An Integrated Methodology for Characterizing Flow and Transport Processes in Fractured Rock

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To investigate the coupled processes involved in fluid and heat flow and chemical transport in the highly heterogeneous, unsaturated-zone (UZ) fractured rock of Yucca Mountain, we present an integrated modeling methodology. This approach integrates a wide variety of moisture, pneumatic, thermal, and geochemical isotopic field data into a comprehensive three-dimensional numerical model for modeling analyses. The results of field applications of the methodology show that moisture data, such as water potential and liquid saturation, are not sufficient to determine *in situ* percolation flux, whereas temperature and geochemical isotopic data provide better constraints to net infiltration rates and flow patterns. In addition, pneumatic data are found to be extremely valuable in estimating large-scale fracture permeability. The integration of hydrologic, pneumatic, temperature, and geochemical data into modeling analyses is thereby demonstrated to provide a practical modeling approach for characterizing flow and transport processes in complex fractured formations.

Hydrogeology and Conceptualization: The modeling-study domain encompasses approximately 40 km^2 of the Yucca Mountain area, Nevada, USA. For hydrological investigations, the UZ geologic formations are categorized into hydrogeologic units, based primarily on their degree of welding (*Montazer and Wilson*, 1984). These units are classified as the Tiva Canyon welded (TCw) hydrogeologic unit; the Paintbrush Tuff nonwelded unit (PTn), consisting primarily of the Yucca Mountain and Pah Canyon bedded tuffs; the Topopah Spring welded (TSw) unit; the Calico Hills nonwelded (CHn) unit; and the Crater Flat undifferentiated (CFu) unit.

The key conceptualizations and assumptions made in analyzing UZ flow patterns are as follows: (1) Ambient water flow in the UZ system is in a quasi-steady-state condition; (2) Hydrogeological units/layers are internally homogeneous, unless interrupted by faults or altered; (3) There may exist capillary barriers in the PTn or other units, causing lateral flow; (4) Perched water results from the permeability barrier effect; and (5) Major faults serve as fast downward flow pathways for laterally diverted flow.

UZ Flow Model: The modeling study for characterizing multiphase flow, chemical transport, and heat transfer through fractured rock is conducted using the UZ flow model (Wu et al. 2004 and 2007). The UZ flow model, built using the TOUGH2 and T2R3D codes (Pruess et al. 1999; Wu et al. 1996), relies on the dual permeability concept to describe fluid flow, chemical transport, and heat transfer between fracture and matrix systems (Pruess and Narasimhan, 1985; Wu and Pruess, 2000). This model uses two 3-D numerical model grids, generated by an irregular, unstructured, 3-D control-volume spatial discretization, used for simulations of UZ fluid flow and heat flow, respectively.

Input parameters in relative permeability and capillary pressure curves are needed for the two media, in addition to other intrinsic fracture and matrix properties (e.g., porosity, permeability, fracture density and geometric parameters), as well as rock thermal and transport properties. Model boundary conditions are described using the ground surface of the mountain as the top model boundary, and the water table as the bottom model boundary. In addition, the top boundary is subject to net infiltration from precipitation. All the lateral boundaries are treated as no-flow (laterally closed) boundaries.

Model Calibration: The complexities of the heterogeneous geological formation and coupled UZ flow and transport processes at the Yucca Mountain UZ have posed serious challenges to modeling investigations. For example, past modeling experiences have shown that one cannot simply input field- and laboratory-measured parameters or 1-D model inverted properties directly into 3-D models and expect reasonable simulation results. This is because of the many uncertainties and significant differences in those input parameters (with respect to spatial and temporal scales) between measurements and model spatial representations. Without further calibration, those parameters observed or determined on one spatial scale are largely inappropriate for use at another spatial scale. In general, a proper model approximation of the actual physical system requires model calibration on the same model scale, from conceptual models to model parameters, as well as an accurate description of the physical processes involved.

Comparisons with Moisture Data: Comparisons between the 3-D UZ model simulations and observed matrix liquid saturation, water potential, and perched water data along the vertical grid column (representing boreholes) generally show reasonable agreement.

Comparison with Pneumatic Data: Calibration of the 3-D UZ model to pneumatic data or gas flow provides a practical method for estimating large-scale fracture permeability within the 3-D UZ system. Note that because of the low percolation flux at the site, moisture data are found to be insensitive to fracture properties under ambient infiltration conditions, and therefore are insufficient for estimating fracture permeability. In this study, gas flow calibration is carried out under a steady-state water flow condition with the present-day infiltration scenario. In these gas–flow calibrations, additional pneumatic boundary conditions are needed on the land-surface boundary for the gas phase, specifically as the time-dependent gas-pressure conditions, based on measured atmospheric barometric pressure data at the site. Since gas flow is a much more rapid process than liquid or heat flow in the UZ, water flow during pneumatic calibration is assumed to be at steady-state conditions, determined by steady-state flow-simulation results under the present-day mean infiltration scenario using the same model grid.

Comparison with Temperature Data: Heat flow simulations use a 3-D thermal model and present-day infiltration rate to simulate advective and conductive steady-state heat-transfer processes within the UZ. The main objective is to analyze the average present-day infiltration rate. Matching measured temperature profiles using simulation results along these boreholes at different locations implies that percolation fluxes (as well as their spatial distributions, as estimated by the 3-D UZ model) are within reasonable range of the actual percolation in the UZ.

Comparison with Geochemical Isotopic Data: The methodology for analyzing percolation flux using geochemical pore-water chloride (Cl) data is based on modeling studies of chloride transport processes in the UZ under different infiltration scenarios. While field-measured moisture data are found to be relatively insensitive to percolation values, geochemical isotopic data, on the other hand, provide valuable information by which to analyze the UZ system and help constrain the UZ percolation flux range (Sonnenthal and Bodvarsson*,* 1999).

Summary: An integrated modeling approach is discussed for characterizing percolation patterns in the unsaturated fractured rock of Yucca Mountain, Nevada. Specifically, a comprehensive modeling effort is made to quantify moisture movement or unsaturated flow patterns at the Yucca Mountain UZ, using an integrated approach to account for the multiple processes within the UZ system, including moisture flow, natural geochemical reaction and transport, and gas and heat flow. The modeling results, based on the integrated modeling approach, provide a better understanding of percolation patterns and flow behavior within the Yucca Mountain UZ. More importantly, integration of different types of field-observed data—such as water potential, liquid saturation, perched water, gas pressure, chloride concentration, and temperature logs—into one single modeling analysis provides a rare opportunity to cross-examine and verify different process model results and various conceptualizations. Such an opportunity may not arise when using only one or two types of data. This study also demonstrates that integrated model calibrations and analyses make it possible to have consistent model predictions for different but interrelated hydrological, pneumatic, geochemical, and geothermal processes in the UZ.

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