

A Two-Scale Model for Coupled Electro-Chemo-Mechanical Phenomena and Onsager's Reciprocity Relations in Expansive Clays: II Computational Validation

CHRISTIAN MOYNE¹ and MÁRCIO A. MURAD²

¹*LEMTA-CNRS-INPL-UHP (UMR 7563) 2, avenue de la Forêt de Haye, 54504 Vandoeuvre lès Nancy Cedex, France*

²*Laboratório Nacional de Computação Científica LNCC/MCT Av Getúlio Vargas 333, 25651-070 Petrópolis, RJ, Brazil*

(Received: 26 October 2004; accepted: 22 January 2005)

Abstract. In Part I Moyne and Murad [*Transport in Porous Media* **62**, (2006), 333–380] a two-scale model of coupled electro-chemo-mechanical phenomena in swelling porous media was derived by a formal asymptotic homogenization analysis. The microscopic portrait of the model consists of a two-phase system composed of an electrolyte solution and colloidal clay particles. The movement of the liquid at the microscale is ruled by the modified Stokes problem; the advection, diffusion and electro-migration of monovalent ions Na^+ and Cl^- are governed by the Nernst–Planck equations and the local electric potential distribution is dictated by the Poisson problem. The microscopic governing equations in the fluid domain are coupled with the elasticity problem for the clay particles through boundary conditions on the solid–fluid interface. The up-scaling procedure led to a macroscopic model based on Onsager's reciprocity relations coupled with a modified form of Terzaghi's effective stress principle including an additional swelling stress component. A notable consequence of the two-scale framework are the new closure problems derived for the macroscopic electro-chemo-mechanical parameters. Such local representation bridge the gap between the macroscopic Thermodynamics of Irreversible Processes and microscopic Electro-Hydrodynamics by establishing a direct correlation between the magnitude of the effective properties and the electrical double layer potential, whose local distribution is governed by a microscale Poisson–Boltzmann equation. The purpose of this paper is to validate computationally the two-scale model and to introduce new concepts inherent to the problem considering a particular form of microstructure wherein the clay fabric is composed of parallel particles of face-to-face contact. By discretizing the local Poisson–Boltzmann equation and solving numerically the closure problems, the constitutive behavior of the diffusion coefficients of cations and anions, chemico-osmotic and electro-osmotic conductivities in Darcy's law, Onsager's parameters, swelling pressure, electro-chemical compressibility, surface tension, primary/secondary electroviscous effects and the reflection coefficient are computed for a range particle distances and sat concentrations.