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Reactive transport simulations of the evolution of a cementitious repository in clay-rich host rocks

Georg Kosakowski, Urs Berner, and Dmitrii A. Kulik
Paul Scherrer Institut, Department of Nuclear Energy and Safety Research, Villigen, Switzerland (georg.kosakowski@psi.ch)

In Switzerland, the deep geological disposal in clay-rich rocks is foreseen not only for high-level radioactive waste, but also for intermediate-level (ILW) and low-level (LLW) radioactive waste. Typically, ILW and LLW repositories contain huge amounts of cementitious materials used for waste conditioning, confinement, and as backfill for the emplacement caverns. We are investigating the interactions of such a repository with the surrounding clay rocks and with other clay-rich materials such as sand/bentonite mixtures that are foreseen for backfilling the access tunnels. With the help of a numerical reactive transport model, we are comparing the evolution of cement/clay interfaces for different geochemical and transport conditions.

In this work, the reactive transport of chemical components is simulated with the multi-component reactive transport code OpenGeoSys-GEM. It employs the sequential non-iterative approach to couple the mass transport code OpenGeoSys (http://www.ufz.de/index.php?en=18345) with the GEMIPM2K (http://gems.web.psi.ch/) code for thermodynamic modeling of aquatic geochemical systems which is using the Gibbs Energy Minimization (GEM) method. Details regarding code development and verification can be found in Shao et al. (2009).

The mineral composition and the pore solution of a CEM I 52.5 N HTS hydrated cement as described by Lothenbach & Wieland (2006) are used as an initial state of the cement compartment. The setup is based on the most recent CEMDATA07 thermodynamic database which includes several ideal solid solutions for hydrated cement minerals and is consistent with the Nagra/PSI thermodynamic database 01/01.

The smectite/montmorillonite model includes cation exchange processes and amphotheric ≡SOH sites and was calibrated on the basis of data by Bradbury & Baeyens (2002). In other reactive transport codes based on the Law of Mass Action (LMA) for solving geochemical equilibria, cation exchange processes are usually calculated assuming that the clay mineral is represented by a X- "(solute) ligand" initially occupied with e.g. Na^+. Our representation of cation exchange is based on a multi end-member ideal solid solution model for the clay which at the same time considers the chemical reactivity of the clay phase in the high pH cement environment.

As a first application, we will present the results of calculations of the interaction between a cement compartment in contact with a clay-rich host rock.

References:

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