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HOMOGENIZATION OF THE ELECTRO-OSMOSIS PHENOMENA IN THE CORTICAL BONE POROUS STRUCTURE

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Abstract: *This note deals with the elector-osmosis phenomena in the cortical bone micro-structure considered as porous medium with one porosity level. The microscopic model is given by the system of equations describing the ionic transport in a canalicular network saturated with a bone ionized fluid. Unfolding homogenization method is used to derive effective equations for the ion concentrations and electric field potentials.*

Keywords: Homogenization, Electro-osmosis, Porous medium, Biomechanics.

1. Introduction

The electro-osmosis in the porous medium is a multiscale phenomenon with numerous applications in geophysics or tissue biomechanics. In particular, the electro-osmosis is responsible for important physiological processes in the cortical bone tissue. Cortical bone is seen as a highly hierarchical structure with multiple porosities on different scale levels of the osteon; usually the following three main levels are distinguished (Moyne and Murad, 2002). The vascular porosity level is the largest one, represented by the Haversian (or osteonal) and the Volkmann canals distributed in the collagen-apatite matrix. This matrix is porous; it incorporates lacunae and canaliculi which form the lacuno-canalicular porosity. Its matrix is formed by porosity associated with the space between collagen and the crystallites of the mineral apatite.

The present work is focused on electro-osmosis phenomena at the lacuno-canalicular porosity level, further referred to as the microscopic level. At this scale the mechanotransduction is an important phenomenon responsible for the bone tissue resorption and deposition (Rohan et al., 2012). Both these processes are related to the strain generated electric potentials which are associated with the electrolyte flows in the pores.

The lacuno-canalicular porosity (characteristic scale $l \approx 10\ nm$) can be modeled as a porous medium with fluid filled pores in the solid matrix. The fluid is a solution with two types of monovalent ions of opposite polarizations (cations Na^+ and anions Cl^-). Further, we consider the solid phase and the solid-fluid interface, both featured by negative electric charges.

In this short text, in Section 2, we present a mathematical model of electro-diffusion relevant to the porosity level and report on the homogenization result in Section 3, to provide an effective model relevant to the macroscopic scale, i.e. the osteon level. The numerical implementation of the two-scale modeling has been made and is illustrated in Section 3.

2. Mathematical Model

This section provides a brief description of mathematical relations describing the electro-osmosis at the microscopic level. The model describing macroscopic behaviour was obtained by homogenization.

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2.1. Model of electro-osmosis

The porous medium occupies the domain Ω with coordinations $x \in R^n$, which is decomposed into solid and fluid parts denoted as Ω_s and Ω_f, respectively. The solid-fluid interface Γ is defined as $\Gamma = \partial\Omega_f \cap \partial\Omega_s$ with the outward normal unit vector, $\mathbf{n}$ in general, thus $\mathbf{n}^s = - \mathbf{n}^f$. Through the text the symbol ∂ denotes a boundary of a domain and subscripts s and f refer to quantities belonging to the solid and fluid parts, respectively. Further, the mathematical model of electro-diffusion is introduced.

$$-\nabla.\alpha_s\epsilon_0\nabla\Phi = \hat{\pi}_s \quad \text{in}\,\Omega_s \tag{1}$$

$$-\nabla.\alpha_f\epsilon_0\nabla\Phi = \pi_f \quad \text{in}\,\Omega_f \tag{2}$$

$$\mathbf{n}\,.\alpha\;\nabla\Phi = 0 \quad \text{on}\,\partial\Omega \tag{3}$$

$$\mathbf{n}^f\,.\;\alpha_f\nabla\Phi|_f = -\,\alpha_\Gamma/e_\Gamma[\Phi]_\Gamma + \rho/2 \quad \text{on}\,\Gamma_f \tag{4}$$

$$\mathbf{n}^s\,.\;\alpha_s\nabla\Phi|_s = -\,\alpha_\Gamma/e_\Gamma[\Phi]_\Gamma - \rho/2 \quad \text{on}\,\Gamma_s \tag{5}$$

