

A dual-porosity model for ionic solute transport in expansive clays

Márcio A. Murad · Christian Moyne

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Abstract A microstructure model of dual-porosity type is proposed to describe contaminant transport in fully-saturated swelling clays. The swelling medium is characterized by three separate-length scales (nano, micro, and macro) and two levels of porosity (nano- and micropores). At the nanoscale, the medium is composed of charged clay particles saturated by a binary monovalent aqueous electrolyte solution. At the intermediate (micro) scale, the two-phase homogenized system is represented by swollen clay clusters (or aggregates) with the nanoscale electrohydrodynamics, local charge distribution, and disjoining pressure effects incorporated in the averaged constitutive laws of the electro-chemo-mechanical coefficients and the swelling pressure, which appear in Onsager's reciprocity relations and in a modified form of Terzaghi's effective principle, respectively. The microscopic coupling between aggregates and a bulk solution lying in the micropores is ruled by a slip boundary condition on the tangential velocity of the fluid, which captures the effects of the thin electrical double layers surrounding each clay cluster. At the macroscale, the system of clay clusters is homogenized with the bulk fluid. The resultant macroscopic picture is governed by a dual-porosity

model wherein macroscopic flow and ion transport take place in the bulk solution and the clay clusters act as sources/sinks of mass of water and solutes to the bulk fluid. The homogenization procedure yields a three-scale model of the swelling medium by providing new nano and micro closure problems, which are solved numerically to construct constitutive laws for the effective electro-chemo-hydro-mechanical coefficients. Considering local instantaneous equilibrium between the clay aggregates and micropores, a quasisteady version of the dual-porosity model is proposed. When combined with the three-scale portrait of the swelling medium, the quasisteady model allows us to build-up numerically the constitutive law of the equilibrium adsorption isotherm, which governs the instantaneous immobilization of the solutes in the clay clusters. Moreover, the constitutive behavior of the retardation coefficient is also constructed by exploring its representation in terms of the local profile of the electrical double layer potential of the electrolyte solution, which satisfies the Poisson–Boltzmann problem at the nanoscale.

Keywords Swelling clay · Homogenization · Dual porosity · Pollutant · Transport · Onsager's relations · Adsorption isotherm · Slip boundary condition · Electro-chemo-mechanical couplings · Retardation coefficient · Disjoining (swelling) pressure · Poisson–Boltzmann

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

C. Moyne
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

1 Introduction

Swelling porous media such as 2–1 lattice clays, hydrophilic polymers, shales, corneal endothelium, and