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Modeling moisture transport by periodic homogenization in unsaturated porous media

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Abstract
In this communication, we establish a macroscopic model of moisture transport in unsaturated porous media using periodic homogenization technique [6]. The dimensional analysis of the continuity equations for both liquid water and water vapor written at the pore scale lets appear dimensional numbers characterizing moisture transport. The asymptotic expansion of these equations leads to the classical Richards equation [4] which is justified rigorously this way. Moreover, we obtain an accurate definition of the homogenized diffusion tensor of moisture involving the geometric properties of the microstructure and known transport properties of the unsaturated porous medium. Finally, the domain of validity of Richards equation is specified through the order of magnitude of the dimensionless number considered.

Résumé
Dans cette communication, nous établissons par homogénéisation périodique [6] un modèle macroscopique du transport d'humidité dans les milieux poreux partiellement saturés. L'analyse dimensionnelle des équations de transport de l'eau liquide et de vapeur d'eau écrites à l'échelle locale fait apparaître des nombres sans dimension caractérisant le phénomène de transfert. Le développement asymptotique des équations conduit l'équation Richards classique [4] qui a été justifié rigoureusement. De plus, on obtient une définition précise du tenseur de diffusion homogénéisé tenant compte de la géométrie de la microstructure et des propriétés de transport connues du milieu poreux partiellement saturé. Finalement, le domaine de validité de l'équation de Richards a été spécifié grâce aux ordres de grandeurs des nombres sans dimension considérés.

1. INTRODUCTION

The mathematical problem of unsaturated water flow in a porous media has receive recently a large attention in the literature. Moisture damage is one of the most important factors liming a building's service life [7]. Indeed, in Civil Engineering, moisture transport in porous materials, as concrete, participates in mechanisms affecting the sustainability of buildings. The penetration of the major aggressive agents (chlorides, carbon dioxide ...) is closely related to the degree of saturation of the material [5].

This coupled transport of moisture and ions often tends to accelerate the mechanisms of chemical and physical degradation, and to reduce the service life of the concrete structures submitted to unsaturated environment. Theoretical studies are then required to model the process of mass transfer in unsaturated porous media to better understand the problems linked to durability of building materials. Many investigations have emphasized the intricate nature of this phenomenon. Among the major difficulties related to the description of transport processes in cement based materials is their intrinsic complexity. The following equation, known as Richards equation:

$$\frac{\partial\theta}{\partial t} - div(D_\theta \, grad\theta) = 0$$

is widely used to model the evolution of water content in a porous material kept in isothermal conditions, where θ is the moisture content. D_θ is the nonlinear moisture diffusivity tensor (or coefficient) which depends in a complicated way on the pore structure and capillary pressure, which in turn depends on the water content.
The main objective of this paper is to establish by periodic homogenization technique equations governing the moisture transport in unsaturated porous media in isothermal condition. Moreover, the approach addressed enables to specify the definition of the effective parameters involved (moisture, diffusivity tensor,...), and to clarify the domain of validity of the model obtained.

2. THE PERIODIC HOMOGENIZATION PROCEDURE

The periodic homogenization technique relies on the assumption that the microstructure of the material can be considered as periodical, i.e as the repetition of an elementary cell whose size and complexity depend on the real microstructure.
In general, even if this assumption is never verified exactly, it constitutes a good approximation of the reality if the elementary cell is sufficiently complex, and constitutes a kind of Representative Elementary Volume (R.E.V) defined by whitaker [8]. Once this assumption admitted, the fields involved (the volumetric mass of liquid water and of water vapor, the velocity of liquid water and of water vapor,...) and their derivatives must be considered as periodical for the problem to be mathematically consistent.

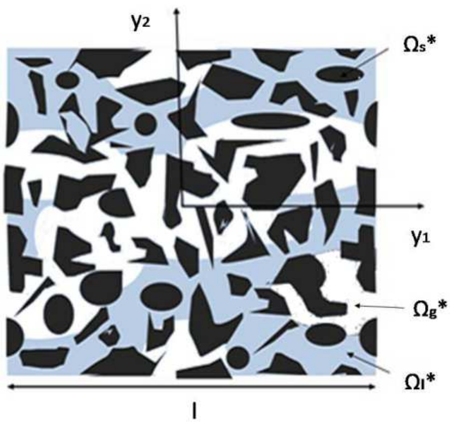

Figure 1: Example of elementary cell constituting the periodic microstructure.

Let us consider at the macroscopic scale that the material studied occupies the domain S^* of the three-dimensional space, whose characteristic length is L. At the macroscopic level, we denote $x^* = (x^*_1, x^*_2, x^*_3)$ a current point of S*. We assume that the material S^* has a periodic microstructure, or equivalently is constituted of the periodic repetition of an elementary cell: $\Omega^* = \Omega_l^*$ U Ω_g^*UΩ_s^*, where Ω_l^* denotes the liquid phase, Ω_g^* the gaseous phase, and Ω_s^* the solid phase (Fig.1). The boundary $\Gamma_l^*$of Ω_l^* is composed of the inner boundary Γ_{ls}^* between the liquid and the solid phases, of the inner boundary Γ_{lg}^* between the liquid and the gaseous phases, and of the part Γ_{ll}^* between the liquid phases of two neighboring cells. The same notations are used for the boundary $\Gamma_g^* = \Gamma_{gl}^*$U Γ_{gs}^*UΓ_{gg}^* of Ω_g^*. At the microscopic level, a current point of the elementary cell Ω^* is noted $y^* = (y^*_1, y^*_2, y^*_3)$. Moreover, the size l of the elementary cell Ω^* is assumed to be very small with respect to the dimension L of the structure. This is a condition of homogenizability of the problem. Thus the aspect ratio $\varepsilon = \frac{l}{L}$satisfies ε <<1.