$$\partial Q^{\pm}/\partial t + \mathbf{w}_f\,.\,\nabla Q^{\pm} - \nabla.\mathbf{D}.\,(\nabla Q^{\pm} \pm (z^{\pm}\,F\,/\,RT)\;Q^{\pm}\,\nabla\Phi) = 0 \quad \text{in}\,\Omega_f \tag{6}$$

$$\mathbf{n}\,.\mathbf{D}^{\pm}\,.\,(\nabla Q^{\pm} \pm (z^{\pm}F/RT)Q^{\pm}\nabla\Phi) = 0 \quad \text{on}\,\Gamma \tag{7}$$

$$Q^{\pm} = Q^{\pm}_0 \quad \text{on}\,\partial\,\Omega \setminus \Gamma \tag{8}$$

Eqs. (1) and (2) are the Gauss-Poisson equations of electrostatics in the solid and fluid, where $\alpha_d, d = f, s$ is relative permitivity, ϵ_0 is permitivity of the void space, π_d is a volume electric charge and by Φ is the electric potential. Using Faraday constant F and the valence of ion particles $z^+ = 1, z^- = -1$, the volume electric charge in the fluid can be expressed, by the definition, as the product between the molar charges and the difference of concentration of cations Q^+ and anions Q^-, thus $\pi_f = F(z^+Q^+ - z^-Q^-)$.

The two boundary conditions (4) and (5) result from one-dimensional electrostatics Dirichlet problem describing charge distribution in a thin layer of thickness e on the solid-fluid interface, where represent modified charge. The condition (3) means that the medium is isolated from outer space.

The movement of ions is described by the Nernst-Planck equation (6), for Newtonian incompressible fluid with vector of convection velocity $\mathbf{w}_f$ and absolute temperature T. Water-ion diffusion coefficients for cations and anions are in form of second-order tensors $\mathbf{D}^{\pm}$ and R is constant of ideal gas. By condition (8) the electroneutrality is preserved, while (7) expresses the flux of ions through Γ.

2.2. Microscopic model

Following the approach introduced in the report Rohan (2012), the upscaling of linearized system (1)-(8) in its dimensionless weak form was performed using the periodic homogenization using the assumption of material periodicity; Ω is assumed to be generated as a periodic lattice based on the so-called representative periodic cell (RPC) Y with coordinates $y = x/\varepsilon$, where ε_0 is the small parameter of the asymptotic analysis, describing the scale between macro- and microscopic coordinates. The dimensionless potentials φ^{ε}_d and concentrations $\upsilon^{\pm,\varepsilon}$ are decomposed into their macro- (denoted by superscript 0) and microscopic (superscript 1) parts as

$$\upsilon^{\varepsilon}(x) = \upsilon^{\varepsilon,0}(x, x/\varepsilon) + \varepsilon\upsilon^{1,\varepsilon}(x, x/\varepsilon) \qquad \varphi^{\varepsilon}(x) = \varphi^{\varepsilon,0}(x, x/\varepsilon) + \varepsilon\varphi^{1,\varepsilon}(x, x/\varepsilon)$$

Knowing osteon micro-structure, namely the canalicular network geometry, the RPC Y is decomposed accordingly to domain Ω, $Y = Y_s \cup Y_f \cup \Gamma_Y$, $Y_f = Y \setminus \overline{Y}_f$, $\Gamma_Y = \overline{Y}_s \cap \overline{Y}_f$. By the homogenization, the local problems on the RPC Y are obtained, as follows: Find $(\varphi^1_f, \varphi^1_s, \upsilon^{1\pm})$ such that for $x \in \Omega$

$$\fint_{\Omega\times Y_f} \mathbb{D}^{\pm}\cdot\left(\nabla_x\vartheta^{0\pm}+\nabla_y\vartheta^{1\pm}\right)\cdot\nabla_y\theta^{1\pm}+\fint_{\Omega\times Y_f}\bar{\beta}(\pm c^{\pm})\mathbb{D}^{\pm}\cdot\left(\nabla_x\varphi_f^0+\nabla_y\varphi_f^1\right)\cdot\nabla_y\theta^{1\pm}=0, \tag{9}$$

