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NUMERICAL SIMULATION OF QUASI-STATIC MODEL OF IONIC TRANSPORT THROUGH DEFORMABLE POROUS MEDIA

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Abstract: The paper deals with the computational model of quasi-static transport of 2-component electrolyte solution transport trough deformable porous medium respecting material microstructure. The multiscale approach is used to derive effective tensors describing macroscopic homogenized body. Numerical simulation are performed in order to test the derived model on the simple microscopic and macroscopic geometries.

Keywords: ionic trasport, homogenization, electro-mechanical coupling

Introduction

Transport of an electrolyte solution through porous media is widely studied problem with numerous applications in geoscience or the research of fuel cells. In the context of geoscience it was explored by authors [3], [4] as a means to model clay swelling.

However, this approach can be also used in modeling of biological tissues, namely the cortical bone tissue. The cortical bone has strictly hierarchical structure with multiple scales. On the canaliculo-lacunar scale it consist of system small interconnected channels saturated by bone fluid, which can be considered as a incompressible solvent of sodium cations and chloride anions. The bone tissue matrix can be consider deformable and it exhibits a small negative charge. At interface between these two phases a separation of positive and negative charge components occurs. This effects lead to a formation of so-called electrical double layer (EDL), which describes the ionic charge distribution in electrolyte in proximity of charged pore surface. Due to the motion or the loading of the bone tissue, there occurs the ionic transport inside the canaliculo-lacunar network. Thus, the ionic transport models are suitable to the modeling of electro-mechanical coupling in the cortical bone tissue.

The aim of this paper is to develop computational model of quasi-static transport of 2-component electrolyte solution transport trough deformable porous medium respecting material microstructure, which may be applied easily to cortical bone tissue modeling in future.

Mathematical model

Mathematical model of the ionic transport through porous media is based on the description of processes in the fluid and solid phases and on their interface. After the literature research of available mathematical models we adopted the model published in [1], which deals with the stationary case and then modified to quasi-stationary case.

Porous medium occupies a bounded domain Ω with characteristic dimension L_c an it is composed of fluid and solid phases. The fluid phase Ω_f consists of the pore space saturated by an electrolyte solution. The solid matrix is then defined as $\Omega_s = \Omega \setminus \overline{\Omega}_f$ and solid-fluid interface as $\Gamma = \partial\Omega_s \cap \partial\Omega_f$. The subscripts $\sqcup_s$ and $\sqcup_f$ will also appear in the rest of the text to denote constants and variables belonging to the respective phase.

For the purpose of the multi-scale modeling we consider macroscopic domain Ω generated as a lattice

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of periodically repeated cell (RPC) Y with characteristic dimension l. It has a composition similar to the Ω, i.e. it is divided into two sub domains Y_s and Y_f with interface Γ_Y, such that

$$Y = Y_s \cup Y_f \cup \Gamma_Y, \quad Y_f = Y \setminus \bar{Y}_s, \quad \Gamma_Y = \bar{Y}_s \cap \bar{Y}_f. \tag{1}$$

The geometry of the RPC Y should reflect the idealized microstructure of domain Ω. It is usually assumed to have a unit side length, i.e. it has the measure $|Y| = 1$.The ration between macroscopic and microscopic scale defines so-called scale parameter $\varepsilon = l/L_c, 0 < \varepsilon \ll 1$ and represents the smallest zoom, by which the microstructure becomes visible from the macroscopic point of view.

Processes in fluid phase

The fluid phase is assumed to be an electrolyte solution of two ionic species (further indexed by $\alpha = 1, 2$) with different valencies $z_1 = -1, z_2 = 1$ and characterized by different concentration c_α. the solvent is considered to be incompressible. The pore surface is charged by small surface charge $-\Sigma$.

Transport of the ions is influenced by three processes. The first one is the convective movement characterized by convective velocity $\mathbf{w}$, the second one is the diffusion of ions in the solvent proportional to diffusivity of the α-th ionic species D_α and the third one is the effect on the movement of electrically charged particles in the electrical field of solid-phase $\mathbf{E}$. There is no ionic exchange between the phases, thus the migration-diffusion fluxes $\mathbf{j}_\alpha$ are zero on the solid-fluid interface.

