

Micromechanical computational modeling of expansive porous media

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Abstract

A modified Terzaghi principle is proposed to describe the influence of locally coupled electro-chemo-mechanical processes in highly compacted swelling clays upon the form of the macroscopic modified effective stress principle. The two-scale model is derived using the homogenization procedure to upscale the microscopic behavior of a two-phase system composed of clay particles saturated by a completely dissociated electrolyte aqueous solution. Numerical experiments are performed to illustrate the results in a particular cell geometry. *To cite this article: M.A. Murad, C. Moyne, C. R. Mecanique 330 (2002) 865–870.*

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porous media / expansive clays / effective stress / homogenization / Poisson–Boltzmann / swelling (disjoining) pressure

Modélisation micromécanique des milieux poreux déformables

Résumé

Un principe de Terzaghi modifié est proposé pour décrire les phénomènes électro-chimico-mécaniques couplés dans des argiles gonflantes fortement compactées. Le modèle à deux échelles utilise la méthode de l'homogénéisation pour un système diphasique composé de particules d'argile saturées par une solution aqueuse d'un sel complètement dissocié. Quelques résultats numériques illustrent les résultats dans un cas particulier. *Pour citer cet article : M.A. Murad, C. Moyne, C. R. Mecanique 330 (2002) 865–870.*

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milieux poreux / argiles expansives / contrainte effective / homogénéisation / Poisson–Boltzmann / pression de (disjonction) gonflement

1. Introduction

The swelling of clay minerals, particularly montmorillonites is of widespread importance in geotechnical and geoenvironmental fields. It is of concern to the civil engineer because of the severe structural damage caused by collapsible and expansive soils. In petroleum engineering, borehole instability in expansive shales is a technical problem in oil and gas drilling in particular using water-based drilling muds. Compacted swelling clays (bentonites) have received great attention because of their use as sealing materials to impede the leakage of radioactive materials from waste repositories into the groundwater supply.

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Clay particles are mostly colloidal aluminosilicates. When water comes in contact with a mass of clay crystals, it penetrates between the layers forcing them apart. As hydration progresses, water is adsorbed by the minerals and the crystals may expand to several times their original thickness. For long-range interactions swelling is dominated by electrostatic forces. In this range the adsorbed fluid is a structureless electrolyte solution consisting of water and an entirely dissociated salt with strong electrolytes Na^+ and Cl^- . At the microscale, ion concentrations and electric potential are governed by the Poisson–Boltzmann equation [1], which reduces to the conventional Gouy–Chapman theory of diffuse double layer in one-dimensional infinite plane geometries [2]. The electrostatic component of the repulsive force between the minerals arises from the overlapping between ionic double layers. Derjaguin [3] described this lyophilic interaction in terms of a *disjoining pressure*, defined as an excess in the normal pressure applied to the mineral surfaces relative to the surrounding bulk phase.

At the macroscale (the homogenized microscale) the complex microstructural solid-fluid physico-chemical interactions are represented in an averaged fashion, with fluid and solid modeled as overlaying continua with averaged properties established at every point in the mixture. At this scale, the expansion of the aggregates is manifested in the experimentally observed *swelling pressure*, defined as an overburden pressure excess that must be applied to a stacked layered arrangement of clay particles to prevent further uptake of water [4].

The development of microscopic models aiming at generalizing the disjoining pressure concept and the Gouy–Chapman double layer theory to non-parallel particles has pursued the numerical solutions of the Poisson–Boltzmann equation in general random domains [5]. On the other hand, macroscopic models for swelling media have been developed within phenomenological approaches [6] or based on the mixture theory [7]. In both frameworks, novel forms of Terzaghi’s effective principle have been postulated aiming at incorporating the influence of physico-chemical effects [6]. In this paper a macroscopic form of Terzaghi’s effective stress principle is derived based on a rigorous scale-up procedure of the local electro-chemo-mechanical microstructural behavior of the clay–water–electrolyte system. For simplicity we consider the case wherein solid, fluid and ions are at thermodynamic equilibrium. We then apply the homogenization procedure to scale up the pore-scale model, given by the Poisson–Boltzmann problem coupled with the fluid equilibrium condition under the action of a body force of Coulombic type and with the elasticity system governing the deformation of the clay particles.