$$\fint_{Y_d}\alpha_d\left(\nabla_x\varphi_d^0+\nabla_y\varphi_d^1\right)\cdot\nabla_y\psi_d^1=0,\qquad d=f,s, \tag{10}$$

for all test function $\theta^{1\pm}$, ψ^1_d in Sobolev space of admissible Y-periodic functions $H^1_\#(Y_d)$. By virtue of the problem linearization, $c^{\pm}$ are given ionic concentrations and $\overline{\beta}=\Phi zF/RT$. Symbol $\fint$ refers to $1/|Y|\int$.

2.3. Homogenized model

Following steps from the report Rohan (2012), the microscopic parts of variables (φ^1_f, φ^1_s, $\upsilon^{1\pm}$) can be express as a linear combinations of so-called corrector basis functions. Those functions represent characteristic response on the RPC Y and are necessary for expressions of effective coefficients $\mathbf{D}^{\pm}_{\mathrm{H}}$, $\mathbf{B}^{\pm}_{\mathrm{H}}$, $\mathbf{A}^{d}_{\mathrm{H}}$, $\mathbf{C}^{\pm}_{\mathrm{H}}$, $\mathbf{S}^{\pm}_{\mathrm{H}}$ approximating characteristics of the macroscopic medium. The homogenized macroscopic form of the electrostatic equation for the potential φ^0_f, φ^0_s in the solid and the fluid yields

$$\begin{aligned}\sum_{d=f,s}\int_\Omega\nabla\psi_d^0\cdot\mathbb{A}_H^d\cdot\nabla\varphi_d^0+\int_\Omega\mathcal{M}_{\Gamma_Y}(\bar{\alpha})(\varphi_f^0-\varphi_s^0)(\psi_f^0-\psi_s^0)-\\-\frac{|Y_f|}{\lambda_D^2|Y|}\int_\Omega\psi_f^0(\vartheta^{0+}-\vartheta^{0-})=\int_\Omega\mathcal{M}_{\Gamma_Y}(\bar{\pi}_s)\psi_s^0+\int_\Omega\frac{\psi_f^0+\psi_s^0}{2}\mathcal{M}_{\Gamma_Y}(\bar{\varrho}),\end{aligned} \tag{11}$$

for all $\psi^0_d\in H^1(\Omega)$. Note, that $\mathcal{M}$ is an operator of a mean value of a variable over the interface. By overline the dimensionless variables are denoted.

The electro-diffusion on the macroscopic scale is described by two equations for concentrations ($\upsilon^{0\pm}$)

$$\begin{aligned}\frac{|Y_f|}{|Y|}\int_\Omega\partial_t\vartheta^{0\pm}\theta^{0\pm}+\int_\Omega\mathbf{C}_H^{\pm}(\mathbf{w_f})\cdot\nabla(\vartheta^{0+}+\vartheta^{0-})\theta^{0\pm}+\int_\Omega\mathbf{S}_H^{\pm}(\mathbf{w_f})\cdot(\nabla\varphi_f^0)\theta^{0\pm}+\\+\sum_{z=+,-}\int_\Omega\nabla\theta^{0\pm}\cdot\mathbb{D}_H^{\pm}\cdot\nabla(\vartheta^{0+}+\vartheta^{0-})+\int_\Omega\nabla\theta^{0\pm}\cdot\mathbb{B}_H^{\pm}\cdot\nabla\varphi_f^0\quad=0\end{aligned} \tag{12}$$

for all $\theta^{0\pm}\in H^1(\Omega)$. If we consider symmetric electrolyte, Eq. (11) becomes independent on the concentration and, thus, can be solved separately from Eqs. (12), now reduced to only one equation for variable υ^0, see (Turjanicová, 2013).