Each of the ionic species (indexed by $\alpha = 1, 2$) fulfills the Eulerian mass conservation law,

$$\frac{\partial c_\alpha}{\partial t} + \nabla \cdot (\mathbf{j}_\alpha + \mathbf{w} c_\alpha) = \frac{\partial c_\alpha}{\partial t} + \nabla \cdot \left(-\frac{c_\alpha D_\alpha}{k_B T} \left(\frac{k_B T}{c_\alpha} \nabla c_\alpha + e z_\alpha \nabla \Psi \right) + \mathbf{w} c_\alpha \right) = 0 \qquad \text{in } \Omega_f \tag{2}$$

$$\mathbf{j}_\alpha \cdot \mathbf{n} = 0 \qquad \text{on } \Gamma, \alpha = 1, 2, \tag{3}$$

where $\mathbf{n}$ is the unit exterior normal to Ω_f.

The electrokinetics of the fluid phase is characterized by electrostatic potential Ψ, which is given as a solution to the Poisson problem,

$$\mathcal{E} \nabla^2 \Psi = -e \sum_{\beta=1}^{N=2} z_\beta c_\beta \quad \text{in } \Omega_f, \tag{4}$$

$$\mathcal{E} \nabla \Psi \cdot \mathbf{n} = -\Sigma \quad \text{on } \Gamma. \tag{5}$$

where $\mathcal{E}$ is dielectric coefficient of the solvent. The corresponding electrical field is $\mathbf{E} = -\nabla \Psi$.

The fluid velocity $\mathbf{v}$ is governed by the equilibrium equation for the fluid,

$$-\nabla \cdot \boldsymbol{\sigma}_f = \mathbf{f} \quad \text{in } \Omega_f, \tag{6}$$

$$\boldsymbol{\sigma}_f = -p\mathbf{I} + 2\eta_f \mathbf{e}(\mathbf{v}) + \mathcal{E} \left(\mathbf{E} \otimes \mathbf{E} - \frac{1}{2} |\mathbf{E}|^2 \mathbf{I} \right), \tag{7}$$

$$\nabla \cdot \mathbf{v} = 0 \quad \text{in } \Omega_f, \tag{8}$$

where $\mathbf{f}$ is the external body force, $\boldsymbol{\sigma}_f$ is the stress tensor of the fluid phase, $\mathbf{e}(\mathbf{v}) = \frac{1}{2} \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^{\mathrm{T}} \right)$, p is the fluid pressure and η_f is the dynamic viscosity of the electrolyte.

Let us note that, in the quasi-stationary problem, the convective velocity takes into account the solid deformation $\mathbf{u}$ extending to the fluid part. Thus, it is defined as $\mathbf{w} = \mathbf{v} - \partial_t \mathbf{u}$.

Processes in solid phase

The porous body is considered to be deformable, with usual assumptions of linear elasticity, small displacement $\mathbf{u}$ and small deformations. As the pores are saturated by electrolyte solution, the continuity of stresses in both the phases on solid-fluid interface has to be ensured. This can be expressed by the following system of equations,

$$-\nabla \cdot \boldsymbol{\sigma}_s = \mathbf{f} \quad \text{in } \Omega_s, \tag{9}$$

$$\boldsymbol{\sigma}_s = \mathbf{A}\mathbf{e}(\mathbf{u}), \tag{10}$$

$$\mathbf{v} = \partial_t \mathbf{u} \quad \text{on } \Gamma, \tag{11}$$

$$\boldsymbol{\sigma}_f \cdot \mathbf{n} = \boldsymbol{\sigma}_s \cdot \mathbf{n} \quad \text{on } \Gamma, \tag{12}$$

where $\mathbf{e}(\mathbf{u}) = \frac{1}{2}\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^{\mathrm{T}}\right)$ is strain tensor and $\mathbf{A} = \{A_{ijkl}\}$ is the symmetric positive definite tensor of elasticity.

Homogenization

Before we perform homogenization procedure, it is beneficial to transform the system of equation 2-12 in its dimensionless form. That can be achieved by the suitable choice of characteristic quantities and by spacial scaling of the operator ∇. The dimensionless scaled quantities are further denoted by $\sqcup^{\varepsilon}$ and forcing terms are further denoted by $\sqcup^{*}$.

The dimensionless system of equations then needs to be linearized. This is possible under the assumption of sufficiently small applied fields $\Psi^{\mathrm{ext},*}$ and $\mathbf{f}^{*}$. Then the system is only slightly perturbed from equilibrium and all the unknowns can be rewritten in terms of their solutions in equilibrium and their perturbations denoted by δ, so that (for any dimensionless quantity φ^{ε})

$$\varphi^{\varepsilon}(x) = \varphi^{\mathrm{eq}}(x) + \delta\varphi^{\varepsilon}(x), \tag{13}$$

where $\sqcup^{\mathrm{eq}}$ indicates equilibrium quantities corresponding to $\mathbf{f}^{*} = 0$ and $\Psi^{\mathrm{ext},*} = 0$.

