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# Numerical modeling of the evolution of a generic clay/cement interface

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The long-term evolution of interfaces between different materials in deep geological repositories for nuclear waste is governed by geochemical interactions in conjunction with mass and energy transport processes. A key role for the design of the multi-barrier system is the knowledge of long term changes at the interfaces between different materials.

Recently, the GEMS-PSI research package (http://gems.web.psi.ch) for thermodynamic modeling of aquatic (geo)chemical systems by Gibbs Energy Minimization was coupled to the T(hermo)-H(ydro)-M(echanical)-C(hemical) transport code Geosys/Rockflow (http://www.ufz.de/index.php?en=11877). The GEM convex programming approach is complementary to the often-used Law of Mass Action (LMA) approach. It is computationally more expensive than LMA and requires more thermodynamic data, but has advantages for describing complex geochemical environments, like aqueous - solid solution equilibria that include two or more multi-component phases. We believe that the use of GEM method in reactive transport codes is a step towards a more realistic description of complex geochemical systems.

The coupled code was verified by a widely used benchmark of dissolution-precipitation in a calcite-dolomite system, the retardation of radium close to a bentontite/cement interface due to incorporation in solid solutions, and the evolution of a generic clay/cement interface. The reactive transport simulations presented in this work were not adapted to specific cement or clay material compositions. We concentrated on a simplified, generic geochemical model and a simplified, diffusion dominated, setup for the transport. This makes it easier to test the coupling of the codes and investigate the effects of the numerical and conceptual parameters (e.g. discretization) on the evolution of the interface.