

A Three-Scale Model of pH-Dependent Flows and Ion Transport with Equilibrium Adsorption in Kaolinite Clays: I. Homogenization Analysis

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Abstract A new three-scale model to describe the coupling between pH-dependent flows and transient ion transport including sorption phenomena in kaolinite clays is proposed. The kaolinite is characterized by three separate nano-micro and macroscopic length scales. The (micro)-scale consists of micro-pores saturated by an aqueous solution containing four monovalent ionic species (Na^+ , H^+ , Cl^- , OH^-) and charged solid particles surrounded by thin electrical double layers. The movement of the ions is governed by the Nernst-Planck equations and the influence of the double layers upon the flow is dictated by the Helmholtz–Smoluchowski slip boundary condition in the tangential velocity. In addition, sorption interface conditions for ion transport are postulated in the sense of Auriault and Lewandowska (Eur. J. Mech. A 15:681–704, 1996) to capture the immobilization of the ions in the electrical double layer and on particle surface due to protonation/deprotonation reactions. The intensity of sorption relative to diffusion effects is quantified by the Damköhler number, whose order of magnitude is estimated by invoking the nanoscopic modeling of the thin EDL based on Poisson–Boltzmann problem for the local electric potential coupled with a non-linear surface charge density with constitutive law dictated by the protonation/deprotonation reactions. The two-scale nano/micro model including sorption and slip boundary condition is homogenized to the core scale leading to a derivation of macroscopic governing equations.

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