A robust and parsimonious model for caesium sorption on pure clay minerals and natural clay materials

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A generic model for Cs sorption onto clays

Published experimental data and models for caesium sorption by pure minerals and natural clay materials were compiled and critically analyzed in an attempt to propose a generic approach. This analysis led to the construction of a new mechanistic model for Cs sorption, which combines surface complexation and cation exchange approaches involving two distinct types of surface sites, frayed edge sites (SO -0.5) and planar sites (X). This model takes into account the cation competitions, as well as the effect of ionic strength and pH. We evaluated our model against Cs sorption data for three reference clay minerals (illite, smectite and kaolinite) and on natural clays materials (e.g. Callovo–Oxfordian Claystones, Hanford sediment) measured under a range of physico-chemical conditions.

Results showed that our model successfully reproduces most of these experimental data both qualitatively and quantitatively. The model account for varying levels of Cs interactions with pure and natural clay substrates, without making any prior adjustment of parameters, offering a major advantage over previously developed models (Fig. 1).

Figure 1: Comparison between Cs sorption models (as Root Mean Square Error (RMSE) and R²)