Title

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An integrated approach to predict coupled processes at a nuclear waste repository

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ABSTRACT: An integrated modeling approach was developed to investigate coupled thermal, hydrological, and chemical (THC) processes around proposed nuclear waste emplacement tunnels at Yucca Mountain, Nevada. The approach involves the development of process models, followed by numerical implementation and validation against field and laboratory experiments, then long-term predictive simulations. An existing reactive transport numerical code was refined and validated to evaluate the chemistry of waters around the tunnels and the effect of water-rock interaction on hydrological behavior around the repository. At liquid saturations significantly larger than residual, no extreme pH or salinity values were predicted. Mineral precipitation around the tunnels consists mainly of silica with minor calcite, trace zeolites and clays. The effect of mineral precipitation on flow depends largely on initial fracture porosity, and results in negligible to significant diversion of percolation around the tunnel. Further analyses of model uncertainty are under way to improve confidence in model results.

1 INTRODUCTION

Assessing the long-term performance of geologic nuclear waste repositories requires evaluating the effects of coupled thermal, hydrological, and chemical (THC) processes for time periods lasting thousands of years. To reach this goal and gain confidence in our predictive ability, an integrated modeling approach was developed (Fig. 1). This approach involves comparing the results of "hard" field and laboratory data to predictive modeling results. This is especially important because reactive transport simulations are computationally intensive, limiting the number of runs that can be performed to assess model uncertainty. As part of this approach, an existing reactive transport numerical code (TOUGHREACT; Xu & Pruess, 2001) was further developed and "validated" for applications specific to nuclear waste disposal (e.g. Xu et al. 2001; Spycher et al. 2003a & b). This simulator considers water, vapor, air, and heat transport; reactive gas, mineral, and aqueous phases; porosity-permeability-capillary pressure coupling; and dual (fracture-matrix) permeability. The simulator and modeling approach were applied to the proposed high-level nuclear waste repository at Yucca Mountain to evaluate seepage water chemistry and the effect on long-term hydrological behavior around the repository, as discussed below.

2 MODELED COUPLED PROCESSES

The proposed repository at Yucca Mountain will be located in fractured, welded volcanic tuffs, several hundred meters above the regional water table. The fracture permeability in these tuffs (10^{-13}–10^{-12} m^2) is several orders of magnitude higher than the rock permeability (10^{-17}– 10^{-19} m^2). In these unsaturated tuffs, water is held mainly in pores of the rock matrix (liquid saturation ~ 0.8–0.9). Upon waste emplacement and subsequent heating (due to radioactive decay), the matrix water will boil and travel as vapor in fractures. In cooler regions around the repository, it will condense and drain back towards the boiling zone. This continuous boiling and refluxing of water is anticipated to induce mineral dissolution and precipitation, and alter the chemical composition of pore waters surrounding emplacement tunnels (drifts). A summary of these processes and references to their study using modeling at Yucca Mountain is given in Spycher et al. (2003a).

The coupled processes were investigated using underground thermal tests and laboratory experiments. THC simulations of the Drift Scale Test (Sonnenthal 2003, Xu et al. 2001) and of plug-flow reactor and fracture sealing experiments (Kneafsey et al. 2001, Dobson et al. 2003) provided the basis for model

