, considering the scope of the model compared to the quality and quantity of the data. Only the first type of measurements listed above allows direct comparison with the model results. Geophysical measurements approximate water saturation data only after data conversion with inverse techniques, which are often a source of uncertainty and only allow for qualitative estimates. Air-permeability data are valuable to qualitatively understand water saturation changes in the fractures (as saturation increases, the conductivity to air decreases). However, fracture-aperture changes as a result of heat-induced stresses have a similar effect on air permeability, making it hard to derive quantitative saturation changes from the measured data. Water retrieval from packed-off boreholes is an important indicator that intense flow processes must have occurred in the adjacent fractures. Not all possible locations will collect water, however, because capillary barrier effects at the borehole wall limit or prevent water from seeping into the borehole interval. Unfortunately, the parameter that is most important for the predictive studies—the change in water flux—can only be inferred

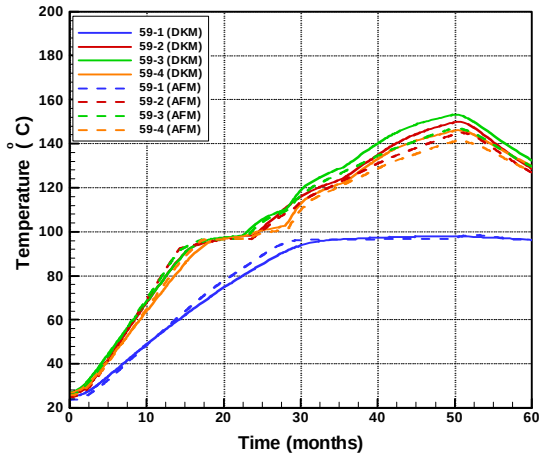
from the supporting data; fluxes cannot be measured in the field.

The question arises whether the quantitative agreements (in temperature, pressure, relative humidity) and the qualitative agreement (in water saturation/collection data) are sufficient to provide confidence in the TH models flux-prediction capability. An important conceptual model uncertainty (with a strong impact on moisture redistribution) is the treatment of fracture-matrix interaction, in particular with respect to the interaction area assumed between these two components. If most of the water condensing in the fractures readily imbibes into the rock matrix, the amount of TH coupling is rather small, as the condensate becomes “trapped” in the low-permeability matrix. In contrast, if imbibition is less important, most of the water remains “mobile” in the fractures, giving rise to fast and intense water flow. Above the emplacement drifts, this flow would be mainly directed back to the drifts, often leading to intensive heat-pipe effects. Below the drifts, most of the condensate would drain downward and away from the repository. While different conceptual models for fracture-matrix interaction—such as the standard dual continuum model versus the AFM—arrive at considerably different flow patterns, it is often not an easy task to define the best-suited model from the available data. This is because the temperature, pressure, and relative-humidity results are not significantly different for both models. The main differences occur in the fracture fluxes and saturations, and these are parameters that cannot be measured directly.

One potential method of reducing the above conceptual model uncertainty is a thorough, detailed analysis of heat-pipe signals in the temperature data. While temperature is rather insensitive to TH coupling due to the dominating effect of heat conduction, the presence, location, intensity, and vertical asymmetry of these subtle signals can be indicative of the relative importance of fracture-matrix interaction (Figure 7). Distinct differences between heat-pipe signals above and below the heater would be expected if condensate remains mostly “mobile” in the fractures; less distinct differences would be indicative of strong imbibition effects. Currently, temperature data from the DST are re-evaluated according to this method, with promising preliminary results. Note that this kind of analysis requires a fine resolution of temperature sensors in all locations where the boiling front resides. Another possibility is to change the design of heater tests such that they allow for a complete water balance; i.e., the amount of water draining away from

the heater should be quantified. This is hard to achieve *in situ*, but could be done in carefully designed laboratory experiments.

Temperatures Above Heated Drift



Temperatures Below Heated Drift

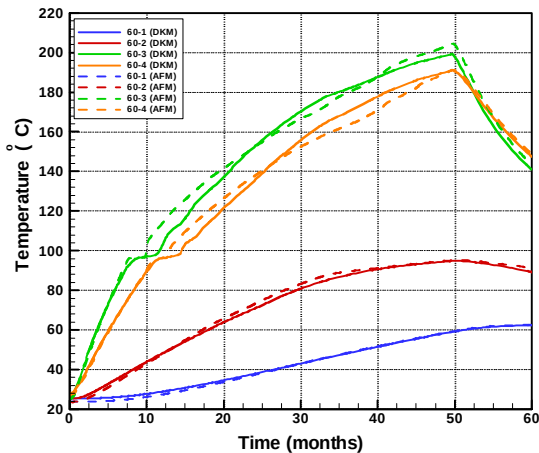


Figure 7. Simulated temperature evolution in the DST (Drift Scale test) using a standard dual-continuum model (DKM) compared to dual-continuum model with AFM. The latter gives rise to less intensive fracture-matrix coupling. The selected boreholes run above (59) and below (60) the heated drift. The main differences in heat-pipe signals between these two models occur below the drift.

