

Identifying important parameters in radionuclide retention in crystalline host rocks: Key findings through establishing a geostatistics-based workflow

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The long-term safety of deep geological repositories for nuclear waste depends on its retention capacity for radionuclides. One barrier part is the host rock, also called the far field. In this study we focus on crystalline rocks as one potential host rock type. A critical aspect of risk assessment is understanding how lithological characteristics and petrological heterogeneity influence radionuclide retention and migration. While simplistic models often assume homogeneous granite, natural crystalline formations exhibit complex mineralogical and structural variations, particularly near intrusion margins and within metamorphic units. These heterogeneities, along with the spatial variability of mineral occurrence and distribution, significantly impact radionuclide sorption and transport behavior.

This study builds upon the SANGUR project (Systematic Sensitivity Analysis for Mechanistic Geochemical Models using Field Data from Crystalline Rock), which integrates geostatistics, geochemical modeling, sensitivity analysis, and experimental data to render radionuclide retention models more realistic. The overall aim is determining which parameters in rock and geochemical modeling are essential, which are secondary but still influential, and which can be reasonably ignored by simplifying (sub)models. This aim is challenged by the inherent uncertainties in mineralogical compositions, fluid chemistry, and sorption processes and also that many parameters rely on estimations and assumptions to fill knowledge gaps.

To address this challenge, we developed a workflow that allows to systematically test through a sensitivity analysis framework how variations in geostatistical rock modeling and different set ups for geochemical simulations influence the calculated K_d value. This approach enables us to assess the relative importance of broad variety of parameters (thermodynamic reaction constants, pore water composition, mineralogical contents) and quantify their influence on radionuclide retention in crystalline host rocks. In this contribution, we will highlight key issues encountered during the development of this workflow, including challenges in parameter selection, uncertainty quantification, and model validation. Additionally, we will present insights gained from applying the workflow to modeled real datasets, demonstrating how sensitivity analysis refines our understanding of radionuclide behavior in geologically complex settings.