

Integration of perched water and chloride data in modeling flow processes within the unsaturated zone of Yucca Mountain, Nevada

Intégration des données relatives aux masses d'eau perchées et aux chlorures dans la modélisation des processus d'écoulement dans la zone non saturée de Yucca Mountain, Nevada

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ABSTRACT

This paper presents a modeling study incorporating field-measured perched water and chloride data into a three-dimensional (3-D) large-scale unsaturated zone (UZ) model of Yucca Mountain, Nevada, a potential underground nuclear waste repository site. This study integrates field measured perched water and pore-water chloride data into a single 3-D flow and transport model through model calibration. Using these field data in model calibration is intended to improve the model's capability to evaluate current conditions and predict future conditions of the unsaturated zone, so as to aid in the performance assessment of the proposed repository system. The calibration results show that the large-scale UZ flow and transport model may be able to predict both moisture and chloride geochemical conditions at the site.

RÉSUMÉ

Cet article présente une étude de modélisation intégrant des données de terrain relatives aux masses d'eau perchées et aux chlorures dans l'eau, dans un modèle 3-D à grande échelle de la zone non-saturée (ZNS) de Yucca Mountain, Nevada, site potentiel pour un stockage souterrain de déchets radioactifs. Cette étude intègre des données de terrain relatives aux chlorures dans les masses d'eau perchées et d'eaux interstitielles, dans un modèle 3-D unique d'écoulement et de transport, au stade de son calage. L'emploi de ces données de terrain au stade du calage du modèle est destiné à améliorer la capacité du modèle à évaluer les conditions du moment et à prédire les états futurs de la zone non saturée, afin de faciliter l'estimation de l'efficacité du système de stockage. Les résultats du calage prouvent que le modèle d'écoulement et de transport en ZNS à grande échelle peut prédire à la fois les conditions d'hydratation et de géochimie des chlorures sur le site.

Keywords: Perched water, chloride, unsaturated zone, Yucca Mountain, geochemistry, infiltration, percolation.

1 Introduction

Quantitative investigation of fluid flow, heat transfer, and radionuclide transport at Yucca Mountain is an essential step for conducting characterization studies of the site, designing the repository, and assessing the natural system's performance. Numerical modeling has played a crucial role in understanding fluid movement in the unsaturated zone for evaluation of hydrogeologic, thermal, and geochemical conditions within the overall waste-disposal system (Wu *et al.*, 1999a,b, 2000, 2002). The numerical models used for performing these site-characterization studies rely critically on, among other factors, incorporation of best-estimate model parameters, normally obtained through model calibration against field and laboratory data.

This paper presents a new study that incorporates fieldobserved perched water and chloride data into the same threedimensional (3-D) unsaturated zone (UZ) flow and transport model. Model calibration using these two types of field data reveals better insight into the UZ flow patterns. The objective of the combined model calibration is to improve the model's capability for evaluating current conditions and predicting future conditions of the unsaturated zone, so as to aid in the performance assessment of the repository system. In comparison, the previous 3-D model-calibration efforts (i.e. Wu *et al.*, 2002) have not incorporated perched water and pore-water chloride data into the same conceptual model.

The modeling approach of the current study is based on a continuum formulation of coupled multiphase fluid flow and tracer-transport processes through fractured porous rock, using a dual-continuum or dual-permeability concept. In this approach, the fractured tuffs at the Yucca Mountain UZ are represented by two continuum media—fracture and matrix—and the two continua are overlapping, globally connected, and interacting to each other. The objectives of this study are to provide a model-calibration methodology and to analyze flow and transport behavior under the current hydrogeological conceptual model and climate. This work is divided into two categories: (1) model calibration with perched-water data and (2) incorporation of pore-water chloride data.

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2 Site description

The domain of the Yucca Mountain UZ model covers a total area of approximately 40 km² (Fig. 1). Depending on the local topography, the UZ thickness varies from 500 to 700 m, overlying a relatively flat water table. The currently proposed repository would be located in the highly fractured Topopah Spring Welded unit, more than 200 m above the water table, with an approximate area of 1000 m east-west and 5000 m north-south. Yucca Mountain is a structurally complex system of Tertiary volcanic rock. Subsurface hydrologic processes in the UZ occur in a heterogeneous environment of layered, anisotropic, fractured volcanic rock (Scott and Bonk, 1984), which consists of alternating layers of welded and nonwelded ash flow and air fall tuffs. These geologic formations have been reorganized into hydrogeologic units based primarily on the degree of welding (Montazer and Wilson, 1984). These are the Tiva Canyon welded (TCw) hydrogeologic unit, the Paintbrush nonwelded unit (PTn) (consisting primarily of the Yucca Mountain and Pah Canyon members and their bedded tuffs), the Topopah Spring welded (TSw) unit, the Calico Hills nonwelded (CHn), and the Crater Flat undifferentiated (CFu) units. The hydrogeological units vary significantly in thickness over the model domain.

