

## Reactive transport in compacted bentonite: porosity concepts, experiments and applications

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### Porosity concepts and scales

Chemical and transport processes in compacted bentonite are operating at the nanometer scale of smectite interlayers but cannot be resolved at this scale by analytical or imaging techniques. Porosity concepts are treated as macroscopic averaged properties but are based on the microscopic scale using electrostatics and explicit or averaged Poisson-Boltzman theory for the distribution of electrolyte species adjacent to mineral surfaces bearing permanent charge. Implementation into reactive transport numerical models is debated, ranging from an averaged single-phase solid-liquid electrolyte [1] to complex multi-porous models assigning transport parameters specific to each type of porosity [2]. Here, we examine the relative merits and limitations of different multi-porous models as applied to experimental data of various complexity.

### Reactive transport modelling of experimental data

A long-term multi-component advective-diffusive reactive transport experiment with compacted bentonite can be modelled satisfactorily with either a dual porous concept (small proportion of charge-balanced “free” electrolyte, large proportion of interlayer-type electrolyte with Donnan approximation), or more complex model assigning separate porosities to the interlayers and a pore space close to external surfaces of smectite particles. Transport of the solvent was additionally constrained by a D<sub>2</sub>O tracer.

Modelling of short-term simple major-component through-diffusion experiments is not discriminating between models of various complexity and leads to a strong dependency of transport coefficients on the porosity concept.

PHREEQC and Crunchflow were used as numerical models, both capable of treating multiple porosities, electrostatics in the form of diffuse-layer theory, and species-specific and porosity-specific transport properties.

**References** [1] Birgersson M. & Karnland O. (2009) *Geochim. Cosmochim. Acta*, **73**, 1908-1923. [2] Tournassat C. & Appelo C.A.J. (2011) *Geochim. Cosmochim. Acta*, **75**, 3698-3710.

## Modeling Eu(III) sorption on granite

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There have been very few researches for the trace elements sorption on complex mineral assemblages such as rocks, sediments and soils. In order to make predictions for the trace elements migration on geologic media, it is crucial to understand the nano-scale interaction of trace elements with complex mineral assemblages, and to construct the thermodynamic sorption models based on the molecular-scale information. In the present study, the batch sorption experiments of Eu(III) on granite were conducted as function of pH and ionic strength. The sorption behavior was modeled based on our microscopic observation (Hasegawa et al. this volume).

The granite sample was collected from a borehole at a depth of 400 m from the Mizunami Underground Research Laboratory constructed by Japan Atomic Energy Agency in central Japan. The granite was visually fresh. However, the microscope observation and the X-ray diffraction analysis of clay fraction show the occurrences of smectite, chlorite, vermiculate, calcite and hydrous iron oxides. Eu(III) sorption experiments on granite in the Teflon vessels were conducted as function of pH (2 to 8), ionic strength (I=0.01 and 0.1) and Eu concentration (1 and 10 μM) under ultra-pure N<sub>2</sub> atmosphere in room temperature.

The experiments and modeling results are shown in the Figure. Sorption ratio of Eu(III) was almost zero at pH 2. They abruptly increase with pH up to 3.5. Above pH 3.5, the sorption ratio indicates almost constant. The sorption strongly depends on ionic strength at the pH more than 3.5. Our microscopic observations show that Eu(III) is selectively scavenged by biotite and that sorption mode of Eu(III) is identified to be exchange reaction with inter-layer K in biotite and Eu(III). The sorption behaviors at pH more than 3.5 are consistent with the cation exchange reaction. At low pH conditions, less than pH 3.5, the release of the Al and/or Fe must occur with dissolution of minerals. The Al and/or Fe should be competed with Eu(III) on the exchange site of biotite. The sorption modeling is simply considering ion exchange reaction and solubility of hydrous iron oxide. The model reasonably reproduces the overall sorption behavior.

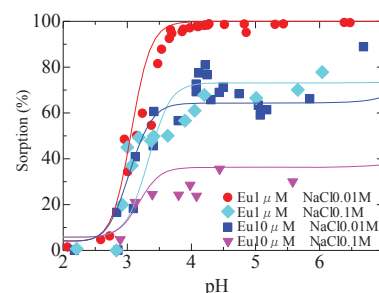


Fig. Sorption behavior of Eu(III) on granite

**Ref.:** Y. Hasegawa, K. Fukushi, K. Maeda, Y. Yamamoto, D. Aosai and T. Mizuno: “Identification and characterization of phase governing Eu(III) uptake in granite by microscopic observations”, In this volume