Eu(III) reactive transport modeling: The "smart-K_d" appraoch

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Spatially and temporally constant sorption coefficients (K_d -values) are currently applied in transport codes for long-term safety analysis of radioactive waste repositories. However, temporally and spatially variable geochemical conditions occuring in natural systems may lead to significant changes in sorption processes of e.g. radionuclides (RN). To account for changing geochemical conditions such constant K_d -values are replaced by so-called "smart K_d -values" which consider the impact of varying geochemical parameters on the sorption behaviour of long-term safety relevant elements; inter alia pH, pCO₂, ionic strength, complexing ions.

We present an overview of the state-of-the-art "smart- K_d " approach to model RN migration with the coupled reactive transport code d^3f ++ [1, 2]. The smart K_d -concept aims to describe complex geochemical and mineralogical systems through detailed geochemical characterization of major components referred to as component additivity approach.

To verify the developed concept, column experiments were conducted to investigate Eu(III) transport processes. Eu(III) serves as a homologue for long-term safety relevant trivalent actinides, e.g. Cm(III) and Am(III). We investigated transport processes through quartz, mica, and feldspar minerals which are ubiquitously presend in Northern Germany. Experiments were conducted in mono-mineral systems and more complex sediments thus covering a variety of geochemical conditions.

We illustrate first results of Eu(III) reactive transport models using the geochemical speciation code PHREEQC [3]. Surface complexation parameters were determined by batch and titration experiments, CXTFIT [4] was applied to assess initial estimates of effective transport parameters. Our analysis provides a comparison of the smart- K_d approach with conventional K_d -values and offers a valuable insight into transport processes of trivalent rare earth elements which are of great relevance for nuclear waste disposal but also in the areas of solar panel construction and wind turbines.

[1] Schneider *et al.* (2016) GRS-392, in press. [2] Noseck *et al.* (2012) GRS-297, 293 pp. [3] Parkhurst, Appelo (1999) U.S. Geological Survey, 312 pp. [4] Toride *et al.* (1999) U.S. Salinity Laboratory, Report No. 137, 118 pp.