Modeling the DR-A in-situ diffusion experiment (Opalinus Clay): Ionic strength effects on solute transport

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In DR-A (Mont Terri URL, CH), synthetic porewater (NaCl-dominated, I = 0.36) containing tracers was circulated through a borehole for 189 days, after which it was replaced with a higher-salinity solution (0.50 M NaCl + 0.56 M KCl) for an additional 540 days, with effects such as the back-diffusion of Cs^+, Ca^{2+}, Mg^{2+} and Sr^{2+} to the borehole resulting from desorption and an increase in the out-diffusion of anions (I^-, Br^-) and also of ^3H (Fig. 1). Modeling has been performed by several teams. CrunchFlowMC, which includes the calculation of the electrical double layer (EDL) on the charged clay surfaces causing anion exclusion and cation excess, together with species-specific diffusion (Nernst-Planck equation), was used here. A 1D radial diffusion model considered a single pore diffusion coefficient (D_p) for cations and ^3H in the bulk porosity, and a smaller D_p for anions. D_p values in the EDL were smaller by ca. an order of magnitude except for Cs^+, which needed a larger D_p. Calculations considered all species in a single run. The model reproduced well back-diffusion of cations due to desorption, and the increase in the out-diffusion of anions and ^3H due to the decrease in EDL porosity with increase in ionic strength.

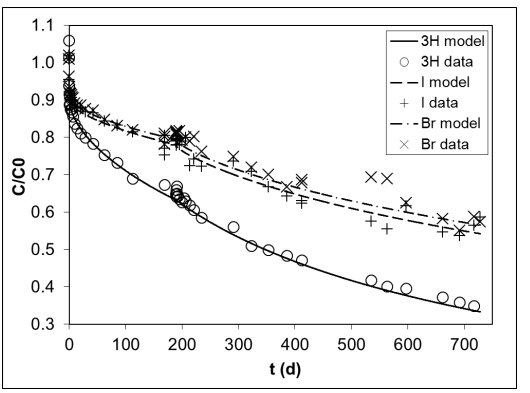

Figure 1: Relative concentrations in the borehole vs. time.