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Reactive Transport of Cesium in Granodiorite: Estimation of Diffusion Coefficients and In-situ Cation Exchange Capacity

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In November 2024, the Nuclear Waste Management Organization (NWMO) selected a granodiorite-tonalite host-rock for a Deep Geological Repository (DGR) for long-term storage of Canada's used nuclear fuel. The host rock for any DGR should be a natural barrier to migration of radionuclides, so it must have low permeability, and the diffusion and reaction properties must be well characterized. By reaction properties, we refer to the tendency for minerals exposed in the pore space of the rock to provide reactive surface sites for attenuation of radionuclides by sorption reactions, specifically, ion exchange and surface complexation. The premise for this study is that a rock's cation-exchange capacity (CEC) is a measure of surface reactivity, and our objective is to estimate the CEC for intact 'granitic' rocks.

Diffusion-reaction experiments were conducted with five cylindrical rock cores (20 mm diameter, 20 mm long) mounted in cells that allow diffusion of a CsCl tracer from bottom to top of the vertical rock cylinders. Diffusion of Cs^+ upward from the lower boundary was monitored in one dimension at one- to two-day intervals using X-ray fluorescence, ending with breakthrough of the tracer at the top boundary. MIN3P was used with the Parameter Estimation code, PEST, to simulate the reactive transport (diffusion + ion-exchange) and estimate the pore diffusion coefficient for Cs^+ (D_p) and the CEC of the rocks.

$D_p = D_0 \times T_f$, where:

D_0 is the free-water diffusion coefficient

T_f is the tortuosity factor ($0 < T_f < 1$)

The X-ray fluorescence data define coherent diffusion profiles for relative concentrations, with C/C_0 values for Cs^+ near the influx boundary that are > 1.0, demonstrating mass accumulation by sorption on the surface of minerals. The estimated D_p values range from 3.33×10^{-11} to 9.33×10^{-11} m^2/s and the CEC values range from 2.20×10^{-3} to 9.92×10^{-2} meq/100g, which are consistent with data obtained from an independent approach. The combined use of reactive transport simulations and parameter estimation represents an effective approach to uniquely determine the diffusion coefficient for a reactive solute and the CEC for intact, low-porosity rocks.