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Modeling multicomponent ionic transport in charged porous media: Multi-continua approach and numerical experiments in heterogeneous sandy-clayey domains

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Low-permeability media are important in many subsurface systems and engineering applications including natural geologic formations, radioactive waste repositories, contaminant transport, and groundwater remediation. Owing to the presence of charged mineral surfaces, such materials can exert a key control on the distribution and movement of charged contaminants and major groundwater ions in porewater. Despite increased recognition of charge-induced electrostatic effects during multicomponent ionic transport in porous media, these processes have not been extensively studied in the context of reactive contaminant transport in groundwater. One possible reason is associated to the unavailability of such mechanisms in conventional solute transport codes.

In this study, we present a multi-continua-based multidimensional reactive transport code (MMIT-Clay), which is capable to accurately capture charge effects during ionic transport in the free water, diffuse layer, and interlayer water of charged porous media [1], and numerical experiments exploring the coupled effects of heterogeneous distribution of physical, chemical, and electrostatic properties on reactive contaminant transport in field-scale groundwater systems including spatially distributed clay zones. The modeling approach is based on a Donnan approximation for the simulation of diffuse layer processes, and the Gaines–Thomas convention for the interlayer processes, whereas the diffusive/dispersive fluxes within each subcontinuum are calculated solving the Nernst–Planck equation while maintaining a net zero–charge flux. Furthermore, the proposed code involves a coupling with the geochemical code PHREEQC, by utilizing the PhreeqcRM module, thus enabling great flexibility to access all PHREEQC's reaction capabilities. The code is used to perform a series of numerical investigations in three distinct heterogeneous sandy-clayey domains with different levels of complexity [2]. In each domain, reactive transport simulations were performed focusing on both forward and back diffusion through the sandy-clayey interfaces. The results illuminate the control of microscopic electrostatic mechanisms on macroscopic mass transfer. Coulombic interactions in the clay's diffuse layer can significantly accelerate or retard a particular species depending on its charge. Neglecting such processes can lead to substantial over- or underestimation of the overall transport behavior.