The 3-D numerical grid used in this study for representing the UZ system is shown in Fig. 1 for the plan view (x-y) (Wu *et al.*, 2000). Note that the 3-D UZ grid uses relatively refined meshes in the vicinity of the repository (relative to grid spacings outside the repository). The repository is located near the center



Figure 1 Plan view of the 3-D UZ model grid, showing the model domain, faults incorporated, and borehole locations at Yucca Mountain.

of the model domain, typical horizontal grid spacings $(\Delta x \times \Delta y)$ are 81 × 162 m within the repository and 200 × 200 m outside (Fig. 1). Each gridblock in the plan view represents a vertical column in the 3-D grid. Also shown in Fig. 1 are the locations of several boreholes used in model calibrations and analyses, and several incorporated major faults.

3 Model description

The simulation results presented in this study were obtained using the TOUGH2 and T2R3D codes (Pruess, 1991; Wu *et al.*, 1996) for flow and transport simulation respectively. Fracture–matrix interactions in the model are handled using the dual-permeability model. The dual-permeability methodology considers global flow and transport occurring not only between fractures but also between matrix gridblocks. In this approach, the rock-volume domain is represented by two overlapping (yet interacting) fracture and matrix continua, and local fracture-matrix flow and transport is approximated as a quasi-steady state. As applied in this study, the traditional dual-permeability concept is further modified using an active fracture model (Liu *et al.*, 1998) to represent fingering flow effects through unsaturated fractures.

In the 3-D model, the ground surface of the mountain is treated as the top boundary and the water table as the bottom boundary. For flow simulations, present-day mean infiltration is applied to the top boundary as a source term and the infiltration rate and its spatial distribution over the mountain were estimated by the US Geological Survey (USGS) scientists (Hevesi and Flint, 2000) for the site. The bottom boundary, the water table, is treated as a Dirichlet-type boundary. All the lateral boundaries, as shown in Fig. 1, are treated as no-flow (laterally closed) boundaries.

The input parameters for fracture–matrix rock and fluid properties include (1) fracture properties (frequency, permeability, van Genuchten (1980) α and *m* parameters, aperture, porosity, and interface area), (2) matrix properties (porosity, permeability, and the van Genuchten α and *m* parameters), and (3) transport properties (grain density, tortuosity, diffusion, decay and sorption coefficients) for each model layer. In addition, special matrix and fracture properties are applied to faults in each TCw, PTn, TSw, and CHn unit. The development of these parameters was presented in several related studies (Ahlers and Liu, 2000; Wu *et al.*, 2000).

4 Results

4.1 Model comparison with perched-water data

Model calibration is a critical step in developing a representative model for the UZ system of Yucca Mountain. Model calibration efforts in this work are focused on matching perchedwater occurrences using the 3-D model (although the matrix liquid saturations and water potentials were matched as well). During field investigations of the site over the past decade, several perched water zones were encountered in the UZ of the site (Rousseau *et al.*, 1998; Wu *et al.*, 1999b), including the observation data from boreholes UZ-14, SD-7, SD-9, SD-12, NRG-7a, G-2, and WT-24 (see Fig. 1 for their locations). These perched-water occurrences were found mostly to be associated with low-permeability zeolites in the CHn or the densely welded basal vitrophyre of the TSw unit.

The presence of perched-water bodies in the vicinity of the potential repository at Yucca Mountain provides invaluable insight into the heterogeneity of the UZ formation, the water movement, and the surface infiltration history of the mountain. A permeability-barrier conceptual model underlying perchedwater occurrence has been used in the UZ flow modeling studies for several years, as summarized in Wu *et al.* (1999b, 2002). The major assumptions with the permeability-barrier concept of perched-water occurrence are: (1) no large-scale vertically connected fractures transect the underlying low-permeability units, (2) both vertical and horizontal permeabilities within and below the perched-water zone are small compared with permeabilities outside perching zones, and (3) sufficient percolation flux (>1 mm/yr) exists.

