Modeling of coupled processes in nanoporous media. From molecular dynamics information to reactive transport modeling

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The physical and chemical properties of nanoporous media are notoriously difficult to characterize. This is especially true for their bulk fluid transport properties and their chemical reactivity. Because of the large specific surface area of these materials, most of the fluid volume in nanoporous media is influenced by the close vicinity of mineral surfaces, which explains the very low transmissivity of these materials. As a result, the experimental characterization of their permeability requires special techniques. Also, the large specific surface area of nanoporous material provides them with very high adsorption capacity. The strong adsorption and resulting confinement of many contaminants by nanoporous material make them ideal for use in natural or engineered barrier systems, but in turn, a good understanding of their chemical reactivity coupled to their transport properties is necessary to predict the long-term evolution of these properties as a function of a range of physical and chemical conditions. In this regard, reactive transport modeling can help bridge the gap between current process knowledge and predictions of the long term evolution of natural and engineered nanoporous materials in geological and industrial settings. However, nanoporous media exhibit a remarkable array of macro-scale properties with marked departures from those observed in conventional porous media such as permeable aquifers, for the study of which reactive transport models and codes have been historically developed. These properties arise from the interactions of charged nanopore surfaces with water and solutes. The presence of an electrostatic potential field at the surface–water interface and of the so–called diffuse layer leads to coupling between flux terms. Reactive transport models have been developed recently to take into consideration the presence of this diffuse layer. In this presentation, we will show how some of the parameters that describe the properties of the diffuse layer porosity can be rooted in small scale information gained from molecular scale modeling methods.