# Modelling transport of sorbed species in clays

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**Abstract**

Due to their low permeability clays are often used as barrier material for waste disposal sites. Migration of contaminants or radionuclides through such clay barriers occurs mainly by diffusion and is affected by (multi-site) sorption processes. The evaluation of diffusion experiments often results in higher diffusion coefficients for cations than for water tracers, especially when sorption is high. This observation cannot be explained consistently by the classical Fickian diffusion concept as implemented typically in transport codes. In order to account for the discrepancy between models and experimental data the concept of surface diffusion was introduced. Surface diffusion accounts for a (full or partial) mobility of sorbed cations, which thus contribute to the overall mass flux. Claysstones such as Opalinus Clay, a formation considered as potential host rock for disposal of radioactive waste, exhibit different sorption sites. Cations sorbed on these sites may contribute differently to the overall observed surface diffusion. To adequately model transport of cations in clays a generalized multisite surface diffusion model[1] is implemented in the reactive transport code FLOTRAN[2]. The model lumps pore and surface diffusion together in one single diffusion coefficient including ion- and site-specific surface mobilities as model parameters. The surface mobilities indicate how mobile sorbed cations on a given site are compared to those in pore water and are not a priori known. In a first step the surface diffusion model is applied to Caesium in-diffusion data in Opalinus Clay with a range of Cs concentrations from $10^{-2}$M to $3.5 \cdot 10^{-8}$M. Cs strongly sorbs onto Opalinus Clay and its sorption behaviour can be described by a three site cation exchange model[3]. Results show that the Cs data can be modeled well over the whole concentration range with one set of surface mobilities, which are used as fitting parameters. The surface diffusion model for Cs with the obtained surface mobilities is now tested against other experimental data in order to evaluate its ability for prediction of Cs diffusion in Opalinus Clay across a wide range of Cs and background solution concentrations.

**References**

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