

How to experimentally improve the predictive capacity of adsorption models of solutes on swelling clays ?

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This presentation will present some perspectives to improve the predictive capacities and/or the validity of the input parameters of models describing adsorption/ion-exchange reactions of inorganic solutes on swelling clay minerals.

Illustration will show that the fact to know the exact morphology of the clayey particles allows to fix in the models the distribution and amount of the different adsorption sites (interlayer *vs* external), and then improve model's robustness. Particle morphology, associated to different physico-chemical parameters of the solution (ionic strength and solid/solution ratio), is known to impact also drastically the organisation of the clay/water system. Such information can be qualitatively assessed from small angle X-ray scattering data [1] and can confirm or not the assumption which is generally made consisting to use the same distribution of sorption sites all along adsorption isotherms [2]. Then, an illustration will show that X-ray diffraction can be used to obtain quantitative information about the reactivity of a specific site (i.e., interlayer sites), and coupled with bulk chemistry analysis to discriminate the properties of the different types of site [1]. Finally, by controlling the hydration state of the particles in water saturated conditions, we will show that interlayer selectivity coefficient obtained from classical batch experiments, associated to self-diffusion coefficients issued from molecular dynamic simulations, can predict correctly diffusion experimental data [3].

[1] Tertre et al. (2011) *J. Colloid Interface Sci.* **363**, 334-347. [2] Robin et al. (2015) *Appl. Geochem.* **59**, 74-84. [3] Tertre et al. (2015) *Geochim. Cosmochim. Acta* **149**, 251-267.