

Electrostatic effects and reactive transport in different clay materials: observations and modelling approaches

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Clayrocks and engineered clay-based materials play a key role in many planned deep geological radioactive waste repositories as host rock or in the engineered barrier. Therefore, transport of solutes in clay must be understood, whatever their origin: naturally abundant solutes in a sequence of geological formations, dissolved species from the engineered barrier, or radionuclides escaping from the waste itself. The negative charge of clay surfaces leads to an inhomogeneous distribution of anions and cations in the saturated pores. Different porosity domains (e.g., diffuse layer on clay grains, interlayer, charge balanced “free” porewater) exhibit different diffusive and advective transport properties. Experimental data on transport in clay show a dependence on porewater composition. This can be explained and modelled with the concept of different porosity domains that dynamically adapt to the porewater, volume changes of reacting minerals, and any mechanical effects.

Tracer transport across different (clay) lithologies can in principle be modelled with a single-component and single-porosity approach, provided an accessible porosity of the tracer for each lithology can be approximated and no significant changes of the pore structure occur.

Diffusive and advective-diffusive laboratory experiments with different clayrocks and porewaters give evidence for a dependence of the transport-accessible porosity fraction on the porewater composition. In extreme cases (e.g., cement-clay interaction), the free porosity may clog completely, but cations still diffuse in the anion-depleted porosity domain, if a cation gradient exists across the clogged zone. Modelling such processes requires coupled multi-porosity, multi-component codes considering electrostatic effects and electrochemical migration.

Transport in saturated swelling clays depends on density and related swelling pressure in addition to the couplings mentioned above. Accordingly, a reactive transport model for instance for bentonite in contact with other materials needs to consider chemo-mechanical coupling as well.

Examples of experimental observations and coupled reactive transport modelling are presented, and related questions are discussed.

Figure: Breakthrough of different species during an advective-diffusive transport experiment with Opalinus Clay. Why do the water tracers break through more slowly than the anions? Which

processes cause the minor but generally observed differences between the two monovalent anionic species, and possibly between the water tracers?

