Mechanically-induced solute transport in a saturated elastic porous medium : analysis by homogenization

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ABSTRACT

Using the homogenization method, we derive a macroscopic model that describes the advective-diffusive transport of a solute within a deformable elastic saturated porous medium. The macroscopic solute transport equation contains a coupling term which reveals a mechanically-induced solute transport mechanism.

INTRODUCTION

A cyclic loading applied on a saturated deformable porous medium is known to increase the solute transport [1]. This effect is of major interest when dealing for instance with the design of drug delivery system [2]. This transport enhancement mechanism also participates in the cell nutrients transfer through avascular biological tissue such as articular cartilage or intervertebral disk [3; 4]. Several experimental and numerical works have focused on the identification of the main parameters (frequency, amplitude, ...) that govern this mechanism. Thus, numerical models are usually based on a poro-elastic formulation coupled to an advective-diffusive equation both written directly at the macroscopic scale. This has been done without wondering if coupling effects between solute transport and mechanical behavior could affect these classical macroscopic equations.

Therefore, we propose to revisit this issue by means of a theoretical upscaling procedure to rigorously determine the macroscopic equations that describe transient advective-diffusive solute transport in a saturated deformable elastic porous media. To upscale the local description, we use the homogenization method for periodic structures, also called the homogenization method of multiple scales asymptotic expansions [5], and the methodology introduced in [6] is applied.

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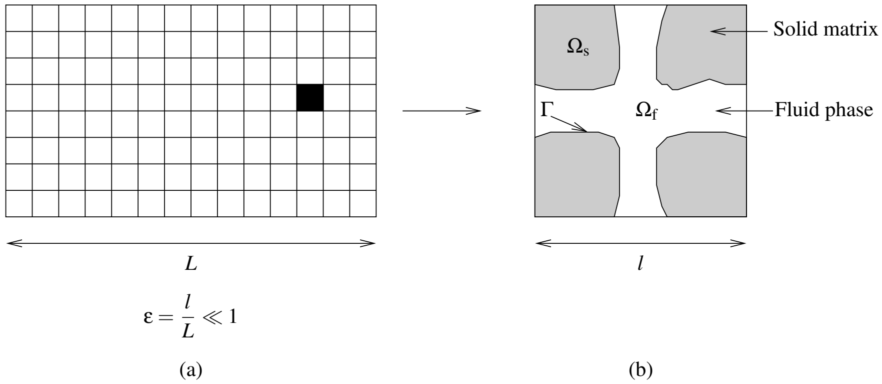

Figure 1 : *Porous medium : (a) Macroscopic sample ; (b) Periodic unit cell.*

HOMOGENEISATION

Medium under consideration

The method of multiple scales is based upon the fundamental assumption of separation of scales. The condition of periodicity is also required, which has no impact upon the form of the macroscopic description. We thus consider a periodic porous medium, of macroscopic characteristic size L, and made of a solid matrix and of a fluid-saturated pore space. We further denote the periodic cell by Ω, its characteristic length by l, and we formulate the condition of separation of scales by $\varepsilon = \dfrac{l}{L} \ll 1$.

Within the periodic cell, we denote by Ω_f the pore domain, by Ω_s the solid matrix, and by Γ their common interface, as depicted in Fig. 1. Using the two characteristic length, l and L, and the physical space variable, $\vec{X}$, we define two dimensionless space variables: $\vec{y} = \vec{X}/l$, $\vec{x} = \vec{X}/L$

Since the condition of separation of scales ($\varepsilon \ll 1$) is supposed to be satisfied, then variables $\vec{y}$ and $\vec{x}$ can be considered as two independent space variables: $\vec{y}$ describes the local scale, while $\vec{x}$ is the macroscopic space variable. As a consequence, the unknown fields (stress tensors, displacements, fluid velocity and pressure, ...) are, a priori, functions of both space variables $\vec{y}$ and $\vec{x}$. Invoking the differentiation rule for multiple variables, the gradient operator with respect to the physical variable, $\vec{X}$, is written as

$$\nabla_X = \frac{1}{l}\nabla_y + \frac{1}{L}\nabla_x \qquad (1)$$

Dimensionless pore-scale description

The methodology introduced in [6] firstly consists in writing the dimensionless pore-scale description, which is the set of dimensionless equations that describe the phenomena being considered within the periodic unit cell depicted in Fig. 1. Each quantity in a dimensionless equation is the ratio of its physical counterpart to its characteristic value (indexed by *). This writing gives rise to dimensionless numbers, which are defined by means of characteristic values. We consider the elasticity equations in the solid domain Ω_s, the equations of flow for a Stokesian fluid and the convection-diffusion equation for the solute in the fluid-saturated pore domain Ω_{f}, together with the boundary conditions over the interface Γ. The dimensionless writing of the equations requires the choice of a characteristic length for the dimensionless writing of space derivatives. We arbitrarily choose L as the reference characteristic length. The dimensionless gradient operator is thus given by:

$$\nabla = L\nabla_X = \varepsilon^{-1}\nabla_y + \nabla_x \tag{2}$$

The dimensionless pore-scale description being considered is given by the equations presented below.