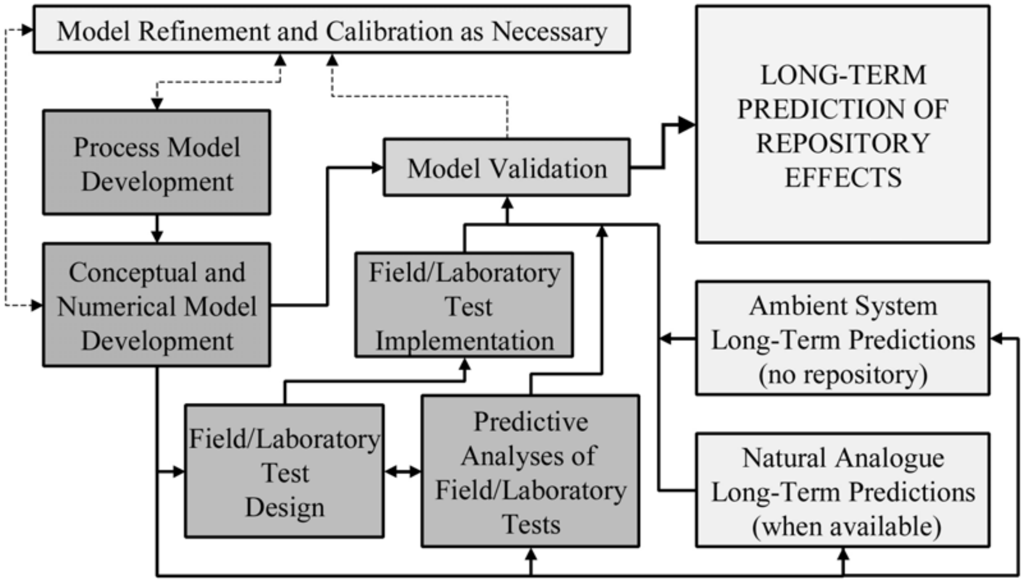

Figure 1. Schematic diagram of integrated modeling approach.

validation. Long-term simulations of the system under ambient thermal and hydrological conditions (without a repository) were also conducted to compare model results with observed data, and further refine the model as necessary to reasonably reproduce these data. Long-term (100,000 years) predictive analyses were then carried out to evaluate the effects of coupled THC processes around a typical nuclear-waste emplacement drift under heat load.

3 SIMULATION RESULTS

Initial results from simulations of long-term coupled THC processes were presented in Spycher et al. (2003a) for two potential repository temperature operating modes. Details on the numerical model and the geochemical system considered can be found in this reference. Here, we use the same model setup and focus on the evolution of water chemistry and mineral alteration in the most liquid-saturated region within fractures above a typical waste emplacement drift, for operating conditions leading to temperatures above boiling (Fig. 2) (Spycher et al. 2003b).

The zone of highest liquid saturation in fractures above the modeled drift is not stationary. Initially, it is adjacent to the drift crown, because percolating water builds up at this location due to the capillary barrier at the wall of the open drift (from ~ 0 to 50 years). As the temperature rises, a boiling front eventually develops and migrates several meters away from the drift wall (~from 50 to 600 years). During this time and until the boiling front collapses back to the drift wall (at ~ 2000 years), liquid saturations build up above the expanding and then receding boiling front (Fig. 3).

Time profiles of predicted temperature and chloride concentrations (Fig. 4) show that fracture water

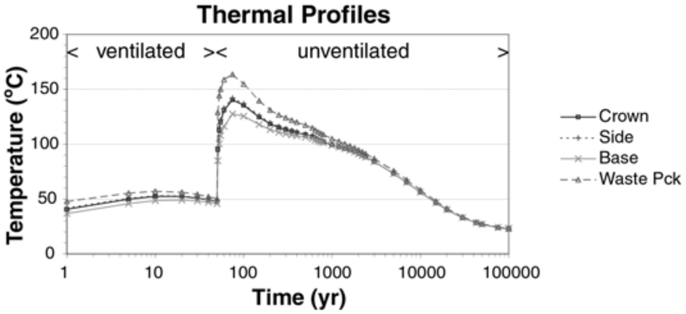

Figure 2. Predicted temperature profiles at the drift wall and waste package surface. Ventilation of the drift occurs for the first 50 years.