It can be shown ([2]), that equilibrium quantities are

$$\mathbf{w}^{\mathrm{eq},\varepsilon} = 0, \qquad p^{\mathrm{eq},\varepsilon} = \sum_{j=1}^{N=2} c_{\beta}^{b} \exp(-z_j \Psi^{\mathrm{eq},\varepsilon}), \tag{14}$$

$$c_{\alpha}^{\mathrm{eq},\varepsilon}(x) = c_{\alpha}^{b} \exp(-z_j \Psi^{\mathrm{eq},\varepsilon}(x)). \tag{15}$$

Since the concentrations have Boltzmann distribution, in equilibrium, they can be computed from the equilibrium potentials. The problem of computing equilibrium potential can be transfered onto the microscopic cell and it needs to be solved before computing cell problems.

The linearization not only simplifies nonlinear terms, but also enables us to solve the three homogenization problems separately: homogenization of electrokinetic system, homogenization of potential perturbation and homogenization of displacement perturbation.

The unfolding homogenization method is used for derivation of the cell problems. This method assumes the periodic microstructure and enables us to translate the problem from domain Ω into the RPC Y. We shall obtain so-called cells problems with solutions constitued by seven families of responses:

- response to the macroscopic pressure gradient $(\boldsymbol{\omega}^{0,k}, \pi^{0,k}\theta_j^{0,k})$,
- response to macroscopic diffusive flux $(\boldsymbol{\omega}^{i,k}, \pi^{i,k}, \theta_{\beta}^{i,k})$,
- response on displacement velocity $(\boldsymbol{\omega}^{u,k}, \pi^{u,k}, \theta_{\beta}^{u,k})$,
- auxiliary cell problem with solution ϖ^{β}
- elastic response on deformation $\mathbf{w}^{ij}$
- response to the pressure $\mathbf{w}^{P}$
- elastic response to the potential perturbation $\mathbf{w}^{i}$

Having obtained the responses on RPC Y as the solutions of thecell problems, we may finally quantify effective tensors.

Macroscopic problem

The homogenization procedure provides the effective tensors. The tensors relevant to the ionic transport are the permeability $\mathbf{K}$, the migration-diffusion tensors $\mathbf{J}_i$, the Onsager tensors $\mathbf{L}_i$, the diffusivity tensors $\mathbf{D}_{ij}$ and two new tensors $\mathbf{U}$ and $\mathbf{M}$ which ensure the stronger coupling between electrokinetic system and elasticity. Further, the modified Biot's poroelasticity coefficients are obtained, the elasticity tensor $\mathbb{A}^H$, the Biot's tensor $\mathbf{B}^H$, and the ionic potential tensor $\mathbf{C}^H$.

The effective tensors related to electrokinetic system read, as follows:

$$J_{lk}^{\alpha} = \fint_{Y_f} \boldsymbol{\omega}^{\alpha,k}(y) \cdot \mathbf{e}^l \,\mathrm{dV}, \tag{16}$$

$$D_{lk}^{\alpha\beta} = \fint_{Y_f} \left(\boldsymbol{\omega}^{\alpha,k}(y) + \frac{z_\beta}{\mathrm{Pe}_\beta} \left(\mathbf{e}^k \delta_{\alpha\beta} + \nabla_y \theta_\beta^{\alpha,k}(y) \right) \right) \cdot \mathbf{e}^l \,\mathrm{dV}, \tag{17}$$

$$K_{lk} = \fint_{Y_f} \boldsymbol{\omega}^{0,k}(y) \cdot \mathbf{e}^l \,\mathrm{dV}, \tag{18}$$

$$L_{lk}^{\alpha} = \fint_{Y_f} \left(\boldsymbol{\omega}^{0,k}(y) + \frac{z_\beta}{\mathrm{Pe}_\alpha} \nabla_y \theta_\alpha^{0,k}(y) \right) \cdot \mathbf{e}^l \,\mathrm{dV}, \tag{19}$$

$$\mathbf{U}_{lk} = \fint_{Y_f} \boldsymbol{\omega}^{u,k}(y) \cdot \mathbf{e}^l \,\mathrm{dV}, \tag{20}$$

$$\mathbf{M}_{lk}^{\alpha} = \fint_{Y_f} c_\beta^{\mathrm{eq}}(y) \left(\boldsymbol{\omega}^{u,k}(y) + \frac{z_\beta}{\mathrm{Pe}_\beta} \left(-h_c \mathbf{e}^k + \nabla_y \breve{\theta}_j^k(y) \right) \right) \cdot \mathbf{e}^l \,\mathrm{dV}. \tag{21}$$

Symbol $\boldsymbol{\Pi}^{ij}$ denotes the so-called transformation vectors $\boldsymbol{\Pi}^{ij} = (\Pi_k^{ij}), i, j, k = 1, \ldots, d, (d = 3)$, which can transform the macroscopic deformation $\delta \mathbf{u}_0(x)$ from Ω into the coordinate system of RPC Y, as follows $\Pi_k^{ij} = y_j \delta_{ik}$.

