

# Modeling radionuclide sorption for crystalline rocks using real samples: Challenges and sources of uncertainty

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In a deep geological repository for nuclear waste, the host rock forms the outermost shell of the multi-barrier system designed to prevent toxic radionuclides from reaching the biosphere and subsequently the food chain. As a natural material, this host rock is characterized by heterogeneities, anisotropies, and different types of fluid pathways. Accordingly, the prediction of radionuclide (RN) migration through the host rock is complex and subject to large uncertainties. Besides salt and clay rocks, crystalline or granitoid rocks can also be considered as host rocks. There, joints and fracture network are very important parameters for the estimation of RN migration. However, microcracks or spatial variability in the mineral composition, especially with respect to exposed mineral surfaces along fluid migration paths, can also significantly increase the uncertainties of the sorption capacity of the host rock. Another important uncertainty component is the scarcity of RN sorption data, namely for mafic minerals like the Biotite group or Amphiboles. Often one has to resort to analogues. Thus, for the calculation of distribution coefficients ( $K_d$  values, see the Smart  $K_d$  concept [1]) for a given combination of RN and rock formation, the results depend both on the knowledge of which mineral phases are actually exposed to pore water (as opposed to average rock compositions) and on the sorption models used.

In our contribution, we present a workflow to use geologic samples to capture the heterogeneity of mineral composition along pathways using an approach from graph theory. Data of these spatially variable mineral compositions obtained from real samples are then used as input parameters for the calculation of  $K_d$  values of uranium. The geochemical modelling was based on background data from sorption and surface complexation models. Furthermore, we show the uncertainties that can arise from measurement artifacts or (incomplete or missing) sorption data for certain mineral phases, especially at different pH levels. This, in turn, paves the way for corresponding sensitivity analyses indicating which input parameters deserve highest priority in future research efforts.

[1] Stockmann et al., Chemosphere. 187 (2017) 277–285. [www.smartkd-concept.de](http://www.smartkd-concept.de)