Another important conceptual model uncertainty arises from the assumption that the fractured rock behaves as a continuous medium for flow and heat transport. Continuum models cannot account for the possibility of small-scale flow processes, such as formation of episodic preferential finger flow in the condensation zone above the heated drifts. These

flow processes do not affect general TH behavior, but could be potentially important for studies on drift seepage because rapid finger flow may penetrate far into the superheated rock above drifts. Because of the vast difference in spatial and temporal scale, it is impossible to include such behavior into drift-scale models addressing long-term changes. A possible method for assessing the impact of flow fingering was presented in Birkholzer et al. (2003b), using a combination of large-scale and small-scale modeling. While a dual-continuum model provides the macroscopic TH behavior over a time period of several hundred years, a microscopic model was applied at selected times during this period to study the fate of episodic finger flow penetrating the superheated rock.

Coupled THM Model

A coupled thermal-hydrological-mechanical (THM) model has been developed to investigate the impact of THM processes on the performance of the proposed repository at Yucca Mountain. Specifically, the coupled THM analysis aims to investigate future mechanical and thermal-mechanical (TM) changes in the hydraulic properties of the rock mass, and its impact on fluid percolation around a repository drift.

Conceptual Model for THM Processes at Yucca Mountain

Coupled THM processes at Yucca Mountain are analyzed using the TOUGH-FLAC simulator (Rutqvist et al., 2002), which is based on a coupling of the two established computer codes TOUGH2 (Pruess et al., 1999) and FLAC3D (Itasca Consulting Group, 1997). A key parameter for the analysis of coupled THM processes is a stress-versus-permeability relationship that dictates how much the permeability will change for a given change in the stress field during the lifetime of a repository. For the Yucca Mountain site, the relationships between hydraulic properties and stress are based on the conceptual model of a highly fractured rock mass that contains three orthogonal fracture sets (as shown in Figure 8.a and b). The permeability in each direction is corrected for changes in stresses normal across each of the three fracture sets, based on an empirical relationship that should be calibrated against *in situ* tests (Rutqvist and Tsang, 2003).

Results from and Lessons Learned about THM Processes at Yucca Mountain

For the coupled THM analysis performed at the Yucca Mountain site, the stress-aperture relationship was calibrated against *in situ* air-permeability tests. Periodic permeability measurements during the ongo-

ing DST are extremely useful for testing of the conceptual model in Figure 8 and for the calibration and validation of the stress-permeability relationship under thermal load. Air-permeability measurements near a drift during its excavation have also been very useful for calibration and validation of the stress-permeability relationship and for quantifying the excavation-disturbed zone around drifts in the highly fractured volcanic tuff at Yucca Mountain. Results from the coupled THM analysis of these tests have shown that the conceptual model in Figure 8 is appropriate. This shows that fracture opening or closing caused by changes in stress normal to the fractures is the dominant mode of stress-induced permeability changes at Yucca Mountain. Current analysis and field observations at the DST do not indicate any significant permeability enhancement by fracture shear.

The conceptual model shown in Figure 8 indicates that a continuum model approach is appropriate for the analysis of THM processes at Yucca Mountain, because the two main stratigraphic layers for the proposed repository (upper middle nonlithophysal (Ttptmn) and the lower lithophysal (Ttptll) units of the Topopah Spring Tuff) are both highly fractured. In these rock units, three dominant sets of fractures are oriented almost orthogonal to each other, two subvertical and one subhorizontal, and the mean fracture spacing is less than 0.3 meters. This structure contrasts with many other fractured rock sites in Canada, Europe, and Asia, where underground tests have been conducted in crystalline sparsely fractured rocks (Rutqvist and Stephansson, 2003). In those formations, fluid flow is dominated by a few widely spaced fractures, which means that a continuum approach may be difficult to apply on the drift scale. In relation to other fractured rock sites, the rock mass at Yucca Mountain is relatively homogenous (homogeneously fractured), with much less variability in rock-mass mechanical and hydraulic properties.

