# Efficient cross-scale modelling of geochemical interactions for nuclear waste geological disposal

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The accurate description of geochemical interactions, and of the coupled mass and radionuclide transport processes in argillaceous rocks and cement barriers, play an important role in understanding and predicting the evolution of the Swiss radioactive waste repositories and of deep geological systems. The geochemical evolution of the repository is controlled by the mass transport across material interfaces and the in-situ chemical conditions. For example, the precipitation-dissolution of minerals from aqueous solutions alters the pore space and its connectivity in a way that has a complex feedback to the ion transport in aqueous phase itself. At the same time radionuclide migration and sorption in clays is strongly dependent on the nanoscale surface distribution of permanent electrostatic charges a process that governs the radiation exposure in the biosphere in the long term. The prediction of the evolution of the technical barriers and of the repository as a whole requires a fully coupled THMC process and provides essential input for the safety assessment.

Fundamental in-depth understanding and better prediction of the underlying processes can be enhanced by a) cross-coupling atomistic models and direct pore-scale modeling, e.g. molecular dynamics and the lattice Boltzmann (LB) method (Prasianakis 2017, Poonoosamy 2016), b) upscaling of transport mechanisms from the pore-level to the field scale simulators e.g. OpenGeoSys-GEM and c) improving the numerical stability and reducing the computational cost of geochemical calculations which usually represent the major computational costs.

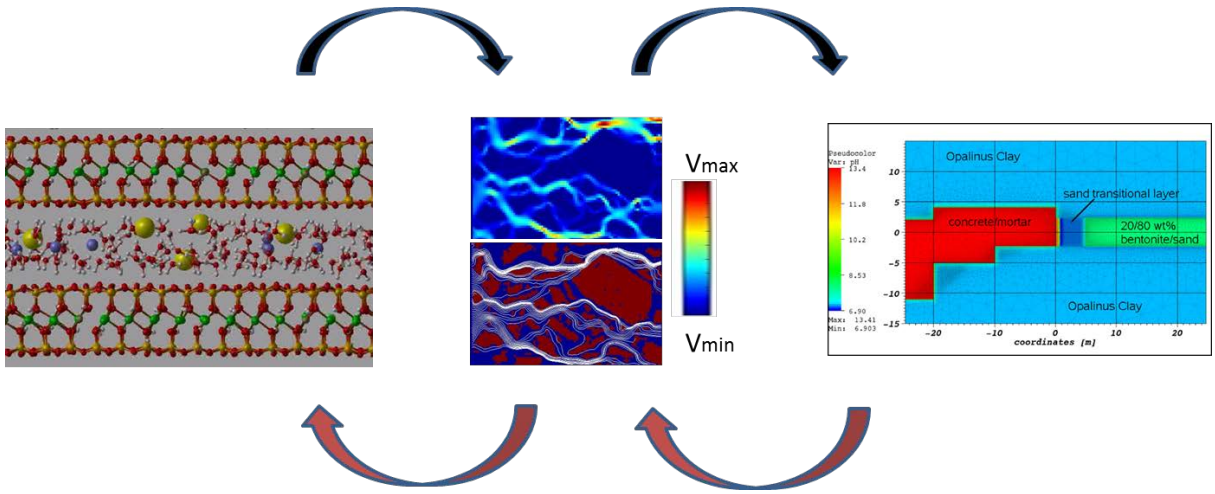


**Fig. 1: Modelling geochemical interactions at different scales. From left to right: molecular dynamics and DFT calculations, lattice Boltzmann pore-level methods and OpenGeoSyS-GEM repository level calculation.**

Molecular dynamics techniques are very powerful in addressing fundamental aspects of diffusive and advective transport of solutes and their retardation (kinetic sorption and sorption competition) in argillaceous rocks and cementitious materials at nano-pore level. Upscaling of results to the micrometer scale heterogeneous poly-mineral rocks has been demonstrated (Churakov 2011). Pore-level microscopic simulations on realistic representations of the actual structures can provide an exact description of porosity evolution and the subsequent effect on the permeability and diffusivity. This in effect allows the derivation of respective correlations that under specific circumstances are more accurate than the generic Kozeny-Carman relationships and Archie's law. Such improved

correlations can pass information to the macroscopic solvers and therefore bridge atomistic, pore-level and macroscopic scales.

For continuum scale calculations OpenGeoSys-GEM is used for the prediction of repository evolution and in-situ conditions. In our method portfolio the newly developed code that combines FEniCS (Alnæs 2015), a finite element solver framework, and the state-of-the-art chemical equilibrium solver Reaktoro (Leal 2016) to model electrochemical transport across reactive interfaces is added. The Nernst-Planck reactive transport solver (NPS) was successfully validated using several benchmarks.

## References


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