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ORIGINAL PAPER

A new methodology for computing ionic profiles and disjoining pressure in swelling porous media

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Abstract A new two-scale computational model is proposed to construct the constitutive law of the swelling pressure which appears in the modified form of the macroscopic effective stress principle for expansive clays saturated by an aqueous electrolyte solution containing multivalent ionic species. The microscopic non-local nanoscale model is constructed based on a coupled Poisson-Fredholm integral equation arising from the thermodynamics of inhomogeneous fluids in nanopores (Density Functional Theory), which governs the local electric double layer potential profile coupled with the ion-particle correlation function in an electrolytic solution of finite size ions. The local problem is discretized by invoking the eigenvalue expansion of the convolution kernel in conjunction with the Galerkin method for the Gauss-Poisson equation. The discretization of the Fredholm equation is accomplished by a collocation scheme employing eigenfunction basis. Numerical simulations of the local ionic profiles in rectangular cell geometries are obtained showing considerable discrepancies with those computed with Poisson-Boltzmann based models for point charges, particularly for divalent ions in calcium montmorillonite. The constitutive law for the disjoining pressure is reconstructed numerically by invoking the contact theorem within a post-processing approach. The resultant computational model is capable of capturing ranges of particle attraction characterized by negative values of the disjoining pressure overlooked by the classical electric double layer theory. Such results provide further insight in the role the swelling pressure plays in the modified macroscopic effective stress principle for expansive porous media.

Keywords Swelling clays · Effective stress principle · Disjoining pressure · Electric double layer · Integral equations · Statistical mechanics · Eigenvalue expansion · Basis eigenfunctions · Collocation schemes

1 Introduction

Swelling ionized porous media are ubiquitous in nature and modern technologies and exhibit tremendous potential for applications in a wide range of fields including geo-environmental and materials sciences, geotechnical engineering, colloid chemistry, medical and life sciences. Historically, research on the computational modeling of such complex systems has focused on describing electro-chemo-mechanical couplings at a particular length scale of interest (ex. nanoscale in colloid science or macroscale in geotechnical engineering). Only recently, bridging between couplings at different scales in media composed of multiple levels of porosity has been accomplished [25, 30].

Understanding and modeling accurately the coupling between the chemistry of aqueous electrolyte solutions and mechanics in electrically charged porous media hinges on various relevant issues which demand strong multi-disciplinary efforts. Applications involve many still open problems in geosciences such as quality of groundwater

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