The prediction of coupled THM processes at the proposed repository at Yucca Mountain shows that the impact of THM processes will last for well over 10,000 years, but the impact of these processes on the performance of a repository is likely to be small. Figure 9 shows the predicted changes in permeability and temperature field at 10,000 years. At this time, the temperature at the repository is about 45°C, which is still significantly higher than the ambient temperature of 24°C. This temperature rise is significant because it creates thermal stresses in the horizontal direction on the order of 10 MPa, which are sufficiently high to close vertical fractures and

thereby reduce their permeability. The thermal-mechanical stresses will make the permeability anisotropic, especially just above the drift where the horizontal permeability is predicted to increase by more than one order of magnitude, while the vertical permeability is predicted to decrease by more than one order of magnitude (Figure 9b). However, despite permeability changes of about one order of magnitude, the impact of hydro-mechanical coupling on the percolation flux around the drift is not significant. The reason is that the water retention curve and the relative permeability, which can change much more than the stress-induced permeability, dictates unsaturated flow. Furthermore, a stress-induced decrease in permeability may be compensated by an increase in relative permeability.

Reduction of Uncertainty in THM Analysis

The above THM analysis should be extended to investigate the impact of THM processes on unsaturated flow in a heterogeneous rock mass. Although the fracture rock at Yucca Mountain is relatively homogeneous, the fracture permeability generally ranges over three orders of magnitude (within each geologic layer). *In situ* tests conducted at Yucca Mountain (as well as at other fractured rock sites world-wide) have indicated that permeability changes most in those parts of the rock mass that have initially low permeability (Rutqvist and Stephansson, 2003). This implies that the impact of mechanical and thermo-mechanical stress may not only change the mean permeability but also the range (or standard deviation) of a heterogeneous permeability field. Furthermore, the distribution of capillary pressure, which depends on the local aperture values, will change with stress. A change in the distribution of permeability and capillary pressure can impact the flow field by increased flow focusing and channeling, which might have some bearing on the possibility of water seeping into a drift.

While the coupled THM model has been convincingly validated for the Ttptmn unit, and the stress-permeability relationship has been well constrained from various tests conducted in the Ttptmn unit, there are still uncertainties regarding the coupled THM model for the Ttptll unit. Recent *in situ* tests show that the rock-mass strength in the Ttptll unit is low because of the presence of lithophysal cavities within a matrix of intensively fractured rock. A low rock-mass strength may lead to larger permanent changes in permeability remaining after the temperature falls to ambient. It will be extremely important to have appropriate *in situ* heater tests in the Ttptll unit for constraining the stress-permeability function and

for predicting possible permanent changes caused by inelastic mechanical responses in that unit.

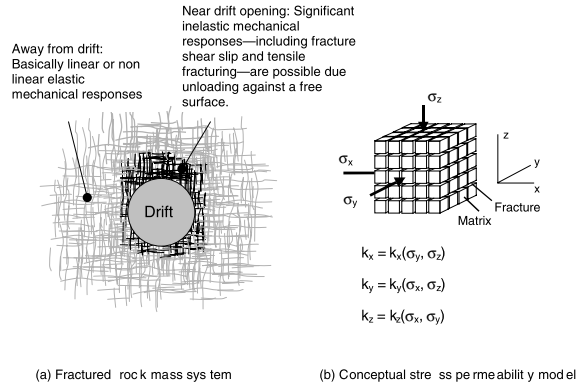


Figure 8. Schematic of the fracture rock system near a drift and the conceptual model used.

SUMMARY AND CONCLUSIONS

In this paper, we discuss five different models of the Yucca Mountain UZ, all of which use the TOUGH2/iTOUGH2 family of codes. For each model, we discussed their basic characteristics and intended use, major assumptions and approximations, and "lessons learned" during their development and application. Although these models consider different processes and spatial scales, the major approximations that cause uncertainties are similar in many cases. One major element of uncertainty in all of the models is the fact that we know little about the detailed flow mechanisms in this unsaturated fractured rock mass. The models perform well and are readily calibrated against field tests with a forcing source, (e.g., seepage tests, heater tests). It is much less certain how well the models actually represent the current, low water flow or the effects of future climate change. We conclude that large-scale behavior can be well predicted, but localized detailed flow patterns cannot. However, the latter may have significant influence on processes involved with seepage or flow behavior during repository heating. Other significant approximations that lead to considerable uncertainties in these models include the continuum approximation, constitutive relationships such as the van Genuchten and, active fracture models and stress versus fracture permeability relationships.

