Diffusion in clays: molecular scale view, continuum scale modeling and importance of microstructure.

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Clay barriers and clay-rocks show a remarkable array of macro-scale properties of interest for high-level radioactive waste management. In clays, small pores hinder water flow and make diffusion the dominant solute-transport mechanism. Most clay mineral structures also exhibit a negative charge that is balanced by an electrostatic diffuse layer at the mineral surface-water interface. This clay mineral property delays cation migration through adsorption processes, decreases the accessible porosity and diffusion fluxes for anions compared to water and cations, and gives rise to semi-permeable membrane properties. While the processes at work are well acknowledged, it is clear nonetheless that there is a need for an improved understanding of how the chemical and mineralogical properties of clay rocks impacts transport through them.

It is at the pore-scale that the chemical properties of clay minerals become important since their electrostatic properties can play a large role. Since the prediction of adsorption and diffusion in clay-rich media is complicated by the similarity between the width of clay nanopores and the thickness of the electrical double layer, it is especially important to build macroscopic continuum models that takes into account as much constraints as possible from molecular and pore scales approaches. This presentation will highlight recent advances in this field, and will show why a detailed characterization and description of the microstructure is necessary to develop accurate predictive diffusion models for clay media.