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A Three-Scale Model of pH-Dependent Flows and Ion Transport with Equilibrium Adsorption in Kaolinite Clays: II Effective-Medium Behavior

Sidarta Araújo de Lima · Márcio A. Murad · Christian Moyne · Didier Stemmelen · Claude Boutin

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Abstract In part I (Lima et al., Transp Porous Media, 2009), a three-scale model governing the movement of an aqueous saline solution containing four monovalent species (Na^+, H^+, Cl^-, OH^-) in kaolinite clays was derived. Unlike purely macroscopic approaches, the novelty of the formulation relied on the double averaging of the nanoscopic electrochemistry of particle/electrolyte solution interface ruled by the electrical double layer coupled with protonation/deprotonation reactions. The passage from the nano to the micro (pore)-scale gave rise to ion-sorbed concentrations and slip velocity at the solid/fluid interface which are coupled with the microscopic Stokes problem and Nernst–Planck equations governing the hydrodynamics and ion transport in the micropores. Application of a formal homogenization procedure led to macroscopic governing equations with effective electro-chemical parameters, such as retardation coefficients, electro-osmotic permeability, and electric conductivity. In this study, we reconstruct the constitutive laws of the macroscopic coefficients by solving the nano and microscopic closure problems. New generalized isotherms for Na^+ and $H^+ - OH^-$ sorption are build-up based on a perturbation approach and the limitations

S. A. de Lima · M. A. Murad (✉)
Laboratório Nacional de Computação Científica LNCC/MCT, Av Getúlio Vargas 333, Petrópolis, RJ 25651-070, Brazil
e-mail: murad@lncc.br

S. A. de Lima
e-mail: sidarta@lncc.br

C. Moyne · D. Stemmelen
LEMTA, Nancy-University, CNRS, 2, avenue de la Forêt de Haye, 54504 Vandoeuvre les Nancy Cedex, France
e-mail: christian.moyne@ensem.inpl-nancy.fr

D. Stemmelen
e-mail: didier.stemmelen@ensem.inpl-nancy.fr

C. Boutin
Univeristé de Lyon, Lab. Geomateriaux, DGCB URA CNRS 1652, Ecole Nationale des Travaux Publics de l'Etat, 69518 Vaulx-en-Velin Cedex, France
e-mail: claude.boutin@entpe.fr