Reactive transport processes in compacted bentonite
Application to a prototype experiment of underground repository for nuclear waste

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**Introduction**
SKB, Swedish Organization for Radioactive Waste (RW) Management, is in the process of license application for the disposal of RW in a deep geological repository. Bentonite clay is planned to be used around the cylindrical RW packages as buffer material. To assess alternative clay materials, SKB started a field experiment in 2006 [1]. A package of 11 different types of compacted bentonite blocks was saturated and heated to target values, and ran for ~2.5y.

**Conceptual model**
- Initial porewater composition in chemical equilibrium for each clay
- Fickian diffusion of only 5 ionic species: Na⁺, Ca²⁺, Mg²⁺, K⁺ and Cl⁻
- Cation-exchange reactions (based on Gaines-Thomas convention)
- Temperature-diffusion coupling based on experimental data (temperature evolves as a function of time)
- Sensitivity scenarios considered: temperature evolution, boundary conditions (No flow, Dirichlet, combination of both)

**Implementation into Subsurface Flow Module**
- Diffusion using the “Solute Transport” Interface
- Cation-exchange through a system of coupled non-linear algebraic differential equations (solved using Newton-Raphson method)
- Transport-Chemistry Coupling using the approach proposed in [2] and solved using Operator Splitting (Sequential Iterative Approach)

**Model verification**
The RTM implemented in COMSOL was satisfactorily benchmarked against the geochemical software Phreeqc:

![Graph showing comparison of exchange composition for a 1D problem using COMSOL (dashed lines) and PHREEQC (solid lines) after 1 year. Zero and 0.1 m distance correspond to no-flux and Dirichlet boundary conditions, respectively.]

**Numerical results**
In conjunction with a composite boundary type (see figure below) based on fracture logging measurements the simple model is capable of reproducing the experimental data with a reasonably good accuracy, especially for Ca and Na (dominant cations). A relatively poorer fit for Mg is observed in the top (although still unclear, it could be due to additional chemical reactions or altered groundwater composition).

**Conclusions**
- A RTM has been successfully implemented into COMSOL
- The model has proved very useful to gain insight in the experiment evolution and served as a basis for discussion with experimentalists
- Comparison of measured patterns of final exchanger composition with RTM results corroborate the hypothesis of distinct regimes of reactive transport in the top and bottom sections of the bentonite column

**References:**

**Objectives of the modeling study**
1. Verify whether a reactive transport model (RTM) coupling diffusion, cation-exchange & temperature evolution can explain the observed homogenisation of cation-exchanger composition
2. Check the feasibility of implementation of a RTM into COMSOL

**Graph showing Initial (before) and final (after the experiment) exchanger composition in terms of unit fraction Na, Ca, Mg and K occupancy (empty: no data available).**

![Graph showing time evolution of Ca unit fraction on the cation exchanger. The time increases from left (initial state) to right (final state – after 880 days).]

**Graph showing post-mortem analysis: initially contrasting cation-exchanger compositions between bentonite blocks significantly homogenized after 880 days [1]:**

**Graph showing schematic representation of the model domain and its boundaries (blue: no-flux, red: constant concentration).**

**Graph showing installation of the package and initial block distribution.**