To calibrate the 3-D model against observed perched-water conditions at Yucca Mountain, modelers must make some local modification of fracture–matrix rock properties. For the perchedwater conceptual model, parameters of fracture and matrix permeabilities within perched zones are manually calibrated from a series of 3-D modeling studies. Matrix permeabilities of potential perched layers/zones are based on average values of the measured matrix permeabilities from the units, while fracture permeabilities used for the northern perched zones are assumed to be 10 times higher than matrix permeabilities. Other than intrinsic permeabilities, van Genuchten's α and *m* parameters, as well as matrix residual saturations within perched zones, are treated as identical to those parameters estimated from the inverse modeling studies using moisture, pneumatic, and geochemical data (Ahlers and Liu, 2000).

In the following, the simulation results of steady-state flow from the 3-D UZ model are presented and discussed in terms of (1) comparisons with matrix liquid saturation and (2) matching with observed perched-water bodies. All simulated results with the perched-water conceptual model have been checked against observed saturation, water potential, and perched-water data at all boreholes where data are available. For brevity, borehole SD-12 is selected to show the match between observed and modeled vertical-saturation and perched-water locations (Fig. 2), respectively.

A further analysis and demonstration of model capabilities is given in Fig. 3. It indicates that the permeability barrier conceptual model can generally capture water-perching conditions, as observed in Yucca Mountain. A simulated perspective view of 3-D perched-water bodies and their volumetric extensions is presented in the figure. It shows fracture water-saturation distributions along the bottom of the TSw or the low basal vitrophyre layer. The blue isosurfaces on the figure reflect the regions near fully liquid-saturated or perched-water zones along the model layer, while the green isosurface represents the portion of the model layer with fracture liquid saturations less than 100%. The model clearly presents several extensive perched-water bodies, separated by faults, in the northern part of the model domain.



Figure 2 Comparison of simulated and observed matrix liquid saturations and perched-water elevations for borehole SD-12, using the three conceptual models with present-day, mean infiltration rate (with the thin-dashed lines representing interfaces between hydrogeological units).



Figure 3 Simulated 3-D view of perched-water bodies along the base of the TSw, using simulation results with present-day, mean infiltration rate (the blue isosurfaces denote the domain with 100% water saturation and the green isosurfaces the areas with less than 100% water saturation).

4.2 Model comparison with chloride data

Geochemical data collected from the UZ provide additional information by which to analyze flow processes of the UZ system. Pore-water chemical concentration data can be used to calibrate the UZ model to bound the infiltration flux, flow pathways, and transport times. The distribution of chemical constituents in both liquid and solid phases of the UZ system depends on many factors, such as hydrological and geochemical processes of surface precipitation, evapotranspiration, the fracture–matrix interactions of flow and transport, large-scale mixing via lateral transport, and the history of climate changes and surface recharge. Evaluation of flow and transport processes from the chloride data is an inverse procedure that involves inferring or assuming the chloride input and transport to produce the measured chloride output. The measured chloride concentration is assumed to represent the average *in situ* pore-water chloride concentration at depth. As in most inverse processes, more than one conceptual model may result in the same chloride distribution. Corroboration from other chemical or physical data is often needed to discriminate between different models and resolve non-unique-solution problems.

In the present chloride-transport modeling, chloride is treated as a conservative (nonadsorbing) tracer transported through the UZ. The mechanical dispersion effect through the fracture– matrix system is ignored, because it was found to be insensitive to modeled results for the flow system considered (Wu *et al.*, 2002). The UZ transport process is assumed to occur under twophase isothermal, steady-state flow conditions for water and air. Steady-state flow fields are provided by the flow simulations using both the perched-water calibration model and nonperchedwater model with the same surface infiltration rate (Wu *et al.*, 2000).