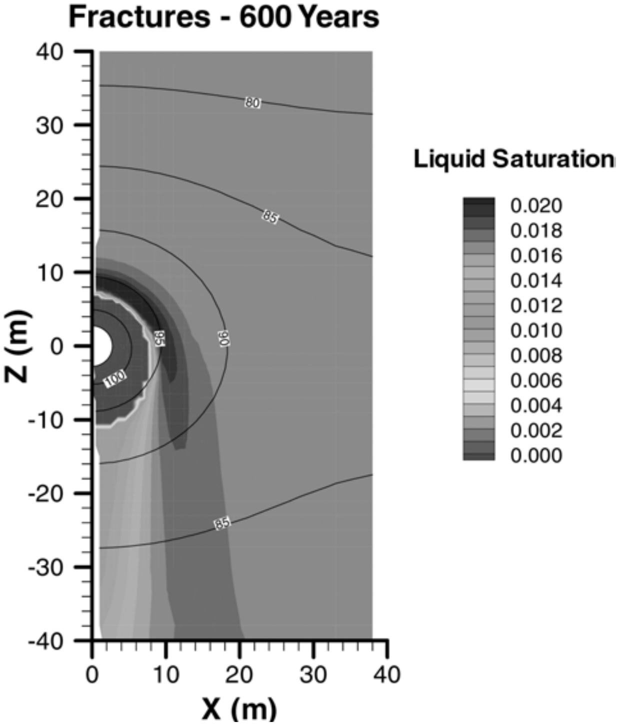

Figure 3. Contour plot of predicted liquid saturation (gray scale) and temperature (contours in °C). The emplacement drift is centered at (0,0) (white circle).

in this dynamic zone undergoes three distinct stages. First, dilution occurs while matrix water boils and condenses in fractures (from ~ 50 to 150 years). Because capillary forces are higher in the matrix than in fractures, the boiling front in the matrix stops expanding earlier than in fractures (at ~ 150 versus 600 years) and, eventually, no more steam is generated from boiling matrix water. Evaporative concentration then takes place (from ~ 150 to 600 years) under near-constant (boiling) temperatures as continuous boiling, condensation and refluxing take place in fractures. Finally, water compositions slowly return to ambient concentrations as the boiling front collapses towards the drift.

Profiles of predicted concentrations of aqueous species divided by chloride concentrations are useful in distinguishing between evaporation/dilution and mineral precipitation/dissolution effects (chloride is not reactive as opposed to other species) (Fig. 5). During the dilution stage, the predicted increase in Ca/Cl is indicative of calcite dissolution by mildly acidic condensate (from CO_2 volatilized from matrix water and then dissolved in condensate in fractures). Na/Cl also increase but much less than Ca/Cl, as the result of minor feldspar dissolution. These trends reverse during the evaporative concentration stage as calcite and sodium aluminosilicates precipitate. Calcium concentrations are slower to return to ambient values because calcite precipitation continues when waters are heated up as they percolate towards the drift.

A thin zone of mineral precipitation forms above the drift resulting in permeability reductions of around 1–2 orders of magnitude, sufficient to deflect the bulk of percolating water around the drift (Fig. 6). This zone consists primarily of amorphous silica and minor calcite (Fig. 7), forming mainly from evaporative concentration at the boiling front. Minor amounts of clay and zeolites also form around the modeled drift from alteration of feldspars, mostly in the rock matrix. These simulations show more precipitation and effect on flow than earlier results (Spycher et al. 2003a) because of model refinement and smaller initial fracture porosity.

