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# A two-scale non-local model of swelling porous media incorporating ion size correlation effects

T.D. Le [a,b], C. Moyne [a,b,*], M.A. Murad [c], S.A. Lima [c]

[a] Université de Lorraine, LEMTA, UMR 7563, Vandoeuvre-lès-Nancy F-54500, France
[b] CNRS, LEMTA, UMR 7563, Vandoeuvre-lès-Nancy F-54500, France
[c] Laboratório Nacional de Computação Científica Av. Getúlio Vargas, 333, Quitandinha, Petrópolis CEP 25651-075, Brazil

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ABSTRACT

A new two-scale model is proposed for derivation of the macroscopic modified effective stress principle for swelling porous media saturated by an electrolyte solution containing finite size ions. A non-local pore-scale model is developed within the framework of Statistical Mechanics in conjunction with the thermodynamic approach based on Density Functional Theory leading to a nonlinear integral Fredholm equation of second kind for the ion/nanopore correlation function coupled with Poisson problem for the electric double layer potential. When combined with the fluid equilibrium condition such non-local electrochemical problem gives rise to a constitutive law for the fluid stress tensor in terms of the disjoining pressure which is decomposed into several components of different nature. The homogenization procedure based on formal asymptotic expansions is applied to up-scale the model to the macroscale leading to a two-scale constitutive law for the swelling pressure appearing in the modified effective stress principle with improved accuracy incorporating the deviations from the Gouy–Chapman Poisson–Boltzmann-based theory due to the finite size short-range ion–ion correlation effects. The integro-differential problem posed in a periodic cell is discretized by collocation schemes. Numerical results are obtained for a stratified arrangement of parallel macromolecules showing that the effects of ion–ion correlation forces give rise to anomalous attraction patterns between the particles for divalent ions.



## 1. Introduction

Swelling-active porous materials are numerous and appear in many applications ranging from geotechnical and chemical engineering to biological and medical sciences. Examples include clays, polymers, biological tissues and cell membranes. Comprehensive understanding of such media is of utmost importance and involves, among others, pollution studies and waste containment. In particular the exposure of swelling soils to free polar fluids (like water) induces stresses that can be very troublesome causing failure of buildings, bridges, rail and heave of tunnel floors leading to complex problems such as broken drainage channels and interference with vehicular traffic during construction. Upon inundation, structures found on collapsible and expansive soils are subject to severe damage ranging from minor cracking to irreparable displacement of footings which often reduce their mechanical stability (Nelson and Miller, 1992). In the petroleum industry, stability of wells

* Corresponding author at: CNRS, LEMTA, UMR 7563, Vandoeuvre-lès-Nancy F-54500, France. Tel.: +33 383595613.
*E-mail addresses:* Tien-Dung.Le@univ-lorraine.fr (T.D. Le), Christian.Moyne@univ-lorraine.fr (C. Moyne), murad@lncc.br (M.A. Murad), sidarta@lncc.br (S.A. Lima).

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