Equations in the solid domain Ω_{s}

$$\nabla \cdot \sigma_{\mathrm{s}} = \vec{0} \tag{3}$$

$$\sigma_{\mathrm{s}} = a : e(\vec{u}_{\mathrm{s}}) \tag{4}$$

Equations of fluid motion in Ω_{f}

$$\mathbb{F}_{\mathrm{L}}\, \Delta \vec{v}_{\mathrm{f}} - \nabla p_{\mathrm{f}} = \vec{0} \tag{5}$$

$$\nabla \cdot \vec{v}_{\mathrm{f}} = 0 \tag{6}$$

where $\mathbb{F}_{\mathrm{L}}$ is a dimensionless number, defined by $\mathbb{F}_{\mathrm{L}} = \dfrac{\mu v_{\mathrm{f}}^{*}}{p_{\mathrm{f}}^{*} L}$

Advective-diffusive solute transport in Ω_{f}

$$\mathbb{N}_{\mathrm{L}} \frac{\partial c}{\partial t} + \mathbb{P}e_{\mathrm{L}} \nabla \cdot (\vec{v}_{\mathrm{f}}\, c) = \Delta c \tag{7}$$

where the dimensionless numbers are defined by $\mathbb{N}_{\mathrm{L}} = \dfrac{L^2}{D t}$ and $\mathbb{P}e_{\mathrm{L}} = \dfrac{v_{\mathrm{f}}^{*} L}{D}$

Conditions over the interface Γ

$$\sigma_{\mathrm{f}} \cdot \vec{n} = \sigma_{\mathrm{s}} \cdot \vec{n} \tag{8}$$

$$\vec{v}_{\mathrm{f}} = \frac{\partial \vec{u}_{\mathrm{s}}}{\partial t} \tag{9}$$

$$\nabla c \cdot \vec{n} = 0 \tag{10}$$

Estimation of the dimensionless numbers

The methodology introduced in [6] consists in estimating the dimensionless numbers with respect to ε. As we are interested in the case which leads to a diphasic macroscopic behavior for the fluid/solid system, the case where fluid motion is generated must be considered, which corresponds to the order [6]

$$\mathbb{F}_{\mathrm{L}} = O(\varepsilon^2) \tag{11}$$

It has been shown in [7] that in rigid porous media, a transient advective-diffusive macroscopic solute transport is obtained when

$$\mathbb{N}_{\mathrm{L}} = O(\varepsilon^0) \qquad \mathbb{P}e_{\mathrm{L}} = O(\varepsilon^0) \tag{12}$$

Homogenization procedure

The homogenization method being used is an asymptotic approach. It is therefore based upon the fundamental statement that the physical unknowns fields can be written in the form of asymptotic expansions in powers of ε:

$$\psi = \psi^{(0)}(\vec{y},\vec{x}) + \varepsilon\psi^{(1)}(\vec{y},\vec{x}) + \varepsilon^2\psi^{(2)}(\vec{y},\vec{x}) + \ldots \tag{13}$$

in which functions $\psi^{(i)}$ are Ω-periodic in variable $\vec{y}$, with $\psi = \sigma_\mathrm{s}$, σ_f, p_f, c, $\vec{v}_\mathrm{f}$, $\vec{u}_\mathrm{s}$. The method consists in incorporating the asymptotic expansions in the dimensionless local description (Eqs. 3-10), while replacing the dimensionless numbers by their orders of magnitude in power of ε (Eqs. 11-12) and taking into account the expression of the dimensionless gradient operator (Eq. 2). This leads to approximated governing equations and boundary conditions at the successive orders, which together with the condition of periodicity define well posed boundary-value problems in the periodic unit cell. Existence of solutions requires that volume averaged equations be satisfied. These latter actually describe the macroscopic behavior at successive orders.

