Diffusion in clays. Continuum and micro-continuum approaches

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The properties of clays have been the subject of longstanding study for several important subsurface energy-related applications. While the low permeability and high adsorption capacity of clay minerals are widely 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. Numerical methods for modeling diffusion processes in clay media with the consideration of the presence of a diffuse layer have met a growing interest in diverse communities in the past years. Information on diffusivity has been sought at the molecular level for the smallest pore sizes, i.e. the interlayer nanopores, and this information has been used to draw a consistent picture of diffusion processes at the mesoscale using up-scaling approaches and pore-scale modeling techniques. These approaches are, however, not yet applicable to the modeling of "laboratory scale" experiments, or to large temporal and spatial scale modeling exercises where numerous coupling with the materials reactivity must also be taken into account. In this respect, reactive transport modeling approaches have the significant advantage to be able to handle complex geometries and chemistry, heterogeneities and transient conditions. In this presentation, we will highlights recent developments of reactive transport modeling that makes it possible to tackle problems on diffusion processes coupled to geochemical reactions at the continuum and the micro-continuum scale.