Coupling clay swelling properties to hydro-geochemical conditions: a reactive transport modeling approach

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The mineralogical and chemical properties of clays have been the subject of longstanding study for the long-term disposal of nuclear wastes in geological repositories. The low permeability of clay materials, including shales, provides at least part of the safety functions for radionuclide contaminants confinement. From a geochemical and mineralogical point of view, the high adsorption capacity of clay minerals adds to the effect of low hydraulic conductivities by greatly increasing the retardation of radionuclides and other contaminants, making clays ideal where isolation from the biosphere is desired. While their low permeability and high adsorption capacity are widely acknowledged, it is clear nonetheless that there is a need for an improved understanding of how the chemical and mineralogical properties of shales impact their macroscopic properties. It is at the pore-scale that the chemical properties of clay minerals become important since their electrostatic properties can play a large role. The negative electrostatic potential field at the clay mineral surfaces results in the presence of porosity domains where electroneutrality is not achieved: cations are attracted by the surfaces while anions are repulsed from them, resulting in the presence of a diffuse ion swarm – or diffuse layer. Numerical methods for modeling macroscopic properties of clay media with the consideration of the presence of a diffuse ion swarm have met a growing interest in diverse communities in the past years. In this presentation we will highlight the complex interplays of mineralogical, chemical and microstructural characteristics of clay materials that are ultimately responsible for a remarkable array of coupled macro-scale properties, including swelling. A coupling scheme for predicting swelling pressure as a function of chemical conditions will be presented in the framework of a reactive transport modeling approach.