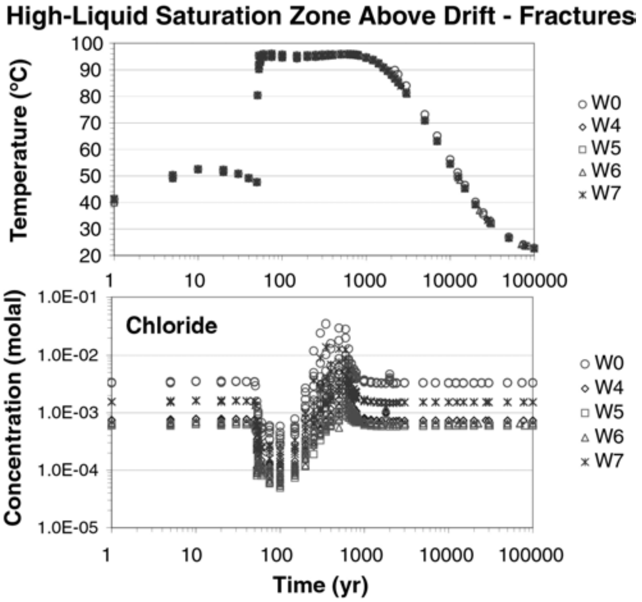

Figure 4. Predicted temperatures and chloride concentrations for five runs using different input water compositions.

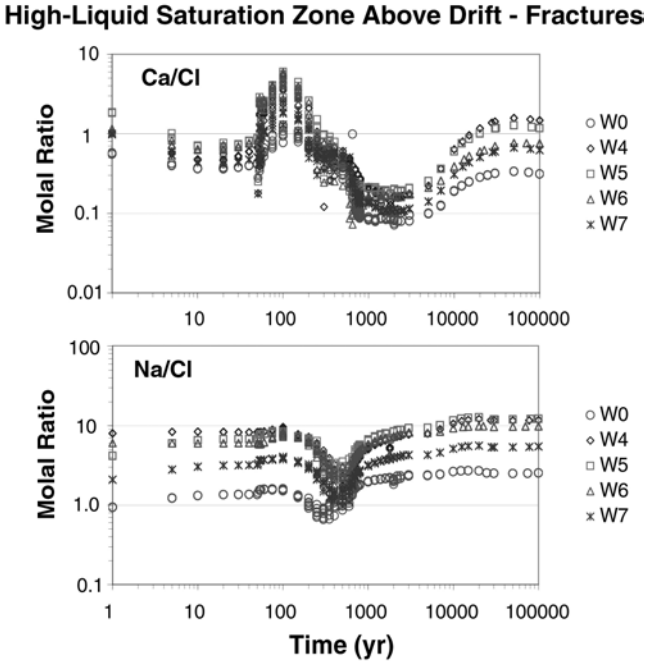

Figure 5. Predicted ratios of calcium and sodium to chloride concentrations for five runs using different input water compositions.

4 SUMMARY & CONCLUSIONS

To improve the level of confidence in long-term simulations of coupled THC processes, predictive modeling studies must be compared with “hard” field and laboratory data. The approach implemented here consisted of: (1) process model development, (2) conceptual and numerical model development, (3) design of field and laboratory tests for model validation, (4) predictive analyses of test results, (5) test implementation, (6) comparisons of experimental results to predictive analyses, (7) model refinement and validation, and (8) model implementation for long-term predictive analyses. Within this framework, an existing simulator was applied and further refined to help evaluate the long-term evolution of water compositions and mineral alteration around waste emplacement drifts at Yucca Mountain.

In fractures above the modeled drift, numerical simulations predict no extreme pH or salinity values while liquid saturations are significantly larger than residual. The effect of mineral precipitation on flow depends largely on initial fracture porosity and original water composition, and can lead to permeability reductions significant enough to affect flow