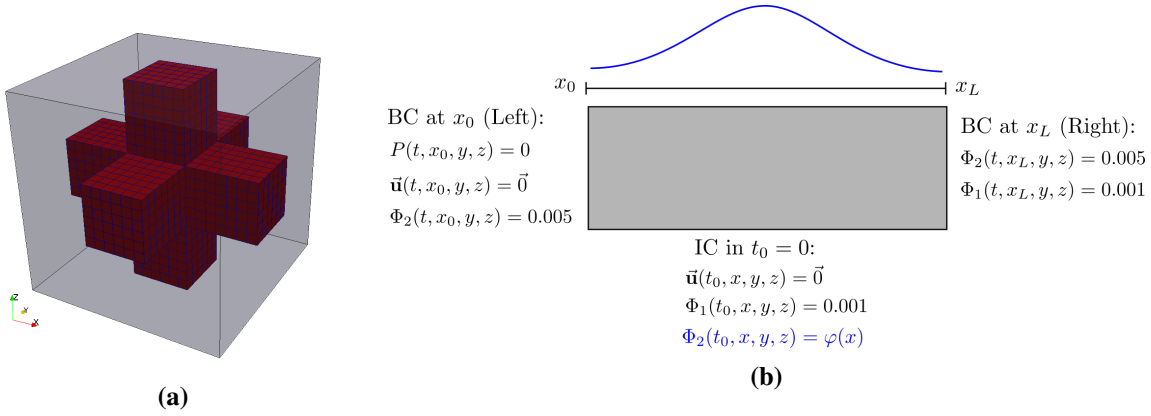
Effective tensors related to extended Biot poroelasticity read

$$A_{ijkl}^H = \fint_{Y_s} \mathbf{A}^* \nabla(\mathbf{w}^{ij} + \boldsymbol{\Pi}^{ij}) : \nabla(\mathbf{w}^{kl} + \boldsymbol{\Pi}^{kl}) \,\mathrm{dV}, \tag{22}$$

$$B_{ij}^H = -\fint_{Y_s} \mathbf{A}^* \nabla(\mathbf{w}^P : \nabla \boldsymbol{\Pi}^{ij}) \,\mathrm{dV}, \tag{23}$$

$$\begin{aligned} C_{ij}^{\alpha} = & \fint_{Y_s} \mathbf{A}^* \nabla(\mathbf{w}^{\alpha}) \,\mathrm{dV} + \sum_{\beta=1}^{N=2} z_\beta \mathbf{I} \fint_{Y_f} c_\beta^0(y) \left(\varpi^\beta(y) + \delta_{\alpha\beta} \right) \,\mathrm{dV} + \\ & + \fint_{Y_f} \frac{1}{\gamma} \left(\nabla_y \Psi^{\mathrm{eq}} \otimes \nabla_y \varpi^\alpha + \nabla_y \varpi^\alpha \otimes \nabla_y \Psi^{\mathrm{eq}} - \nabla_y \Psi^{\mathrm{eq}} \cdot \nabla_y \varpi^\alpha \mathbf{I} \right) \,\mathrm{dV}. \end{aligned} \tag{24}$$

Now we can state the dimensionless macroscopic homogenized system of equations, where all ex-



(a) **(b)**

Figure 1: (a): Geometry of RPC Y used in numerical simulations; (b): Boundary and initial conditions used in numerical simulation

ternal forces are omitted: Find $(P^0, \Phi^0_\beta, \delta\mathbf{u}^0), \beta = 1, 2$, such that

$$\int_\Omega \mathbf{K}\nabla_x P^0 \nabla_x q \,\mathrm{dV} - \sum_{\beta=1}^{N=2} \int_\Omega \mathbf{J}^\beta \nabla_x \Phi^0_\beta \nabla_x q \,\mathrm{dV} + \int_\Omega \mathbf{U}\delta\mathbf{u}^0 \nabla_x q \,\mathrm{dV} = 0, \quad (25)$$

