

**MODELING COUPLED THERMAL, FLOW, TRANSPORT AND GEOCHEMICAL  
PROCESSES CONTROLLING NEAR FIELD LONG-TERM EVOLUTION**

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Bentonite is planned for use as a buffer material in the Swedish nuclear waste disposal concept (KBS-3). Upon emplacement, the buffer is expected to experience a complex set of coupled processes involving heating, resaturation, reaction and transport of groundwater imbibed from the host rock. The effect of these processes may eventually lead to changes in desirable physical and rheological properties of the buffer, but these processes are not well understood. In this paper, a new quantitative model is evaluated to help improve our understanding of the long-term performance of buffer materials. This is an extension of a previous study [1] that involved simple thermal and chemical models applied to a fully saturated buffer.

The thermal model in the present study uses heating histories for spent fuel in a single waste package [2]. The model uses repository dimensions, such as borehole and tunnel spacings [2], which affect the temperature distribution around the waste package. At the time of emplacement, bentonite is partially saturated with water having a different composition than the host-rock groundwater. The present model simulates water imbibition from the host rock into the bentonite under capillary and hydraulic pressure gradients. The associated chemical reactions and solute transport are simulated using Äspö water composition [3]. The initial mineralogy of bentonite is assumed to be dominated by Na-smectite with much smaller amounts of anhydrite and calcite. Na-smectite dissolution is assumed to be kinetically-controlled while all other reactions are assumed to be at equilibrium. All equilibrium and kinetic constants are temperature dependent. The modeling tool used is TOUGHREACT, developed by Lawrence Berkeley National Laboratory [4]. TOUGHREACT is a numerical model that is well suited for near-field simulations because it accounts for feedback between porosity and permeability changes from mineral precipitation/dissolution and solute transport.

Preliminary results show that during the early heating phase, reactions strongly depend on the magnitude of the temperature gradient across the buffer. As the temperature gradient diminishes, reactions are increasingly dominated by groundwater solutes diffusing into the bentonite pore water from the host rock. Bentonite effective diffusion coefficient plays an important role in long-term solute transport.

[1] Arthur, R., W. Zhou, and B. Stromberg, (2003), "THC modeling of the non-isothermal phase of near-field evolution" in *Proceedings of the 10<sup>th</sup> International High-Level Radioactive Waste Management Conference*, March 30-April 2, 2003, Las Vegas, Nevada, USA.

[2] Hökmark, H. and B. Fälth, (2003), *Thermal dimensioning of the deep repository*, SKB TR-03-09, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

[3] Bruno, J. D. Arcos, and L. Duro, (1999), Processes and features affecting the near field hydrochemistry, SKB TR-99-29, Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.

[4] Xu, T., E. Sonnenthal, N. Spycher, and K. Pruess, (2003), *TOUGHREACT User's Guide: A Simulation Program for Non-isothermal Multiphase Reactive Geochemical Transport in Variably Saturated Geologic Media*, LBNL-55460, Lawrence Berkeley National Laboratory, Berkeley, California, USA.