# Simulation of Reactive Transport Processes in Compacted Bentonite: Application to a Prototype Experiment of Underground Repository for Nuclear Waste

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## Abstract

The Swedish Organization for Radioactive Waste (SKB) is considering disposal of High Level Waste in a deep underground repository in crystalline rocks. Bentonite clay is planned to be used in the near-field of the waste packages as buffer material. The buffer is expected to provide a favourable environment with limited radionuclide migration due to slow diffusion and retardation by sorption and cation-exchange. SKB is investigating several alternative buffer materials. To this end, the field experiment Alternative Buffer Materials (ABM) was started at the Äspö URL in 2006. Three packages of eleven different compacted bentonite blocks in different configurations have been tested over varying time periods. The packages were saturated and heated to target values. This work is concerned with the evolution of Package 1, which ran for about 2.5 years. Post-mortem examination after retrieval showed that the initially contrasting cation-exchanger compositions between different bentonite blocks became significantly homogenized. A modeling study has been undertaken to verify whether a reactive transport model that couples solute diffusion with cation-exchange can explain the observed experimental patterns in cation-exchanger composition. The feasibility of implementing a relatively simple reactive transport model into COMSOL has been tested. To this end, the Subsurface Flow Module has been coupled to a set of differential-algebraic equations (DAE) representing the chemical reactions. Reactive transport was implemented using a conservative component formulation. Temperature dependence of the effective diffusion coefficient and a variety of boundary conditions were represented in a simplified way and their effect tested. Despite major simplifications of the chemical system, the reactive transport model has proven largely successful in reproducing experimental results. In particular, the model is capable of capturing the observed homogenization patterns in cation-exchanger populations and pore water chloride concentrations. Moreover, when physically reasonable assumptions about groundwater boundary conditions are made, the model results match most of the measured values with satisfactory accuracy (Figure 1). However, a discrepancy between the modelled and experimental Mg-exchanger occupancy (not shown) may suggest that additional chemical processes relevant to Mg behaviour may operate. The results indicate that pore-water solute diffusion coupled to temperature evolution and cation-exchange are the main processes of solute reactive transport during the experiment. A sensitivity study has shown that temperature evolution and boundary conditions are the key controls of the model behaviour. The presented work demonstrates the feasibility of implementing a coupled reactive transport model in COMSOL using the Subsurface Flow Module

and a set of DAE. The results obtained agree well with observed experimental data and provide insight into the processes and controls behind solute transport in the bentonite column. The results of this study help to better understand and quantify processes responsible for radionuclide transport in the near-field of a HLW repository.

## Figures used in the abstract

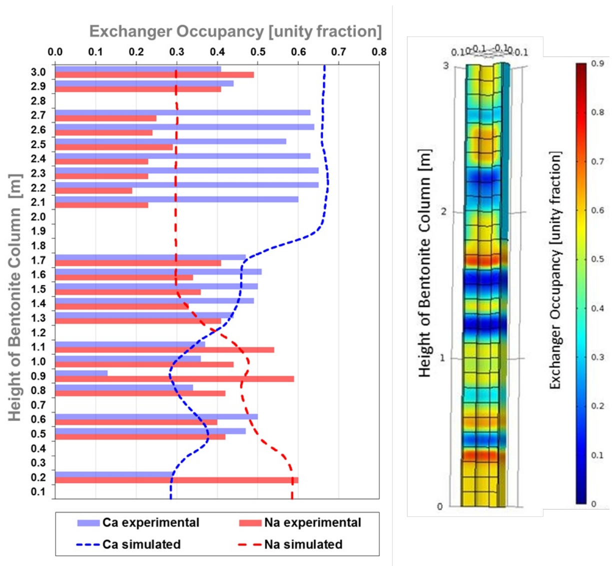


**Figure 1**: Left – example comparison between modelled and experimental (measured) values of Ca and Na unit fraction occupancy on the exchanger after 2.5 years (end of experiment). Right – Na unit fraction occupancy halfway through the simulation (1.25 years).