The homogenization procedure is capable of capturing the precise correlation between macroscopic swelling pressure and microscopic disjoining pressure. By discretizing the local cell problems by the finite element method, numerical results are presented illustrating the potential of the proposed procedure in computing the behavior of the swelling pressure in a general cell geometry. Further work is in progress to treat the general non-equilibrium case of electro-chemo-mechanical coupled phenomena.

2. Microscopic description of the problem

Consider at the microscale the expansive medium a biphasic aggregate composed of clay particles and an aqueous dilute solution consisting of water and an entirely dissociated salt with strong electrolytes (for example Na^+ (cations) and Cl^- (anions)) whose volumetric concentrations in the fluid phase are denoted by c^+ and c^- . The solution is at thermodynamic equilibrium with an outer saline bath (with salinity c_b). The equality between the electro-chemical potentials leads to the classical Boltzmann distributions $c^\pm = c_b \exp(\mp F\varphi/RT)$, where φ is the electrical potential, F the Faraday constant, T the absolute temperature and R the universal gas constant [8]. If $\tilde{\epsilon}_0$ and $\tilde{\epsilon}$ designate the vacuum permittivity and the relative dielectric constant of the solvent and $q \equiv F(c^+ - c^-) = -2Fc_b \sinh(F\varphi/RT)$ the net charge density, the electric potential is governed by the Poisson–Boltzmann problem (Eq. (1) with $\epsilon = 1$) [8]. Denoting $\mathbf{E} = -\nabla\varphi$ the electric field satisfying $\tilde{\epsilon}\tilde{\epsilon}_0\nabla \cdot \mathbf{E} = q$ and $\{p, \sigma_f\}$ the hydrodynamic pressure and the stress tensor of the electrolyte solution, the equilibrium of the fluid is dictated by the electric body force of Coulombic type $q\mathbf{E}$. Further, if \mathbf{I} and \otimes designate the unit tensor and the tensorial product between

vectors, the Maxwell stress tensor is classically defined as $\boldsymbol{\tau}_M \equiv (1/2)\tilde{\epsilon}\tilde{\epsilon}_0(2\boldsymbol{E} \otimes \boldsymbol{E} - E^2\boldsymbol{I})$ (see [9]). This form is motivated by the property $\nabla \cdot \boldsymbol{\tau}_M = q\boldsymbol{E}$ which can be obtained from the above definitions. Whence, neglecting gravity, the fluid equilibrium is represented by (2). The solid phase is supposed isotropic and linear elastic with Lamé parameters λ_s and μ_s . The displacement \mathbf{u} , stress tensor $\boldsymbol{\sigma}_s$ and deformation $\boldsymbol{\mathcal{E}}(\mathbf{u}) \equiv (\nabla\mathbf{u} + (\nabla\mathbf{u})^T)/2$ satisfy (3). Finally, denoting Γ and \mathbf{n} the common interface and the unit normal exterior to the fluid domain and $\sigma < 0$ the fixed surface charge of the solid particles, continuity of the normal component of the stress tensor together with the charge balance on Γ are represented by (4) (with $\epsilon = 1$).

