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Title
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ABSTRACT

This paper presents a field modeling study characterizing fluid flow and tracer transport in the unsaturated zone of Yucca Mountain, Nevada, a proposed underground repository for storing high-level radioactive waste. The 500 to 700 meter thick unsaturated zone of Yucca Mountain consists of highly heterogeneous layers of anisotropic, fractured ash flow and air fall tuffs. Characterization of fluid flow and heat transfer through such a system has been a challenge due to the heterogeneities prevalent on various scales. Quantitative evaluation of water, gas, and heat flow by means of numerical simulation is essential for design and performance assessment of the repository.

A three-dimensional numerical flow and transport model will be discussed. The model has been calibrated against field-measured data and takes into account the coupled processes of unsaturated flow and tracer transport in the highly heterogeneous, unsaturated fractured porous rock. The modeling approach of the model is based on a dual-continuum formulation of coupled multiphase fluid and tracer transport through fractured porous rock. As application examples, effects of current and future climates on the unsaturated zone processes are evaluated to aid in the assessment of the proposed repository's system performance.

INTRODUCTION

Since the 1980s, significant progress has been made in characterizing flow and transport processes in fractured rock of the unsaturated zone (UZ) of the highly heterogeneous, fractured tuff at Yucca Mountain, Nevada, a proposed subsurface repository for storing high-level radioactive waste. Numerical models have played an important role in these site characterization studies to evaluate UZ hydrological conditions. Modeling studies before the 1990s primarily used one- and two-dimensional models for understanding basic flow and transport behavior (Rulon et al. 1986). In the 1990s, Wittwer and co-workers (1995) started effort of developing a three-dimensional (3-D) model that incorporated many geological and hydrological complexities. Ahlers et al. (1995a; 1995b) continued developing the site-scale UZ model with increased spatial resolution and more physical processes of gas and heat flow analyses. Since then, more comprehensive model calibrations and studies, using the mountain-scale numerical model, were made to study liquid flow and radionuclide transport processes in the Yucca Mountain UZ (e.g., Viswanathan et al., 1998; Wu et al., 1999a; 1999b; 2002).

The modeling studies of this paper represent our continuing effort in development of the mountain-scale UZ Flow Model (Wu et al., 2003), which is in turn built on the analysis and results of the above-referenced work as well as many other studies. This work presents a methodology of comprehensive 3-D model calibrations using field-measured geochemical isotopic, geothermal, and pneumatic data in addition to moisture and perched-water data. In addition, the present work demonstrates how to use a numerical model to analyze flow behavior and to predict system response to future climate conditions in the Yucca Mountain UZ.

MODEL DESCRIPTION

The aerial domain of the UZ Model encompasses approximately 40 km^2 of the Yucca Mountain area (Figure 1). The UZ is between 500 and 700 m thick and overlies a relatively flat water table. The primary

UZ geological formations from the land surface down consist of the Tiva Canyon, Yucca Mountain, Pah Canyon, and the Topopah Spring tuffs of the Paintbrush Group. Underlying these units are the Calico Hills Formation, and the Prow Pass, Bullfrog, and Tram Tuffs of the Crater Flat Group. These geological formations have been categorized into hydrogeologic units based on the degree of welding (Montazer and Wilson 1984): the Tiva Canyon welded (TCw) hydrogeologic unit; the Paintbrush nonwelded unit (PTn); the Topopah Spring welded (TSw) unit; the Calico Hills nonwelded (CHn); and the Crater Flat undifferentiated (CFu) units.