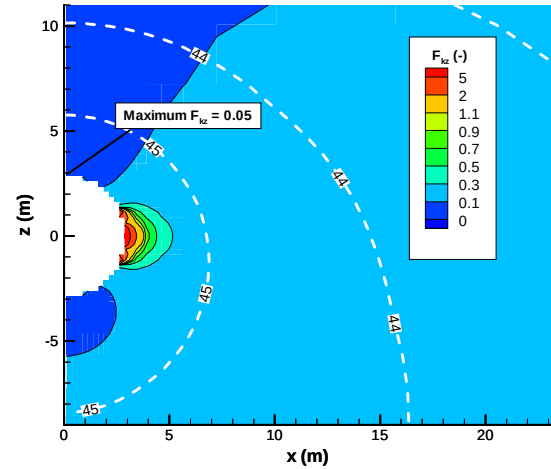
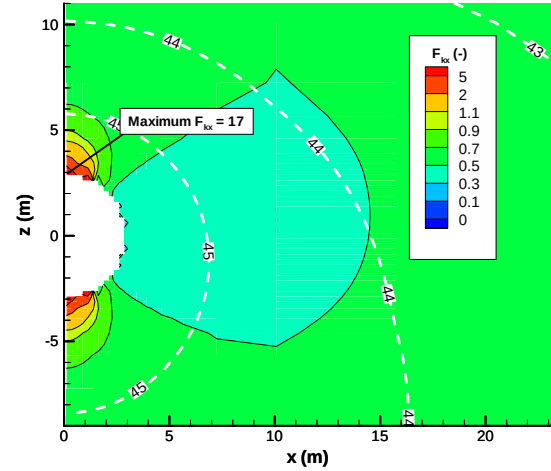


Figure 9. Calculated permeability correction factors around an emplacement drift in the Tptpmn unit at 10,000 years. Permeability. Correction factors are defined as $F_{kz} = k/k_{zi}$ and $F_{kx} = k/k_{xi}$ where index i means initial conditions before excavation of the drift.

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REFERENCES

- Bandurraga, T.M., and G.S. Bodvarsson. 1999. Calibrating hydrogeologic parameters for the 3-D site-scale unsaturated zone model of Yucca Mountain, Nevada, *J. Contam. Hydrol.*, 38, 47–46.
- Birkholzer, J., S. Mukhopadhyay, Y.W. Tsang, Analysis of the vaporization barrier above waste emplacement drifts, Proceedings: 10th IHLRWM Conference, Las Vegas, NV, March 30 – April 2, 2003a.
- Birkholzer, J., S. Mukhopadhyay, Y.W. Tsang, Modeling water seepage into heated waste emplacement drifts at Yucca Mountain, Proceedings: TOUGH Symposium 2003, Berkeley, Calif., May 12–14, 2003b.
- Birkholzer, J.T., Y.W. Tsang, Modeling the thermal-hydrologic processes in a large-scale underground heater test in partially saturated fractured tuff, *Water Resources Research*, 36(6), 1431–1447, 2000.
- Bodvarsson, G.S., H.H. Liu, R. Ahlers, Y.S. Wu and E. Sonnenthal. 2000. Parameterization and upscaling in modeling flow and transport at Yucca Mountain, in *Conceptual Models of Unsaturated Flow in Fractured Rocks*, National Academy Press, Washington, D.C..
- Finsterle, *iTOUGH2 User's Guide*, Report LBNL-40040, Lawrence Berkeley National Laboratory, Berkeley, Calif., 1999.
- Finsterle, S., 2000. Using the continuum approach to model unsaturated flow in fractured rock, *Water Resour. Research*, 36(8), 2055–2066.
- Ghezzehei, T.A., R.C. Trautz, and S. Finsterle, Evaluating the effectiveness of liquid diversion around an underground opening when evaporation is non-negligible, *Proceedings: TOUGH Symposium 2003*, Lawrence Berkeley National Laboratory, Berkeley, Calif., 2003.
- Itasca Consulting Group, 1997. *FLAC-3D Fast Lagrangian Analysis of Continua in 3 Dimensions*, Version 2.0. Five Volumes. Minneapolis, Minnesota: Itasca Consulting Group.
- Liu, H. H., C. Doughty, and G. S. Bodvarsson. 1998. An active fracture model for unsaturated flow and transport in fractured rocks. *Water Resour. Res.* 34, 2633–2646.
- Liu, H. H., and G. S. Bodvarsson. 2001. Constitutive relations for unsaturated flow in fracture networks. *J. of Hydrology*, 252, 116–125.
- Liu, H. H., Doughty, C., and Bodvarsson, G. S., 1998, An active fracture model for unsaturated flow and transport in fractured rocks, *Water Resource Research*, 34, 2633–2646.
- Liu, H.H., and C.F. Ahlers. Calibrated properties model. Rep. MDL-NBS-HS-000003. BSC, Las Vegas, Nevada, 2003.
- Liu, H.H., C. B. Haukwa, F. Ahlers, G. S. Bodvarsson, A. L. Flint, and W. B. Guertal. 2003a. Modeling flow and transport in unsaturated fractured rocks: An evaluation of the continuum approach. *J. Contam. Hydrol.* (in press).
- Liu, H.H., G. Zhang and G.S. Bodvarsson, 2003b The active fracture model: Its relation to fractal flow behavior and a further evaluation using field observations, *Vadose Zone Journal* (in press).
- Liu, H.H., G.S. Bodvarsson and S. Finsterle. 2002. A Note on unsaturated flow in two-dimensional fracture networks. *Water Resour. Res.*, 38 (9), 1176, doi:10.1029/2001WR000977.
- Mukhopadhyay, S., Y.W. Tsang, Understanding the anomalous temperature data from the Large Block Test at Yucca Mountain, Nevada, *Water Resources Research*, 38(10), 28.1–28.12, 2002.
- National Research Council, *Rock Fractures and Fluid Flow: Contemporary Understanding and Applications*. National Academy Press, Washington, D.C., 1996.
- Neuman, S.P. 1994. Generalized scaling of permeabilities: Validation and effect of support scale. *Geophys. Res. Lett.*, 21, 349–352.
- Pruess, K., Oldenburg, C., Moridis, G., *TOUGH2 User's Guide*, Version 2.0, Lawrence Berkeley National Laboratory Report LBLN-43134, Berkeley, Calif., 1999.
- Pruess, K., On vaporizing water flow in hot sub-vertical rock fractures, *Transport in Porous Media*, 28, 335–372, 1997.
- Rulon, J., Bodvarsson, G. S. and Montazer, P., *Preliminary Numerical Simulations of Groundwater Flow in the Unsaturated Zone, Yucca Mountain, Nevada*. LBL-20553. Berkeley, California: Lawrence Berkeley Laboratory, 1986.
- Rutqvist J. and Stephansson O. The role of hydro-mechanical coupling in fractured rock engineering. *Hydrogeology Journal* (in press) Jan (2003).
- Rutqvist J. and Tsang C.F. Analysis of thermal-hydrologic-mechanical behavior near an emplacement drift at Yucca Mountain. *J. of Contam. Hydrol.*, (in press), 2003.