3. Homogenization

We upscale to the macroscale using the homogenization procedure. Following the classical framework of [10], the swelling clay is comprised of a spatially periodic porous structure. Two disparate length scales are introduced; a microscopic scale ℓ of the order of the pore size and a macroscopic one L of the overall dimensions of the swelling medium. Their ratio $\epsilon \equiv \ell/L$ is a small parameter. The periodic bounded domain Ω^ϵ is composed of spatially repeated unit disjoint parallelepiped periods, Y^ϵ , congruent to a standard Y , formed by the union of cell domains Y_f and Y_s occupied by the fluid and solid respectively, whereas the reference interface Γ is given by the union of ∂Y_{fs} interfaces. The basic problem is to investigate the asymptotics of the solution as $\epsilon \rightarrow 0$ and obtain the homogenized limit as the scale of the inhomogeneity tends to zero. In what follows, the microscopic governing equations are written in dimensionless form thoroughly using reference values (denoted by the subscript “ref”) and the magnitudes of the dimensionless parameters involved are investigated. The reference characteristic length ℓ_{ref} is chosen of the order of the macroscopic medium, i.e., $\ell_{\text{ref}} \equiv L$ such that the macroscopic length L is used to normalize the spatial differential operators. The choice of the reference electric field E_{ref} is based on boundary condition (4)(a) which suggests $E_{\text{ref}} \equiv \sigma/\tilde{\epsilon}\tilde{\epsilon}_0$. In addition, the reference value of the electric potential is selected $\varphi_{\text{ref}} = \ell E_{\text{ref}}$. From the overall condition of electroneutrality (5), the net charge q counterbalances the surface charge σ and therefore the reference concentration is selected as $c_{\text{ref}} = \sigma/(F\ell)$. The choice of the reference solid displacement u_{ref} is based on (4)(b) together with the constitutive equations for the stresses in (2) and (3). This suggests the choice $(\lambda_s + 2\mu_s)(u_{\text{ref}}/L) = \max(p_{\text{ref}}, 0.5\tilde{\epsilon}\tilde{\epsilon}_0 E_{\text{ref}}^2)$. By rephrasing the micromodel in dimensionless form, three dimensionless quantities naturally appear namely $N = F\sigma\ell/(\tilde{\epsilon}\tilde{\epsilon}_0 RT)$, $M_1 = \sigma^2/(\tilde{\epsilon}\tilde{\epsilon}_0 p_{\text{ref}})$ and $M_2 = (\tilde{\epsilon}\tilde{\epsilon}_0 E_{\text{ref}}^2 L)/(2u_{\text{ref}}(3\lambda_s + 2\mu_s))$. The former measures the ratio of electric energy to the thermal energy of an ion whereas the two latter parameters measure the magnitude of Maxwell stresses relative to the fluid pressure and stresses in the solid particles. From the conventional Gouy–Chapman theory of diffuse double layer, the magnitude of the physico-chemical forces is of the same order as the contact forces and thus we choose the three parameters of $\mathcal{O}(1)$. Making use of the above scaling laws, the micromechanical model is rephrased below with a formal ϵ^n factor to indicate the order of magnitude of each term.

- Poisson–Boltzmann:

$$\epsilon^2 \nabla^2 \varphi = -\frac{q}{\tilde{\epsilon}\tilde{\epsilon}_0} = \frac{2Fc_b}{\tilde{\epsilon}\tilde{\epsilon}_0} \sinh\left(\frac{F\varphi}{RT}\right) \quad (1)$$

- Equilibrium of the electrolyte solution

$$\nabla \cdot \boldsymbol{\sigma}_f = \nabla \cdot (-p\boldsymbol{I} + \boldsymbol{\tau}_M) = -\nabla p + q\boldsymbol{E} = -\nabla p - q\nabla\varphi = 0 \quad (2)$$

- Elasticity equation for the solid phase

$$\nabla \cdot \boldsymbol{\sigma}_s = 0; \quad \boldsymbol{\sigma}_s = \lambda_s \nabla \cdot \mathbf{u}\boldsymbol{I} + 2\mu_s \boldsymbol{\mathcal{E}}(\mathbf{u}) \quad (3)$$

