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A Two-Scale Computational Model of *p*H-Sensitive Expansive Porous Media

We propose a new two-scale model to compute the swelling pressure in colloidal systems with microstructure sensitive to pH changes from an outer bulk fluid in thermodynamic equilibrium with the electrolyte solution in the nanopores. The model is based on establishing the microscopic pore scale governing equations for a biphasic porous medium composed of surface charged macromolecules saturated by the aqueous electrolyte solution containing four monovalent ions (Na^+, Cl^-, H^+, OH^-)*. Ion exchange reactions occur at the surface of the particles leading to a pH-dependent surface charge density, giving rise to a nonlinear Neumann condition for the Poisson–Boltzmann problem for the electric double layer potential. The homogenization procedure, based on formal matched asymptotic expansions, is applied to up-scale the pore-scale model to the macroscale. Modified forms of Terzaghi's effective stress principle and mass balance of the solid phase, including a disjoining stress tensor and electrochemical compressibility, are rigorously derived from the upscaling procedure. New constitutive laws are constructed for these quantities incorporating the pH-dependency. The two-scale model is discretized by the finite element method and applied to numerically simulate a free swelling experiment induced by chemical stimulation of the external bulk solution.*
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Keywords: swelling porous media, disjoining pressure, Poisson–Boltzmann, pH, homogenizaton, ion exchange reactions, finite element method, nonlinear surface charge, effective stress principle

1 Introduction

In the past few decades there has been an increasing interest in the comprehensive understanding of the response of swelling porous media under various loading conditions induced by electro-chemo-mechanical-thermal stimulations. Applications are widespread in nature and in modern technologies involving diverse fields such as: soil science, hydrogeology, geotechnical and petroleum engineering, chemical and mechanical sciences, colloid chemistry, pharmaceutical and life sciences, biomechanics, clinical, and medical fields.

Historically, owing to its critical role in the quality of groundwater, swelling of clay-rich formations, particularly montmorillonites, during moisture imbibition and sorption of ionic species has been widely reported in the literature [1]. The exposure of swelling soils to free polar fluids induces stresses which can be very troublesome to foundations, leading to the failure of buildings, bridges, highways, and runways. Upon inundation structures founded on collapsible and expansive soils are subject to severe damage ranging from minor cracking to irreparable displacements of footings, which may reduce the stability of land slopes [2,3]. In the petroleum industry swelling/contraction of clay-rich rocks such as shales, which are strongly dependent on the water-based drilling mud concentrations, has been responsible for most of the stability problems of drilled boreholes [4]. Swelling can also be explored for beneficial purposes. For instance bentonitic based compacted expansive clays play a critical role in the safety assessments of their capacity to act as a host rock of high-level long lived radioactive waste disposal sites. In addition, they act as a geochemical filter for environmental protection to inhibit the migration of contaminants from hazardous wastes in sanitary landfills [5].

Swelling polymers have numerous technological applications in the development of smart drug delivery substrates, in contact lenses, and in many biological and biomedical devices [6]. In particular, the osmotic induced swelling of cross-linked ionized hydrogels characterized by a stable microstructure [7] make them very attractive as sensor devices [8,9].

In biomedical technology, articular cartilage reinforced by collagen fibers illustrates the enormous complexity inherent to the modeling of electrically charged swollen soft tissues. The tissue fabric consists of a multiphasic hydrated mixture mainly composed of proteoglycan, collagen, and water [10]. The proteoglycans are negatively charged biomacromolecules, which play a crucial role in the load-bearing capacity of the cartilage by dictating the magnitude of the shear and compressive modulus and determining the ability to develop prestresses in the articulating joints and damping the dynamic forces in the human body. Thus, it is imperative that any macroscopic model describing the complex electro-chemo-mechanical interactions inherent to swelling systems is capable of capturing their complex response to different types of stimulation.

Expansive materials have a multiphasic porous microstructure in common, which is composed of a charged solid matrix, identified as a mixture of macromolecules (polymers, active clay particles, and proteoglycans) and an interstitial fluid, which is either adsorbed to the macromolecules in the form of a thin film (or electrolyte solution) or in a bulk state where the electroneutrality condition is fulfilled pointwisely [11]. The electrochemical properties of macromolecules/water interfaces have been intensively studied and have a tremendous impact on the volume, stiffness, strength, conformational properties, and the permeability of reactive porous media [12,13]. Electrically charged interfaces in colloidal system are very sensitive to several mechanisms of different natures, such as electro-osmosis, chemico-osmosis, streaming current, streaming potentials, and electric currents, which may induce severe alterations in the ionic structure and charge distribution in the medium [14].

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