$$\frac{|Y_f|}{|Y|}\int_\Omega \partial_t c^{\mathrm{eq}}_\alpha + \int_\Omega \mathbf{L}^\alpha \nabla_x P^0 \nabla_x s \,\mathrm{dV} - \sum_{\beta=1}^{N=2} \int_\Omega \mathbf{D}^{\alpha\beta} \nabla_x \Phi^0_\beta \nabla_x s \,\mathrm{dV} + \int_\Omega \mathbf{M}^\alpha \delta\mathbf{u}^0 \nabla_x s \,\mathrm{dV} = 0, \quad (26)$$

$$\int_\Omega \mathbb{A}^H e_x(\delta\mathbf{u}^0) : e_x(\mathbf{r}) \,\mathrm{dV} + \int_\Omega \hat{\mathbf{B}}^H P^0 : e_x(\mathbf{r}) \,\mathrm{dV} - \sum_{j=1}^{N=2} \int_\Omega \mathbf{C}^\beta \Phi^0_\beta : e_x(\mathbf{r}) \,\mathrm{dV} = 0, \quad (27)$$

for any test functions $q \in L^2(\Omega)$, $s \in L^2(\Omega)$ and $\mathbf{r} \in H^1(\Omega)^d$ and where $\hat{\mathbf{B}}^H = |Y_f|\mathbf{I} - \mathbf{B}^H$.

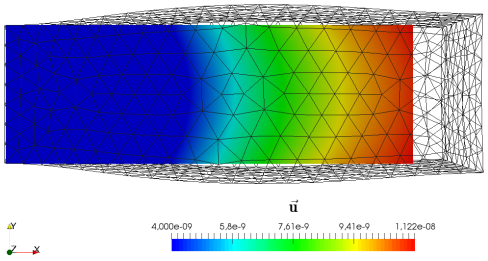
Numerical simulations

The numerical implementation of the homogenization procedure and the homogenized model completed by suitable choice of initial and boundary conditions was made in python based FEM software *SfePy*. For the homogenization, the simple geometry of RPC Y was used as to represent interconnected system of channels through cortical bone, see Fig.1a. Computed effective tensors were then used in implementation of the macroscopic problem.

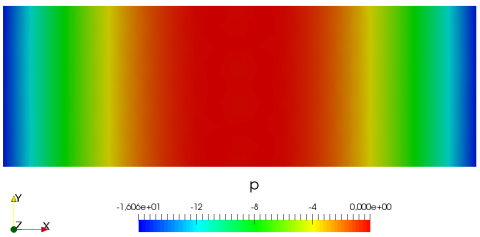
Macroscopic equations were completed by a set of boundary and initial conditions, which can be found in Fig.1b. Macroscopic problem was computed on the simple cuboid geometry. Resulting macrosopic fields $(P^0, \Phi^0_\beta, \delta\mathbf{u}^0), \beta = 1, 2$ are shown in Fig.2. It is evident that the shape of function $\varphi(x)$ prescribed as initial condition of Φ^0_2 influences the resulting shape of pressure P^0 and potential Φ^0_1 as well. The visualization of macroscopic displacement $\mathbf{u}^0$ shows swelling in response to the potential Φ^0_2 distribution.

Conclusion

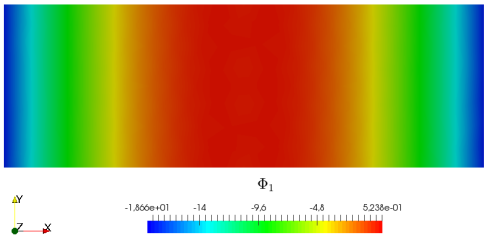
Based on the literature research, suitable model considering rigid porous medium which can be easily expanded to the case of deformable porous medium was adopted. Mathematical model was transformed into dimensionless form and then linearized, which simplified the homogenization procedure. Then, unfolding homogenization method was used to derive effective tensors and macroscopic problem equations.



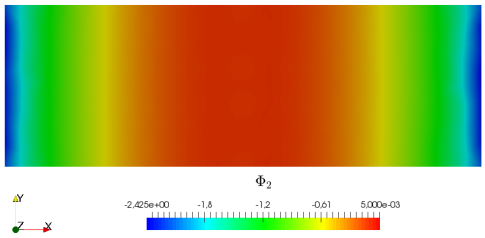
(a) Distribution of displacement $\mathbf{u}^0$, $10^8\times$ enlarged



(b) Distribution of global pressure P^0



(c) Distribution of ionic potential Φ_1^0



(d) Distribution of ionic potential Φ_2^0

Figure 2: Solution of homogenized macroscopic problem

The local microscopic as well as the macroscopic problems were implemented in the open source software *SfePy*. The simple geometrical representation of microstructure was used so that homogenization results can be easily interpreted. The resulting effective coefficients were used in the solution of Dirichlet boundary macroscopic problem.

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