- Boundary conditions

$$-\boldsymbol{E} \cdot \mathbf{n} = \epsilon \nabla\varphi \cdot \mathbf{n} = \frac{\sigma}{\tilde{\epsilon}\tilde{\epsilon}_0}; \quad \boldsymbol{\sigma}_f \mathbf{n} = \boldsymbol{\sigma}_s \mathbf{n} \quad (4)$$

- Electroneutrality condition

$$\int_{Y_f} q \, dY = \tilde{\epsilon} \tilde{\epsilon}_0 \int_{Y_f} \nabla \cdot \mathbf{E} \, dY = \tilde{\epsilon} \tilde{\epsilon}_0 \int_{\partial Y_{fs}} \mathbf{E} \cdot \mathbf{n} \, d\Gamma = - \int_{\partial Y_{fs}} \sigma \, d\Gamma \quad (5)$$

Within the classical approach based on perturbation, two independent variables \mathbf{x} and \mathbf{y} , denoting macroscopic and microscopic coordinates, are introduced. The formal method based on asymptotic expansions consists in postulating a development in series of the small parameter ϵ for each variable in the form $\psi = \sum_k \epsilon^k \psi^k$. After replacing the differential operator ∂/∂_x by $\partial/\partial_x + \epsilon^{-1} \partial/\partial_y$ and collecting the powers of ϵ , local cell problems parametrized by \mathbf{x} are obtained. The homogenized results include a Poisson–Boltzmann equation for φ^0 and the macroscopic modified Terzaghi’s decomposition. To pursue the two-scale version of these results begin by noting that an important consequence of the scaling factor ϵ^2 in (1) is the “shrinking” of the homogenized result which preserves the original form of the unscaled Poisson–Boltzmann problem, but is posed locally within each unit cell, as is easily seen from (1) and (4) at $\mathcal{O}(\epsilon^0)$

$$\begin{aligned} \tilde{\epsilon} \tilde{\epsilon}_0 \Delta_{yy} \varphi^0 &= -q^0 = 2F c_b \sinh(F\varphi^0/RT) \quad \text{in } Y_f \\ -\tilde{\epsilon} \tilde{\epsilon}_0 \mathbf{E}^0 \cdot \mathbf{n} &= \tilde{\epsilon} \tilde{\epsilon}_0 \nabla_y \varphi^0 \cdot \mathbf{n} = \sigma \quad \text{on } \partial Y_{fs} \end{aligned} \quad (6)$$

together with periodicity conditions on the frontier of the unit cell. Hence, the zeroth order electric potential depends on the fast variable \mathbf{y} . This characterizes φ^0 and \mathbf{E}^0 as highly oscillatory quantities. Notably this fact is consistent with the electrical double layer results at equilibrium where these quantities vary in the pore fluid domain [1]. Moreover, from (2) at $\mathcal{O}(\epsilon^{-1})$ p^0 also varies across the fluid domain as $\nabla_y p^0$ balances the local variation of the Coulomb term $q^0 \nabla_y \varphi^0$. On the other hand one may introduce a non-oscillatory apparent bulk phase pressure by rewriting the Coulomb term in (2) at $\mathcal{O}(\epsilon^{-1})$ along with (6) as

$$q^0 \nabla_y \varphi^0 = \nabla_y \int_0^{\varphi^0} q^0 \, d\varphi = -2F c_b \nabla_y \int_0^{\varphi^0} \sinh\left(\frac{F\varphi^0}{RT}\right) \, d\varphi = -2c_b RT \nabla_y \left[\cosh\left(\frac{F\varphi^0}{RT}\right) - 1 \right] \quad (7)$$