Macroscopic model for the fluid/solid system

Homogenization of the fluid/solid equations has been performed in [8]. It leads to the following macroscopic model, which is identical to Biot's model of consolidation:

$$\nabla_x \cdot < \sigma^{(0)} > \; = \; \vec{0} \tag{14}$$

$$< \sigma^{(0)} > \; = \; \mathbf{C} : e\left(\vec{u}_\mathrm{s}^{(0)}\right) - \alpha\, p_\mathrm{f}^{(0)} \tag{15}$$

$$\nabla_x \cdot \left(< \vec{v}_\mathrm{f}^{(0)} > - \phi \frac{\partial \vec{u}_\mathrm{s}^{(0)}}{\partial t} \right) \; = \; \alpha\, tr\left(\dot{e}\left(\vec{u}_\mathrm{s}^{(0)}\right)\right) - \beta \frac{\partial p_\mathrm{f}^{(0)}}{\partial t} \tag{16}$$

$$< \vec{v}_\mathrm{f}^{(0)} > - \phi \frac{\partial \vec{u}_\mathrm{s}^{(0)}}{\partial t} \; = \; -\mathbf{K}\, \nabla_x p_\mathrm{f}^{(0)} \tag{17}$$

where $< \sigma^{(0)} >$ is the first-order averaged total stress tensor, $\mathbf{C}$ is the effective elastic tensor, α represents the elasticity coefficient of Biot, β is the medium compressibility, $\mathbf{K}$ denotes the permeability tensor. The term $< \vec{v}_\mathrm{f}^{(0)} > - \phi \frac{\partial \vec{u}_\mathrm{s}^{(0)}}{\partial t}$ is the fluid relative velocity. The porosity ϕ is defined by:

$$\phi = \frac{| \Omega_\mathrm{f} |}{| \Omega |} \tag{18}$$

The distinct avegares being introduced are defined by:

$$< \psi > = < \psi >^\mathrm{s} + < \psi >^\mathrm{f} \tag{19}$$

where

$$< \psi >^\mathrm{s} = \frac{1}{| \Omega |} \int_{\Omega_\mathrm{s}} \psi \, d\Omega \qquad < \psi >^\mathrm{f} = \frac{1}{| \Omega |} \int_{\Omega_\mathrm{f}} \psi \, d\Omega \tag{20}$$

Details on the derivation of the above model can be found in [8].

Homogenization of transport equations

Determination of $c^{(0)}$ and $c^{(1)}$

At the first two orders, we get boundary-value problems which are identical to those obtained in a rigid porous medium [7]. They lead to:

$$c^{(0)} = c^{(0)}(\vec{x},t) \quad \text{and} \quad c^{(1)} = \vec{\chi}\cdot\nabla_x c^{(0)} \tag{21}$$

where $\vec{\chi}$ is defined by the local problem to be solved on the unit cell:

$$\left\{\begin{array}{rcll} \nabla_y\cdot(\nabla_y\vec{\chi}+\mathbf{I}) & = & \vec{0} & \text{in } \Omega_\text{f} \\ (\nabla_y\vec{\chi}+\mathbf{I})\cdot\vec{n} & = & \vec{0} & \text{on } \Gamma \\ <\vec{\chi}>^\text{f} & = & \vec{0} & \text{and} \quad \vec{\chi} \text{ is } \Omega\text{-periodic} \end{array}\right. \tag{22}$$

Determination of the first-order macroscopic description

At the third-order, transport equations lead to the following system:

$$\left\{\begin{array}{rcll} \dfrac{\partial c^{(0)}}{\partial t} - \nabla_y\cdot\left(\nabla_y c^{(2)} + \nabla_x c^{(1)} - c^{(0)}\vec{v}_\text{f}^{(1)} - c^{(1)}\vec{v}_\text{f}^{(0)}\right) & & & \\ -\nabla_x\cdot\left(\nabla_y c^{(1)} + \nabla_x c^{(0)} - c^{(0)}\vec{v}_\text{f}^{(0)}\right) & = & 0 & \text{in } \Omega_\text{f} \\ \left(\nabla_y c^{(2)} + \nabla_x c^{(1)}\right)\cdot\vec{n} & = & 0 & \text{on } \Gamma \\ \vec{v}_\text{f}^{(0)} & = & \dfrac{\partial \vec{u}_\text{s}^{(0)}}{\partial t} & \text{on } \Gamma \end{array}\right. \tag{23}$$

