Surface complexation modelling: Sorption of Ni on quartz and orthoclase

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Retardation processes such as radionuclide sorption on mineral surfaces are of high relevance in long-term safety assessments of radioactive waste repositories. Spatially and temporally variable geochemical conditions may lead to significant changes in sorption behaviour of radionuclides. To address this in reactive transport codes the smart-K_d-concept (www.smartkd-concept.de) has been developed [1]. For this purpose mineral and element specific thermodynamic sorption data are required.

In the present study, batch experiments were conducted to investigate sorption processes of Ni on natural quartz and orthoclase minerals under varying geochemical conditions: pH 5-8, 0.01, 0.2 M $NaClO_4$ and 0.066 M Na_2SO_4 background solution, initial concentration $C_{(Ni,\ 0)}$ of 5×10^{-7}, 10^{-6}, 10^{-5} mol L^{-1} Ni and solid-liquid-ratios in a range of 25 to 200 g L^{-1}. Non-radioactive Ni was used as a suitable chemical equivalent of Ni-59, which is a long-lived activation product in radioactive waste, and is hence relevant for long-term safety assessments [1].

PHREEQC [2] coupled with UCODE [3] is applied to determine so-called surface complexation parameters (SCP) via the adaption of mechanistic surface complexation models. Ni surface complex formation constants (logK-values) are estimated for selected surface species by means of inverse modelling using the collected batch sorption data.

Sorbed Ni fractions show significant dependencies on pH, $C_{(Ni,\ 0)}$ and solid-liquid-ratios. In terms of quartz and orthoclase log K_d-values range from -1.2 to 2.0 and -0.8 to 2.8 L kg^{-1}, respectively. Moreover, results show a disctinct impact of ionic strength and no influence of sulfate as a ligand on Ni sorbed fractions on both minerals.

Batch experiment and surface complexation modelling results of Ni batch sorption data will be discussed.

[1] Noseck et al. (2012), GRS-297, 293 p. [2] Parkhurst & Appelo (2013), Techniques and Methods 6-A43, 497p. [3] Poeter et al., (2008), Techniques and Methods 6-A11, 283 p.