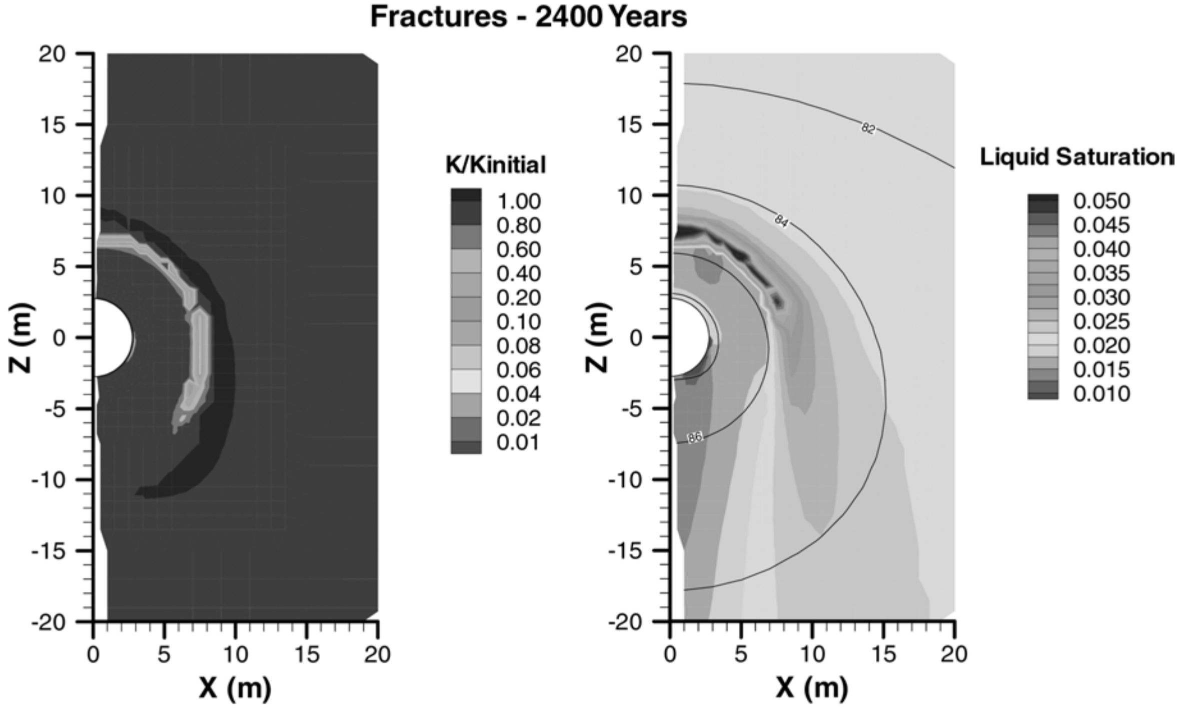

Figure 6. Predicted permeability reduction and effect on flow. The liquid saturation plot also shows temperature contours in °C.

around the drift. Investigations are under way to further assess model uncertainty and the implications for long-term evaluation of repository performance.

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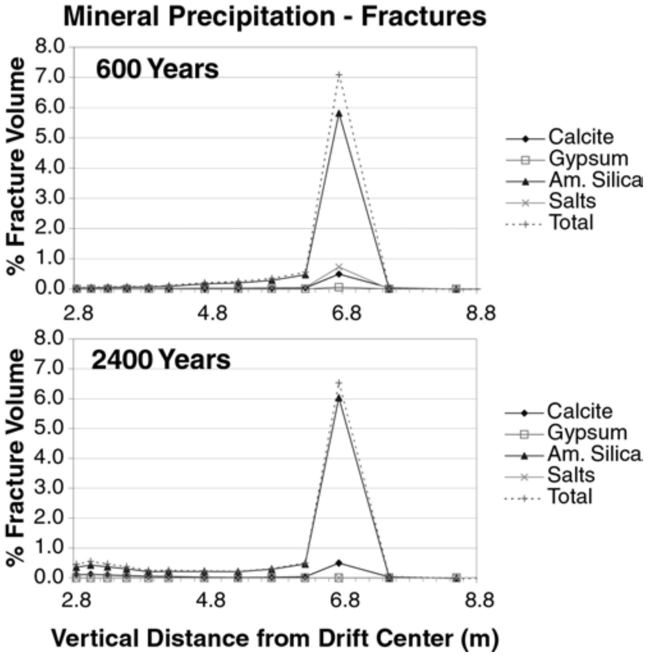

Figure 7. Dominant minerals predicted to precipitate in the zone of permeability reduction above the modeled drift (Figure 6). Note that the modeled fracture continuum initially contains 50% solids, such that the decrease in fracture porosity is actually twice that shown.