- Rutqvist J., Y.-S. Wu, C.-F. Tsang, and G. Bodvarsson A Modeling Approach for Analysis of Coupled Multiphase Fluid Flow, Heat Transfer, and Deformation in Fractured Porous Rock *Int. J. Rock mech. Min. Sci.*, 39, 429-442 (2002).
- Tsang, Y., J. Birkholzer, Predictions and observations of the thermo-hydrological conditions in the Single Heater Test, *Journal of Contaminant Hydrology*, 38, 385-425, 1999.
- Van Genuchten, M. 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soil. *Soil Sci. Soc. Amer. J.*, 44, 892-898.
- Wang, J.S.Y., R.C. Trautz, P.J. Cook, S. Finsterle, A.L. James, and J. Birkholzer, Field tests and model analyses of seepage into drifts, *J. Contam. Hydrol.*, 38, 323-347. 1999.
- Wittwer, C., Chen, G., Bodvarsson, G. S., Chornack, M., Flint, A., Flint, L., Kwicklis, E., and Spengler, R., *Preliminary Development of the LBL/USGS Three-Dimensional Site-Scale Model of Yucca Mountain, Nevada*. LBL-37356. Berkeley, California: Lawrence Berkeley Laboratory, 1995.
- Wu, Y.S.; Haukwa, C.; and Bodvarsson, G. S., A Site-Scale Model for Fluid and Heat Flow in the Unsaturated Zone of Yucca Mountain, Nevada. *Journal of Contaminant Hydrology*. 38 (1-3), 185-217, 1999.
- Wu, Y.S.; Pan, L., Zhang, W. and Bodvarsson, G.S., "Characterization of Flow and Transport Processes within the Unsaturated Zone of Yucca Mountain, Nevada ." *Journal of Contaminant Hydrology* 54, 215-247, 2002.
- Zhang, K., Y.S. Wu, G.S. Bodvarsson and H.H. Liu, 2003. Determination of unsaturated flow paths in fracture networks, World Water Environmental Resources Congress 2003, Philadelphia.
- Zhou, Q., H.H. Liu, G.S. Bodvarsson and C. Oldenburg, Unsaturated flow and transport in fractured rocks: Effects of multi-scale heterogeneities. *J. of Contam. Hydrology*, 60 (1), 1-30, 2003.