MODELLING Ni(II) SORPTION IN GRANITIC GROUNDWATER

M.E. MALMSTRÖM[1,2], E. DOCAMPO CABALEIRO[1]
AND S. REGENSPURG[1]

[1] Industrial Ecology, Royal Institute of Technology (KTH),
    SE-1004 Stockholm, Sweden;
[2] malmstro@ket.kth.se

Retention by sorption on to geological materials constitutes a potentially important barrier for radionuclide migration in case of failure of deep repositories for radioactive wastes. Due to the inaccessibility of the geosphere for characterization and the extremely long time perspectives of these deposits, modelling constitutes an important path for assessing pollutant fate in case of release to the groundwater.

In current reactive-transport models for radionuclide migration, the geochemical retention processes are commonly quantified through site-specific conditional K_d-values. However, process-based models are expected to have a larger predictive capability and to apply over a wider range of geochemical conditions than K_d-based models. For sorption, such models explicitly handle the dependence of K_d on ionic strength, pH, E_h, and speciation of the tracer, as well as effects of surface saturation and competition between different metal ions for the surface sites.

In this study, we model Ni^{2+} sorption (representing the radionuclides ^{63}Ni and ^{59}Ni) onto the geological material typically found in the vicinity of a fracture in the granitic rock at the Äspö Hard Rock Laboratory in southern Sweden, including gouge material, fracture coatings, alteration zones, and the fresh host rock. We use a Component Additive (CA) approach for surface complexation [1], where the sorption properties of the rock are assumed to be a linear combination of those of the minerals in the rock, weighted by their volume fractions. We quantify the sorption reactions using a Non Electrostatic Model (NEM) [1] in combination with published sorption data for Ni^{2+} on pure minerals.

We show that site specific model predictions of K_d-values reasonably well agree with published, experimental values for granite from the vicinity of the Äspö HRL. Despite the presence of clay and iron (hydr)oxide minerals in the granite, model results indicate chlorite and biotite to be dominating the Ni^{2+} sorption. We identify important lack of sorption data for pure minerals and of specific surface area for granitic materials. Using the PHREEQC and the PHAST reactive-transport codes [2], we compare results from K_d-based and surface complexation-based geochemical models, for identical pollution and transport scenarios in the fracture.

References
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