3. Results

The homogenization procedure and homogenized problem on macroscale was implemented in the software *SfePy*. The canalicular level was represented by cubic RPC with three connected channels in directions of main axes. The homogenized problem given by Eqs. (11) and (12) was solved on the simple prismatic geometry, representing small part of osteonal wall. The left side of Fig. 1 illustrates the macroscopic solutions (φ^0_f, φ^0_s, υ^0) alongside the y-coordinate of test problem with boundary and initial conditions $\varphi^0_s(x, l, z) = 100$, $\varphi^0_f(x, l, z) = 0$, $\upsilon^0_f(x, l, z, t) = 10$, $\upsilon^0(x, y, z, 0) = 10$. On the right in the Fig. 1 is shown recovered microscopic diffusion flux on the RPC Y representing microstructure.

4. Conclusions

This work reports on the two-scale modeling of electro-osmosis phenomenon in the cortical bone osteon. The microscopic model with only one porosity level was introduced, whereby the flow problem was treated as decoupled. The homogenized model enables to describe distribution of voltage in both solid and fluid phases and the ionic concentrations at the macroscopic level of bone osteon. By virtue of the corrector results, the microscopic distribution of electric fields and concentration fluxes can be recovered.

It is possible to assess influence of the geometrical arrangement of the fluid channels in the microstructure on the effective material properties and the local electro-osmosis processes. In the further research an extension of the model for coupled fluid-solid interaction will be pursued and the role of the solid piezoelectricity will be reviewed in the context of the recent work (Lemaire et al., 2011), where an alternative upscaling approach was used.

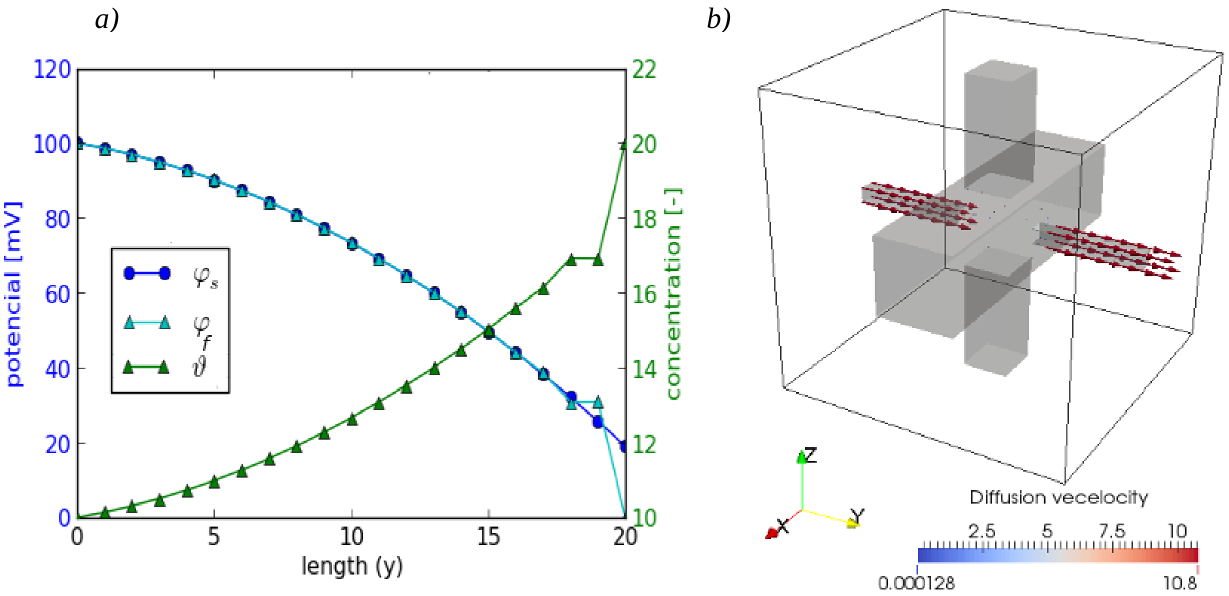

Fig. 1: a) Solutions $(\varphi^0_f, \varphi^0_s, \upsilon^0)$ *of homogenized problem;*
b) Recovered microscopic diffusion velocity on the RPC Y.

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