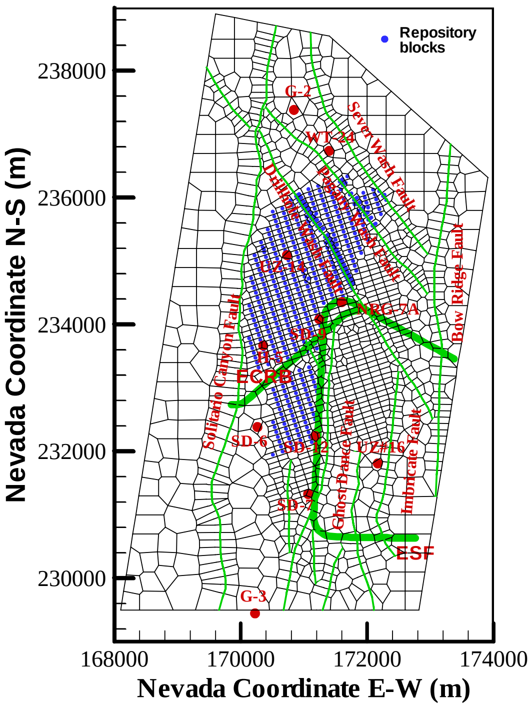

Figure 1. Plan View of the 3-D UZ Model Grid, Showing the Model Domain, Faults Incorporated, Proposed Repository Layout, and Several Borehole Locations.

The 3-D mountain-scale UZ model domain, as well as the numerical grid for this study, is shown in plan view in Figure 1. The UZ model grid is primarily designed for the purpose of model calibrations and investigations of UZ flow behavior. Also shown in Figure 1 are the locations of several boreholes used in model calibrations and analyses. The model domain is selected to focus on the study area of the repository area and to investigate the effects of different infiltration scenarios and major faults on moisture flow around and below the proposed repository. In the model grid, faults are represented in the model by vertical or inclined 30 m width zones. The model grid, as shown in Figure 1, has 2,042 mesh columns (or gridblocks per layer) of both fracture and matrix continua, and averages 59 computational grid layers in the vertical direction, resulting in 250,000 gridblocks and 1,000,000 connections in a dual-permeability grid.

Model calibration and simulation results in this work are carried out using TOUGH2 and T2R3D codes (Pruess, 1991; Wu et al., 1996). The single active liquid-phase flow module of the TOUGH2 code is used to calibrate the UZ flow, while tracer transport and chloride studies are performed using the module of T2R3D. On the other hand, the dual-permeability concept is used for handling fracture-matrix flow and interaction.

Both the top (ground surface) and bottom (water table) boundaries of the model are treated as Dirichlet-type conditions with a specified constant (but spatially distributed) pressure and constant liquid saturation values along these surfaces. For flow simulations surface infiltration is applied using a source term in the fracture gridblocks within the second grid layer from the top. This is because the first layer is assigned as a Dirichlet-type boundary with constant pressure, saturation, or temperature to represent average atmospheric conditions at the mountain. All lateral boundaries (Figure 1) are treated as no-flow (closed) boundaries.

Net infiltration from precipitation at land surface is the major control on overall hydrological and thermal-hydrological conditions within the Yucca Mountain UZ. To cover the various possible scenarios and uncertainties of future climates at Yucca Mountain, a total of nine net infiltration maps (Hevesi and Flint, 2000) are incorporated into modeling studies, including present-day (modern), monsoon, and glacial transition—three climatic scenarios, each of which consists of lower-bound, mean, and upper-bound infiltration rates. A plan view of the spatial distribution of the present-day mean infiltration map, as interpolated onto the model grid, is shown in Figure 2, with an average rate of 4.43 mm/yr over the model domain. The figure shows patterns of flux distributions with higher infiltration rates in the northern part of the model domain and along the mountain ridge east of the Solitario Canyon Fault from south to north.