Integrating the first equation over the period yields:

$$\phi\frac{\partial c^{(0)}}{\partial t} - \nabla_x\cdot\left(\mathbf{D}^{eff}\nabla_x c^{(0)}\right) + \left(<\vec{v}_\text{f}^{(0)}> - \phi\frac{\partial \vec{u}_\text{s}^{(0)}}{\partial t}\right)\cdot\nabla_x c^{(0)} + \frac{\partial \vec{u}_\text{s}^{(0)}}{\partial t}\cdot\mathbf{T}\,\nabla_x c^{(0)} = 0 \tag{24}$$

where the effective diffusion tensor $\mathbf{D}^{eff}$ and the tortuosity tensor $\mathbf{T}$ are defined by:

$$\mathbf{T} = \frac{1}{|\,\Omega\,|}\int_{\Omega_\text{f}} (\nabla_y\vec{\chi}+\mathbf{I})\; d\Omega \qquad \text{and} \qquad \mathbf{D}^{eff} = D\mathbf{T} \tag{25}$$

CONCLUSIONS AND PERSPECTIVES

By means of a homogenization procedure, the macroscopic solute transport equation (Eq. 24) that describe transient advective-diffusive solute transport in an elastic porous media can be written in a simpler manner:

$$\phi\frac{\partial c}{\partial t} + \phi\left(\vec{V}_\text{f} - \vec{V}_\text{s}\right)\cdot\nabla c + \vec{V}_\text{s}\cdot\mathbf{T}\,\nabla c = \nabla\cdot\left(\mathbf{D}^{eff}\nabla c\right) \tag{26}$$

where $\vec{V}_\text{f}$ and $\vec{V}_\text{s}$ denote the fluid and solid intrinsic macroscopic velocities. Besides the usual accumulation, advection and effective diffusion terms, the coupling term $\vec{V}_\text{s}\cdot\mathbf{T}\,\nabla c$ is emerging from the scale transition. This term is associated with the no-slip boundary condition at the fluid-solid interface and characterizes a mechanically-induced solute transport mechanism. It can be seen as a convective transport in the boundary layer moving at the solid phase velocity. It is weighted by the tortuosity tensor **T** that represent a geometrical property of the unit cell micro-structure, for isotropic porous media it comes down to a scalar ranging from 0 to 1. An important feature of this coupling term is that it occurs only whenever there exits macroscopic advection: it does not appear in the case of a purely diffusive solute transport.

The influence of this additional term should be negligible in classical cases of consolidating porous media. Nevertheless, when focusing on solute transport in porous media submitted by cyclic loading, the cumulative effect of this mechanically-induced transport mechanism may become predominant. Experimental evidence of this term may be tricky to bear out. However, a numerical approach would bring some interesting features. These development have been done with specific orders of the dimensionless numbers $\mathbb{F}_L$, $\mathbb{N}_L$ and $\mathbb{P}e_L$ (Eqs. 11 and 12). Future works will include the analysis of different cases and particularly for higher Péclet number where dispersive effects come up.

References

1. Mauck, R.L., C.T. Hung, and G.A. Ateshian. 2003. "Modelling of neutral solute transport in a dynamically loaded porous permeable gel: implications for articular cartilage biosynthesis and tissue engineering," *J Biomech. Eng.* 125:602–614.

2. Urciuolo, F., G. Imparato, and P. A. Netti. 2008. "Effect of Dynamic Loading on Solute Transport in Soft Gels Implication for Drug Delivery," *AIChE J.* 54:824–834.

3. Evans, R.C. and T.M. Quinn. 2006. "Dynamic Compression Augments Interstitial Transport of a Glucose-Like Solute in Articular Cartilage," *Biophysical Journal* 91:1541–1547.

4. O'Hara, B.P., J. Urban, and A. Maroudas. 1990. "Influence of cyclic loading on the nutrition of articular cartilage," *Ann Rheum Dis.* 49:536–539.

5. Sanchez-Palencia, E. 1980. *Non Homogeneous Media and Vibration Theory*. Lecture Notes in Physics, Springer-Verlag, New-York.

6. Auriault, J.-L. 1991. "Heterogeneous medium: is an equivalent macroscopic description possible?," *Int. J. Eng. Sci.* 29:785–795.

7. Auriault, J.-L. and P. Adler. 1995. "Taylor Dispersion in porous media: analysis by multiple scale expansions," *Advances in Water Resources* 18:217–226.

8. Auriault, J.-L. and E. Sanchez-Palencia. 1977. "Etude du comportement macroscopique d'un milieu poreux saturé déformable," *Journal de Mécanique* 16:37–53.