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RESEARCH PAPER

A three-scale model for pH-dependent steady flows in 1:1 clays

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Abstract A new three-scale model to describe the coupling between electro-chemistry and hydrodynamics in non-swelling kaolinite clays in steady-state conditions is proposed. The medium is characterized by three separate nano-micro and macroscopic length scales. At the pore (micro)-scale the portrait of the clay consists of micropores saturated by an aqueous solution containing four monovalent ions (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 hydrodynamics is modeled by a slip boundary condition in the tangential velocity governed by the Stokes problem. To capture the correct form of the interface condition we invoke the nanoscopic modeling of the thin electrical double layer based on Poisson–Boltzmann problem with varying surface charge density ruled by the protonation/deprotonation reactions which occur at the surface of the particles. The two-scale nano/micro model is homogenized to the macroscale leading to a precise derivation of effective governing equations. The macroscopic model is discretized by the finite volume method and applied to numerically simulate desalination of a clay sample induced by an external electrical field generated by the placement of electrodes. Numerical results indicate strong pH-dependence of the electrokinetics.

Keywords Electrical double layer · Electrokinetics · Homogenization · Kaolinite · Nernst–Planck · Poisson–Boltzmann · Protonation reactions

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1 Introduction

Electrokinetic phenomena in electrically charged porous media have received considerable attention with an enormous variety of applications in different fields of science and engineering. Among the broad range of applications, particular emphasis has been given in the current literature to the modeling of subsurface contamination phenomena. In this area the correct description of the electrokinetic couplings involved is of utmost importance in predicting the effectiveness of some clean up technologies [67]. In this context, the strong coupling between hydraulic and charge transport gives rise to electroosmotic flows in contaminated fine-grained soils and slurries which pose a significant issue to the environment giving rise to major technological challenges. Applications of electroosmosis in geotechnical engineering are widespread involving dewatering of clay mineral waste tailings [63], clean up by electrokinetic remediation techniques [67] and contaminant transport mitigation in the sub-surface environment [52]. It is well known that classical clean up techniques such as soil flushing, chemical treatment and bioremediation have been found ineffective when applied to clayey soils with low permeability [42]. Electrokinetic remediation is a