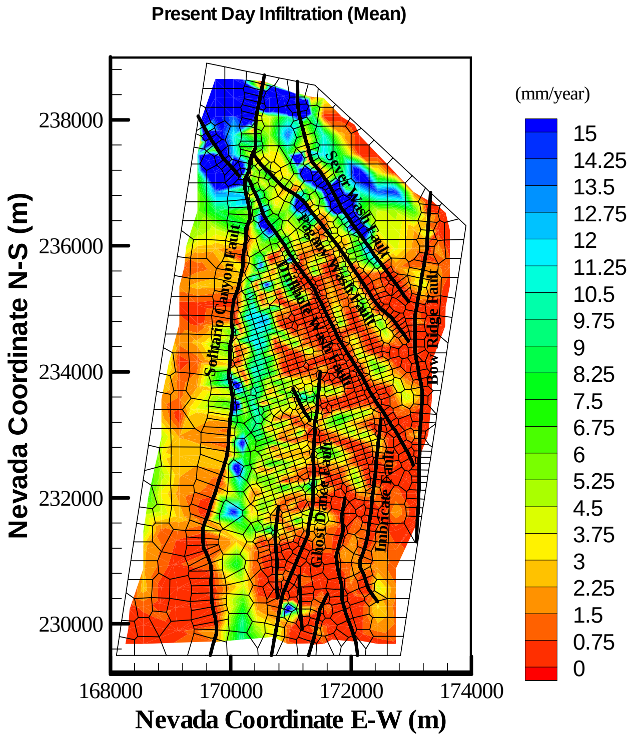

Figure 2. Plan View of Net Infiltration Distributed over the 3-D UZ Flow Model Grid for the Present-Day, Mean Infiltration Scenario.

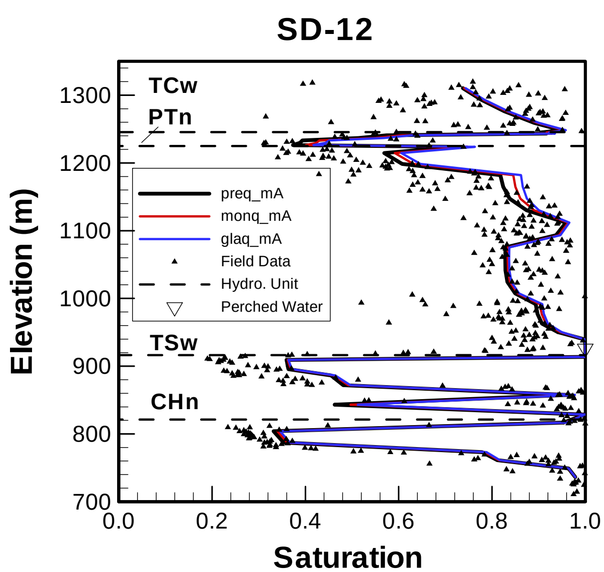

Figure 3. Comparison to Simulated and Observed Matrix Liquid Saturations and Perched-Water Elevations for Borehole SD-12, Using the Results of the Simulations with Three Mean Infiltration Rates.

Input parameters for the rock and fluid properties of each model layer as well as fault-fracture properties in this work are taken from those parameters estimated using a 1-D inversion modeling approach (Liu, 2002). Then the 1-D model estimated properties are calibrated and modified through a series of 3-D model calibrations using field-measured moisture, perched water, pneumatic, temperature, and chloride data. Using a hybrid, dual-permeability approach, we treat all of the geological units, including fault zones, as fracture-matrix systems (except for CHn vitric zones, which is treated as single-porosity matrix.)

MODEL CALIBRATION AND APPLICATION

Model calibration has been a critical step in developing the mountain-scale UZ flow models of Yucca Mountain (Wu et al., 1999a and 2002). It is part of the important iterative process of model development and verification, which derives model-scale related parameters and increase confidence in model predictions. This modeling effort uses an integrated approach to match all the available hydraulic, geochemical, pneumatic, and geothermal data with a 3-D model. In particular, we present an example of using moisture data below.

Measured matrix liquid saturation, water potential data, and perched-water elevations from all sampling boreholes have been compared to 3-D model results. This has resulted in model parameter adjustment in several model layers and zones. Simulated and observed matrix liquid saturation and perched water data along a vertical column for borehole SD-12 are compared in Figure 3, for the three mean infiltration rates. In general, as shown in Figure 3, the modeled results from all simulations after calibration are in good agreement with the measured saturation and water-potential profiles, as well as perched water levels.

