Implementing an explicit diffuse layer in reactive transport simulations by using the Nernst-Planck equation

P. ALT-EPPING, T. GIMMI, P. WERSIN, A. JENNI

Institute of Geological Sciences, RWI-Group, University of Bern, Baltzerstrasse 3, CH-3012, Bern, Switzerland, alt-epping@geo.unibe.ch

Bentonite clay is considered as backfill/buffer material for underground repositories. When in contact with water, bentonite begins to swell, thus filling voids in the backfilled underground facility and, owing to its high swelling pressure and low permeability, forming an effective barrier to advective groundwater flow. Thus solute transport in bentonite is dominated by diffusion.

Bentonite clay is composed predominantly of montmorillonite with few accessory minerals. One important characteristic of montmorillonite crystals is their negative surface charge. The effective diffusion coefficient of an ion in bentonite depends on the pore structure of the bentonite as well as on the electrostatic properties of the dominant clay minerals, the polarity and valence of a specific ion as well as on the ionic strength of the solution. In reactive transport simulations the electrostatic effects of clay surfaces on ion transport are commonly implemented via a Donnan equilibrium formulation. A recent benchmark proposal by Alt-Epping *et al.* [1] has shown, that the Donnan approach is appropriate to reproduce experimentally determined breakthrough curves of ions in a bentonite core.

Here we us an approach first proposed by Gimmi [2] to simulate reactive transport in a bentonite involving Donnan equilibrium which is based on the Nernst-Planck equation and does not explicitly solve for Donnan equilibrium. We use this approach to rerun the benchmark proposal by Alt-Epping *et al.* [1] and to test the implications of two underlying assumptions of the explicit Donnan formulation: 1) the same activity coefficients in and 2) instantaneous diffusive equilibrium between the free water and the EDL pore water. In additional simulations we apply this method to the multibarrier KBS-3 repository design developed by Posiva (Finland) and SKB (Sweden) to determine sulphide fluxes released from the bentonite backfill which could cause the corrosion of copper canisters containing the spent fuel.

[1] Alt-Epping, *et al.* (2014) Computational Geosciences. doi:10.1007/s10596-014-9451-x. [2] Gimmi, T. (2016) Simulating Donnan equilibria in clays based on the Nernst-Planck equation. (in prep.)