



Electro-osmosis in kaolinite with pH-dependent surface charge modelling by homogenization

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Manuscript received on June 17, 2008; accepted for publication on January 19, 2009

ABSTRACT

A new three-scale model to describe the coupling between *pH*-dependent flows and transient ion transport, including adsorption phenomena in kaolinite clays, is proposed. The kaolinite is characterized by three separate nano/micro and macroscopic length scales. The pore (micro)-scale is characterized by micro-pores saturated by an aqueous solution containing four monovalent ions 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 on the tangential velocity. In addition, an adsorption interface condition for the Na^+ transport is postulated to capture its retention in the electrical double layer. The two-scale nano/micro model including salt adsorption and slip boundary condition is homogenized to the Darcy scale and leads to the derivation of macroscopic governing equations. One of the notable features of the three-scale model is the reconstruction of the constitutive law of effective partition coefficient that governs the sodium adsorption in the double layer. To illustrate the feasibility of the three-scale model in simulating soil decontamination by electrokinetics, the macroscopic model is discretized by the finite volume method and the desalination of a kaolinite sample by electrokinetics is simulated.

Key words: electrical double layer, electro-osmosis, homogenization, kaolinite, Nernst-Planck, Poisson-Boltzmann.

INTRODUCTION

The quality of groundwater in clayey soils is strongly influenced by the electrochemistry, which is dictated by the electrochemical interactions that occur between the pore fluid and the minerals. Hydrogeochemical processes, including dissolution, precipitation, ion-exchange, hydrolysis, electroosmosis, electromigration, sorption and desorption, control the variation in chemical composition of groundwater (Mitchell 1993,

Selected paper presented at the IUTAM Symposium on Swelling and Shrinking of Porous Materials: From Colloid Science to Poromechanics – August 06-10 2007, LNCC/MCT.

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