Modeling of Thermal-Hydrological-Chemical Laboratory Experiments

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Research Objectives
The emplacement of heat-generating nuclear waste in the potential geologic repository at Yucca Mountain, Nevada, will result in enhanced water-rock interaction around the emplacement drifts. Water present in the matrix and fractures of the rock around the drift may vaporize and migrate via fractures to cooler regions where condensation would occur. The condensate would react with the surrounding rock, resulting in mineral dissolution. Mineralized water flowing under gravity back towards the heat zone would boil, depositing the dissolved minerals. Such mineral deposition would reduce porosity and permeability above the repository, thus altering the flow paths of percolating water. The objective of this research is to use coupled thermal-hydrological-chemical (THC) models to simulate previously conducted laboratory experiments involving tuff dissolution and mineral precipitation in a boiling, unsaturated fracture.

Approach
Numerical simulations of tuff dissolution and fracture plugging were performed using a modified version of the TOUGHREACT code developed at LBNL by T. Xu and K. Pruess. The models consider the transport of heat, water, gas and dissolved constituents, reactions between gas, mineral and aqueous phases, and the coupling of porosity and permeability to mineral dissolution and precipitation. The model dimensions and initial fluid chemistry, rock mineralogy, permeability, and porosity were defined using the experimental conditions. A 1-D plug-flow model was used to simulate dissolution resulting from reaction between deionized water and crushed ash flow tuff. A 2-D model was developed to simulate the flow of mineralized water through a planar fracture within a block of ash flow tuff where boiling conditions led to mineral precipitation. Matrix blocks were assigned zero permeability to confine fluid flow to the fracture, and permeability changes in the fracture were specified using the porosity cubic law relationship.

Accomplishments
Simulations were conducted for both the tuff dissolution and fracture plugging experiments. Predicted concentrations of the major dissolved constituents for the plug-flow reaction were within a factor of 2 of the measured average steady-state compositions, with the 60 μm grain size model providing the best match. The fracture plugging experiment simulations are ongoing, with initial model results indicating the precipitation of a narrow band of silica at the base of the boiling front. While the overall reduction of fracture porosity is small (~2-3% over 5 days), fracture permeability is reduced by over an order of magnitude due to the highly focused silica precipitation.

Significance of Findings
Predicting changes in permeability and porosity resulting from water-rock interaction is important in the evaluation of long-term performance of nuclear waste repositories and

for geothermal reservoir engineering. This study demonstrates that carefully constructed THC models can successfully replicate laboratory experiments, thus validating the use of similar models in the prediction of changes in permeability, porosity and resulting fluid flow for the potential nuclear waste repository at Yucca Mountain.

Related Publications
Kneafsey, T. J., J. A. Apps, and E. L. Sonnenthal, Tuff dissolution and precipitation in a boiling, unsaturated fracture, Proceedings of the 9th International High-Level Radioactive Waste Management Conference, April 29-May 3, 2001, Las Vegas, Nevada, American Nuclear Society, La Grange Park, IL, 2001.

Sonnenthal, E.L., and N. Spycher, Drift-scale coupled processes (DST and THC seepage) models, Report MDL-NBS-HS-000001 REV01, Lawrence Berkeley National Laboratory, Berkeley, CA; CRWMS M&O, Las Vegas, NV, 2001.

Figure 1. Comparison of measured and simulated results of tuff dissolution plug-flow experiment. Legend descriptions refer to versions 2.2 and 2.3 of TOUGHREACT, use of 60 and 120 μm grain size models, and variations in model mineralogy. Plots show variations with time for Na (a) and SiO_2 (b).

(a)

Legend:
- ● 1999 LBNL tuff dissolution experiment
- —— v2.2, 60 um, pot. fsp as microcline
- — – · v2.2, 120 um, pot. fsp as microcline
- ········ v2.3, 60 um, no k-smecite, pot. fsp as microcline
- — — v2.3, 60 um, no k-smectite, pot. fsp as k-spar
- — – · v2.3, 60 um, k-smectite added to illite, pot. fsp as k-spar

Na (mg/l) vs Time (days)

(b)

Legend:
- ● 1999 LBNL tuff dissolution experiment
- —— v2.2, 60 um, pot. fsp as microcline
- — — · v2.2, 120 um, pot. fsp as microcline
- ········· v2.3, 60 um, no k–smectite, pot. fsp as microcline
- ·········· v2.3, 60 um, no k–smectite, pot. fsp as k–spar
- — — v2.3, 60 um, k–smectite as illite, pot. fsp as k–spar

Axis labels: SiO2 (mg/l) vs Time (days)