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Mountain-Scale Coupled Thermal-Hydrological-Chemical Processes Around the Potential Nuclear Waste Repository at Yucca Mountain

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Research Objectives

The objectives of this study were to evaluate the thermal-hydrological-chemical (THC) effects on flow and geochemistry in the unsaturated zone (UZ) at Yucca Mountain at a mountain scale. The major THC processes important in the UZ are (1) mineral precipitation/dissolution affecting flow and transport to and from the potential repository, and (2) changes in the compositions of gas and liquid that may seep into drifts.

Approach

The conceptual model developed for THC processes provides the basis for modeling mineral-water-gas reactions, as they influence the chemistry of water and gas and associated changes in mineralogy and hydrologic properties. Data incorporated in the model include hydrologic and thermal properties, geologic layering from the UZ 3-D flow and transport model, geochemical data (fracture and matrix mineralogy, water and gas geochemistry), and thermodynamic and kinetic data. Simulations included coupling among heat, water, and vapor flow; aqueous and gaseous species transport; kinetic and equilibrium mineral-water reactions; and feedback of mineral precipitation/dissolution on porosity, permeability, and capillary pressure for a dual permeability (fracture-matrix) system. Simulations were performed using TOUGHREACT V2.3.

The effects of coupled THC processes on the evolution of flow fields and water and gas chemistry in the UZ were evaluated for an above-boiling thermal operating mode. A cross section was chosen from the UZ 3-D flow and transport model that follows a north-south trend through the potential repository. Minerals include calcite, silica phases, feldspars, zeolites, clays, gypsum, fluorite, and iron oxides with the relevant aqueous species. The gas phase consists of air, water vapor, and CO₂. The composition of the initial and infiltrating water was derived from the matrix pore water extracted from the Topopah Spring welded tuff near the ongoing Drift Scale Test.

Accomplishments

The simulations revealed that by 5,000 years, most of the region above and directly below the potential repository undergoes a small reduction in fracture porosity of less than 1 percent (Figure 1). Above the northern edge, a region of slight porosity increase persists, owing to enhanced vapor convection and condensation. The areas that show the most effect as a result of heating are in the zeolitic units below the potential repository, where calcic zeolites dissolve to form alkali feldspars, leading to increased aqueous calcium concentrations and increased porosity. The predicted range in pH from 7 to 9 is linked to changes in gas-phase CO₂ concentrations induced by heating of pore waters.

Significance of Findings

The results of these simulations, based on a limited range of input parameters, suggest that mineral precipitation/dissolution will not significantly affect the percolation flux above the potential repository compared to the effects on flow induced solely by increased temperature. Edge effects owing to gas convection produce mineral precipitation below the drifts at the potential repository edge and in wider ranges in water and gas compositions than has been observed in drift-scale THC simulations. The results of this modeling will be used to bound uncertainties in potential repository performance.

Related Publications

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, California, 2001.

Acknowledgements

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Figure 1. Porosity changes and temperature contours after 5000 years. Crosses represent potential repository drift locations.