Modeling the chloride distribution requires either the known concentration in infiltrating water or the total surface flux pattern (Sonnenthal and Bodvarsson, 1999). The chloride flux includes dissolved material in rain and snow, and a contribution from windblown dust (Meijer, 1995; Fabryka-Martin et al., 1996, 1997; Triay et al., 1996; Tyler et al., 1996). The strong vertical and lateral heterogeneity in field-measured pore-water chloride concentrations indicates that the waters have undergone differing degrees of evaporation, interacted with waters flowing through fractures and the matrix pore-water, and may have been involved in large-scale mixing via lateral flow. Chloride has lower concentrations in regions of high infiltration below thin soil and higher concentrations beneath thick alluvial deposits, assuming that little surface runoff has taken place. On the other hand, the amount of water, to reflect the large variations in chloride concentrations and spatial variations by evapotranspiration, must be included in estimating the chloride concentrations in infiltrating. Both the chloride fluxes and concentrations must be considered, because areas of higher fluxes may have lower concentrations (owing to increased infiltration), and thus less evaporative concentration. Runoff will result in areas with higher surface water-fluxes and thus higher chloride fluxes. These higher chloride fluxes could lead to high concentrations in infiltrating water if evapotranspiration is high, or low concentrations if little evaporation takes place, resulting in the infiltration of a large volume of diluted water. Precipitation rates were calculated using the spatially varying precipitation data provided at a 30 m gridblock resolution (Flint et al., 1996).

Precipitation and infiltration fluxes were calculated for the 3-D model boundary by averaging all points enclosed in a circular



Figure 4 Comparison of simulated and observed chloride concentrations at the ECRB cross drift tunnel, using perched-water and nonperched-water conceptual model results.

area equivalent to the model grid (column) block surface area. Combining the mean annual precipitation of about 170 mm/year calculated for Yucca Mountain (Flint *et al.*, 1996) with the present-day chloride deposition rate of 106 mg/m²/year given by Fabryka-Martin *et al.* (1996) yields a mean chloride concentration of about 0.62 mg/L (Fabryka-Martin *et al.*, 1997; Sonnenthal and Bodvarsson, 1999). Boundary conditions for chemical transport are treated similar to those for flow simulations, except that the additional chloride mass fluxes are applied on the surface. The diffusion coefficients used were those for chemical ions at 25°C and infinite dilution in water (Lasaga, 1998).

In this study the results of 3-D chemical transport simulations were compared with measured pore-water chloride concentration data. The data available and applied were from samples collected at boreholes (NRG-6, NRG-7A, SD-6, SD-7, SD-9, SD-12, UZ#4, UZ-14, and UZ#16), the Enhanced Characterization of the Repository Block (ECRB) cross drift tunnel, and the Exploratory Studies Facility (ESF) tunnel, including South Ramp, North Ramp, and Main Drift. Detailed descriptions of these data were given in several reports (Fabryka-Martin *et al.*, 1998; Yang *et al.*, 1998).

Modeled chloride concentrations are compared with the measured field data, with the results shown in Figs 4–7 at the ECRB tunnel and boreholes SD-9, SD-12, and UZ#16, respectively. As can been seen from these figures, the model results are close in trend with or in reasonable agreement with the field data, and the perched-water model results are in general superior to the nonperched-water model results. This indicates that perched water zones may have a large impact on chloride transport and distribution in the UZ.

5 Summary and conclusions

A large-scale, 3-D modeling study incorporating perched-water and chloride data has been presented for characterizing fluid flow and tracer/radionuclide transport processes in the unsaturated zone of Yucca Mountain, NV, a potential site for a high-level



Figure 5 Comparison of simulated and observed chloride concentrations at borehole SD-9, using perched-water and nonperched-water conceptual model results.



Figure 6 Comparison of simulated and observed chloride concentrations at borehole SD-12, using perched-water and nonperched-water conceptual model results.



Figure 7 Comparison of simulated and observed chloride concentrations at borehole UZ#16, using perched-water and nonperched-water conceptual model results.

nuclear waste repository. The methodology used in the study includes (1) manually calibrating the fluid and rock parameters in the perched zones to match the observed perched-water body and (2) forward simulations to match the measured chloride porewater concentration data at depths. These efforts are devoted to improving model capabilities for evaluating current conditions and predicting future conditions of the Yucca Mountain UZ system, enabling it to contribute to performance assessment of the proposed repository system.

This modeling study has constituted an important step in understanding and characterizing flow and transport processes at Yucca Mountain. There are, however, still considerable limitations and uncertainties associated with the current model and corresponding results. These limitations and uncertainties include accuracy of estimated model properties, other types of input data, and hydrogeological conceptual models, such as the geological and conceptual models used, the large-scale volume-average modeling approach, and the available field and laboratory data. These model limitations need to be identified, constrained, and perhaps quantified through continued investigations with combined modeling and field studies, as demonstrated in this work.

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