Hence, defining the Donnan osmotic pressure $\pi^0 \equiv 2c_b RT [\cosh(F\varphi^0/RT) - 1]$ one may define a local apparent bulk phase pressure $p_b^0 \equiv p^0 - \pi^0$. Note that using (7), Eq. (2) at order $\mathcal{O}(\epsilon^{-1})$, $\nabla_y p^0 + q^0 \nabla_y \varphi^0 = 0$ can be rephrased as $\nabla_y p_b^0 = 0$ or $p_b^0 = p_b^0(\mathbf{x})$. This shows that, in contrast to p , p_b^0 does not oscillate. This result can be exploited to derive the modified Terzaghi’s effective principle. To this end begin by noting that (3) at $\mathcal{O}(\epsilon^{-2})$ implies that $\mathbf{u}^0 = \mathbf{u}^0(\mathbf{x})$. Denoting $\langle \cdot \rangle \equiv |Y|^{-1} \int_{Y_\alpha} \cdot \, dY_\alpha$ ($\alpha = f, s$) the volume average operator over the unit cell Y , we begin by averaging the fluid and solid equilibrium conditions and use boundary condition (4)(b) at $\mathcal{O}(\epsilon^1)$. Denoting $\sigma_T^0 \equiv \langle \sigma_f^0 \rangle + \langle \sigma_s^0 \rangle$ the overall stress tensor of the mixture, using the divergence theorem and the periodicity we obtain the overall equilibrium $\nabla_x \cdot \sigma_T^0 = 0$. Further to obtain a local cell problem for \mathbf{u}^1 , we consider the elasticity problem at $\mathcal{O}(\epsilon^{-1})$ together with boundary condition (4)(b) and the constitutive equation for the stress tensors at $\mathcal{O}(\epsilon^0)$, with $p^0(\mathbf{x}, \mathbf{y})$ replaced by $p_b^0(\mathbf{x})$. Denoting δ_{ij} the Kronecker delta and \mathbf{c}_s the fourth-order tensor with components $c_{ijkl} = \lambda_s \delta_{ij} \delta_{kl} + \mu_s (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})$ we have

$$\nabla_y \cdot (\mathbf{c}_s \mathcal{E}_y(\mathbf{u}^1)) = 0 \quad \text{in } Y_s \quad (8)$$

$$- [p_b^0(\mathbf{x}) \mathbf{I} + \mathbf{\Pi}^0(\mathbf{x}, \mathbf{y})] \mathbf{n} = \mathbf{c}_s [\mathcal{E}_x(\mathbf{u}^0(\mathbf{x})) + \mathcal{E}_y(\mathbf{u}^1)] \mathbf{n} \quad \text{on } \partial Y_{fs} \quad (9)$$

where $\mathbf{\Pi}^0$ is a disjoining stress tensor which incorporates the chemico-osmotic pressure π^0 and Maxwell stresses τ_M^0

$$\mathbf{\Pi}^0 = \pi^0 \mathbf{I} - \tau_M^0 = 2c_b^0 RT \left[\cosh\left(\frac{F\varphi^0}{RT}\right) - 1 \right] \mathbf{I} - \frac{\tilde{\epsilon} \tilde{\epsilon}_0}{2} [2\mathbf{E}^0 \otimes \mathbf{E}^0 - E^{02} \mathbf{I}] \quad (10)$$

When comparing the cell problem (8) for \mathbf{u}^1 with the similar Neumann problems which typically arises in the homogenization derivation of Biot’s equations of poroelasticity (see [11]), the novelty is the appearance of the disjoining tensor $\mathbf{\Pi}^0$ which incorporates the influence of physico-chemical effects on the traction

boundary condition in (9). By linearity we have

$$\mathbf{u}^1(\mathbf{x}, \mathbf{y}) = \boldsymbol{\zeta}(\mathbf{y})p_b^0(\mathbf{x}) + \boldsymbol{\xi}(\mathbf{y})\mathcal{E}_x(\mathbf{u}^0(\mathbf{x})) + \mathbf{u}_\pi^1(\mathbf{x}, \mathbf{y}) + \widehat{\mathbf{u}}^1(\mathbf{x}) \quad (11)$$