Figure 4 shows an example of percolation fluxes simulated at the repository level for the present-day climate. Percolation fluxes at the repository horizon have been analyzed using 18 3-D UZ flow simulation results, with nine infiltration maps and each infiltration map having a base case (A) and alternative case (B) (Wu et. al., 2003). A comparison of the calculated repository percolation fluxes

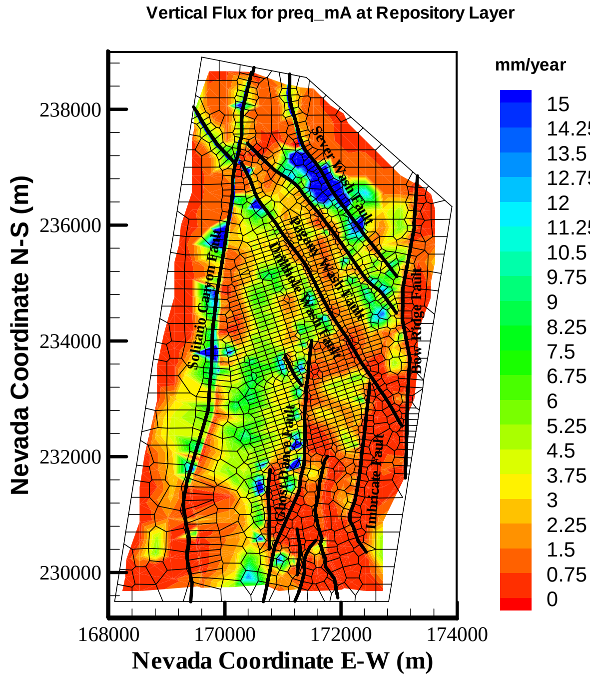

Figure 4. Simulated Percolation Fluxes at the Proposed Repository Horizon under Present-Day, Mean Infiltration.

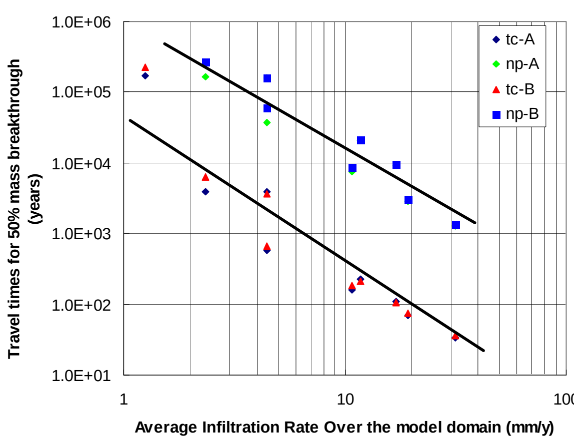

Figure 5. Correlation of Average Infiltration Rates and Groundwater Travel or Tracer Transport Times at 50% Mass Breakthrough for the 36 Tracer-Fracture-Release Simulation Scenarios.

(Figure 4) with the surface infiltration map (Figure 2), described as the top boundary condition, indicates that percolation fluxes at the proposed repository are different from surface infiltration patterns. This is because a substantial amount of large-scale lateral flow occurs when flowing across the PTn unit.

Groundwater travel times (since release from the repository to the water table) may be analyzed using statistics for groundwater travel or tracer transport times of 50% mass breakthrough at the water table. The tracer transport simulations are conducted under steady-state flow conditions using a total of 18 3-D flow fields of three climates and nine infiltration scenarios. There are two tracer transport runs, one for conservative and one for sorbing tracer, for each of the 18 flow fields. The distribution coefficient K_d (cc/g) of the sorbing tracer is 4.0 for zeolitic layer in the CHn, 1.0 for other layers, and no sorption in fractures. Figure 5 correlates average infiltration rates and groundwater travel or tracer transport times at 50% mass breakthrough for the 36 simulation scenarios of tracer-fracture release. The statistical data of Figure 5 shows the following:

- Groundwater travel times are inversely proportional to average surface infiltration (net water recharge) rate. When an average infiltration rate increases from 5 to 35 mm/yr, average groundwater travel (50% breakthrough) times decrease by more than one order of magnitude for both adsorbing and nonsorbing species.
- Nonsorbing tracers migrate one to two orders of magnitude faster than adsorbing tracers when traveling from the proposed repository to the water table under the same infiltration conditions.

SUMMARY AND CONCLUSIONS

This paper presents a modeling study using a 3-D mountain-scale UZ model, which has been calibrated using an integrated approach of incorporating all available data observed and measured from the site, including field-measured saturation, water potential and perched water data, temperature profiles, and pneumatic and geochemical data. These model-calibration efforts provide us with more confidence that the numerical UZ model can be used to predict hydrological conditions and flow processes in the UZ system of Yucca Mountain.

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