The canonical cell problems for the third-order tensor $\boldsymbol{\xi}$ and the vector $\boldsymbol{\zeta}$ are classical [11]. The novelty in (11) is the appearance of the component \mathbf{u}_π^1 which measures the particle displacement component arising from the traction induced by the physico-chemical tensor $\boldsymbol{\Pi}^0$, i.e.,

$$\begin{aligned} \nabla_y \cdot (\mathbf{c}_s \mathcal{E}_y(\mathbf{u}_\pi^1)) &= 0 \quad \text{in } Y_s \\ (\mathbf{c}_s \mathcal{E}_y(\mathbf{u}_\pi^1))\mathbf{n} &= -\boldsymbol{\Pi}^0 \mathbf{n} \quad \text{on } \partial Y_{fs} \end{aligned} \quad (12)$$

Denoting $\mathbf{C}_s \equiv \langle \mathbf{c}_s(\mathbf{I}\mathbf{I} + \mathcal{E}_y(\boldsymbol{\xi})) \rangle$ the macroscopic elastic modulus, by averaging the constitutive equation for $\boldsymbol{\sigma}_s^0$ and using (11) we obtain $\langle \boldsymbol{\sigma}_s^0 \rangle = \mathbf{C}_s \mathcal{E}_x(\mathbf{u}^0) + \langle \mathbf{c}_s \mathcal{E}_y(\boldsymbol{\zeta}) \rangle p_b^0 + \langle \mathbf{c}_s \mathcal{E}_y(\mathbf{u}_\pi^1) \rangle$. Denoting n_α ($\alpha = f, s$) the volume fraction of the α -phase, in terms of $p_b^0(\mathbf{x})$ the averaged constitutive equation for $\boldsymbol{\sigma}_f^0$ is given as $\langle \boldsymbol{\sigma}_f^0 \rangle = -n_f p_b^0 \mathbf{I} - \langle \boldsymbol{\Pi}^0 \rangle$. Using the above results in the definition of $\boldsymbol{\sigma}_T^0$ gives

$$\begin{aligned} \boldsymbol{\sigma}_T^0 &= -\boldsymbol{\alpha} p_b^0 + \mathbf{C}_s \mathcal{E}_x(\mathbf{u}^0) - \boldsymbol{\Pi}_*^0 \\ \boldsymbol{\Pi}_*^0 &= \langle \boldsymbol{\Pi}^0 \rangle + n_s \boldsymbol{\Pi}_S^0, \quad \text{where } \boldsymbol{\Pi}_S^0 \equiv -\langle \mathbf{c}_s \mathcal{E}_y(\mathbf{u}_\pi^1) \rangle^s \text{ with } \langle \cdot \rangle^s \equiv n_s^{-1} \langle \cdot \rangle \end{aligned} \quad (13)$$

and $\boldsymbol{\alpha} \equiv n_f \mathbf{I} - \langle \mathbf{c}_s \mathcal{E}_y(\boldsymbol{\zeta}) \rangle$ is the Biot coefficient for the particles. Eq. (13) is nothing but Terzaghi's decomposition for the swelling clay. In addition to the pore pressure p_b^0 and contact stresses $\mathbf{C}_s \mathcal{E}_x(\mathbf{u}^0)$, it incorporates physico-chemical component $\boldsymbol{\Pi}_*^0$. This latter quantity may be decomposed into the averaged counterpart of $\boldsymbol{\Pi}^0$ and the additional component $\boldsymbol{\Pi}_S^0$, which consists of chemical stresses in the particles due to the traction induced by $\boldsymbol{\Pi}^0$ in (12). Since $\boldsymbol{\Pi}_S^0$ represents stresses acting effectively in the solid phase, it may be viewed as the physico-chemical component which dictates the expansion of the aggregates. Whence, this quantity shall be referred to as *swelling stress tensor*, as it plays the role of a tensorial generalization of the swelling pressure to incorporate deviatoric effects. Hence, we remark the strong potential of the proposed formulation in providing a precise microstructural representation for the macroscopic expansive stresses and their role in the modified effective stress principle [6].

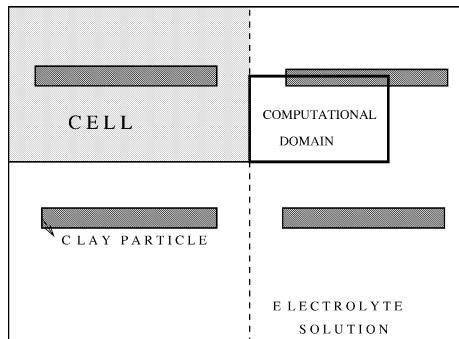


Figure 1. Periodic unit cell and computational domain (square of side H).

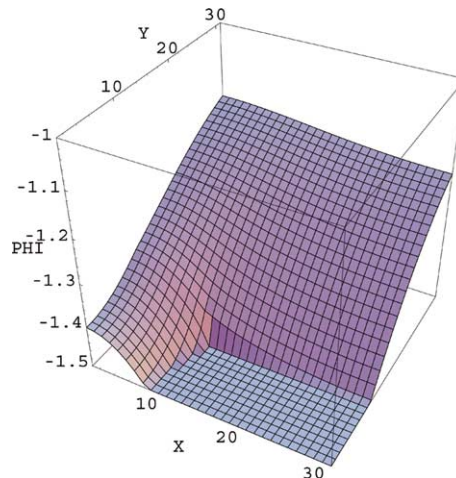


Figure 2. Dimensionless electric potential elevation (the constant value $\varphi^* \approx -1.5$ at the particle surface is extended over the solid domain).

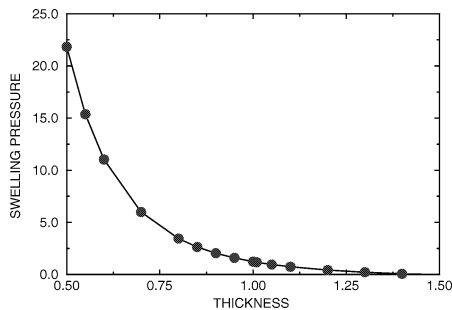


Figure 3. Dimensionless swelling pressure as a function of the interlayer spacing.

4. Numerical results

To illustrate the capability of the micromechanical approach in furnishing an accurate portrait of the swelling stress tensor, in what follows we consider the finite element approximation of the aforementioned cell problems. To this end we begin by solving the discrete version of the local PB problem (6) in its Debye–Hueckel linearized form [1,2] to obtain discrete φ^0 and \mathbf{E}^0 fields. Disjoining stresses are then computed within a post-processing using (10) and subsequently used as input traction boundary conditions in (12), (13) to obtain swelling stresses. The computational square domain (side H) together with the periodic cell geometry are depicted in Fig. 1. Fig. 2 shows the behavior of the normalized electric potential $\varphi^* \equiv \varphi^0 \tilde{\varepsilon} \tilde{\varepsilon}_0 / \sigma L_D$ (where $L_D \equiv \tilde{\varepsilon} \tilde{\varepsilon}_0 RT / 2c_b F^2$ is the Debye length [1,2]) as a function of the dimensionless coordinate $\mathbf{x}^* = \mathbf{x} / H$ (with $H = L_D$). As expected it reaches a maximum negative value near the solid surface. For completeness, the values of φ^0 over the solid surface are extended using the maximum negative value at the surface. Lastly Fig. 3 shows the normal component of the dimensionless swelling stress $\Pi_S^* \equiv (2\Pi_S^0 \tilde{\varepsilon} \tilde{\varepsilon}_0 / \sigma^2)$ as a function of the interlayer spacing H / L_D . As expected disjoining effects are highly pronounced for small interlayer spacings.

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