3. TRANSPORT EQUATIONS IN UNSATURATED POROUS MEDIA

The continuity equations for the liquid water and for the water vapor with the associated boundary conditions at the local scale classically write:

$$\frac{\partial^* \rho_l^*}{\partial t^*} + div^*(\rho_l^* V_l^*) = 0 \quad \text{in} \quad \Omega_l^* \tag{1}$$

$$\frac{\partial^* \rho_v^*}{\partial t^*} - div^*(D_v^*\, grad^*\, \rho_v^*) = 0 \quad \text{in} \quad \Omega_g^* \tag{2}$$

where ρ_l^* and ρ_v^* denote respectively the mass of liquid water and water vapor per unit volume. D_v^* is the self-diffusion coefficient of water vapor in the gaseous phase and V_l^* the convection velocity of the liquid water. The liquid-solid interface Γ_{ls}^* is considered as a passive surface and the boundary conditions associated with equations (1) write:

$$V_l^*.n_{ls}^* = 0 \quad \text{on} \quad \Gamma_{ls}^* \tag{3}$$

where n_{ls}^* denotes the unit normal vector directed from the liquid domain Ω_l^* toward the solid domain Ω_s^*. The solid-gas interface Γ_{sg}^* is considered also as a passive interface and the boundary conditions associated with equation (2) write:

$$D_v^*\, grad^* \rho_v^*.n_{gs}^* \;=\; 0 \quad \text{on} \quad \Gamma_{gs}^* \tag{4}$$

where n_{gs}^* denotes the unit normal vector directed from the gas domain Ω_g^* toward the solid domain Ω_s^*. This Neumann boundary condition means that there is no exchange of water vapor between the solid and the gaseous phases. The boundary conditions at the liquid-gas interface Γ_{lg}^* are more complex. The flux of water vapor is directly linked to the evaporation / condensation velocity:

$$-D_v^*\, grad^* \rho_v^*.n_{gl}^* = \rho_v^*\, V_v^*.n_{gl}^* \quad \text{on} \quad \Gamma_{lg}^* \tag{5}$$

where n_{gl}^* denotes the unit normal vector directed from the gas domain Ω_g^* toward the liquid domain Ω_l^*. Moreover, the mass conservation (or the jump condition) associated with equations (1) and (2) writes:

$$(\rho_l^* V_l^* - \rho_l^* \omega_{lg}^*).n_{lg}^* = (D_v^* grad^* \rho_v^* + \rho_v^* \omega_{gl}^*).n_{gl}^* \tag{6}$$

4. DIMENSIONAL ANALYSIS OF EQUATION AND REDUCTION TO A ONE- SCALE PROBLEM

We define dimensionless physical data and dimensionless unknowns of the problem:

$$\begin{aligned} y &= \frac{y^*}{l}, \quad x = \frac{x^*}{L}, \quad t = \frac{t^*}{T_r}, \\ \rho_l = \frac{\rho_l^*}{\rho_r^l}, \quad D_v &= \frac{D_v^*}{D_v^r}, \quad \rho_v = \frac{\rho_v^*}{\rho_r^v}, \end{aligned} \tag{7}$$

$$V_l = \frac{V_l^*}{V_l^r}, \quad \omega_{lg} = \frac{\omega_{lg}^*}{\omega_{lg}^r}, \quad V_v = \frac{V_v^*}{V_v^r}$$

where the variabl ies and the new variables which appear (without a star) are dimens ss variables previously defined in equations (1)-(6), we obtain the dimensionless problem:

$$\tau_l \frac{\partial \rho_l}{\partial t} + div\,(\,\rho_l\, V_l\,) = 0 \quad \text{in} \quad \Omega_l \tag{8}$$

$$\tau_v \frac{\partial \rho_v}{\partial t} - div\,(\,D_v\, grad\rho_v\,) = 0 \quad \text{in} \quad \Omega_g \tag{9}$$

with the associated boundary conditions :

$$V_l.n_{ls} = 0 \quad \text{on} \quad \Gamma_{ls} \tag{10}$$

$$D_v\, grad\, \rho_v.n_{gs} = 0 \quad \text{on} \quad \Gamma_{gs} \tag{11}$$

$$-D_v\, grad\rho_v.n_{gl} = \gamma\, \rho_v\, V_v.n_{gl} \quad \text{on} \quad \Gamma_{lg} \tag{12}$$

and the dimensionless mass conservation on Γ_{lg}:

$$(\,\lambda\, \rho_l\, V_l - \zeta\, \rho_l\, \omega_{lg}\,).n_{lg} = (\,D_v\, grad\rho_v + \delta\, \rho_v\, \omega_{gl}\,).n_{gl} \tag{13}$$

Hence, the dimensional analysis of the transport equations of liquid water and water vapor naturally leads to the following dimensionless numbers characterizing moisture transfer in unsaturated porous media:

$$\begin{aligned} \tau_l &= \frac{t_l^{conv}}{T_L^r}, \quad \tau_v = \frac{t_v^{dif}}{T_V^r}, \quad \lambda = \frac{\lambda_l^{conv}}{\lambda_v^{dif}} \\ \zeta &= \frac{\omega_{lg}^r}{V_l^r}\lambda, \quad \delta = \frac{\rho_v^r}{\rho_l^r}\zeta, \quad \gamma = \frac{V_v^r}{\omega_{gl}^r l}\,\delta \end{aligned} \tag{14}$$

where

- τ_l represents the ratio of the characteristic time of convection $t_l^{conv} = \frac{l}{V_l^r}$ of the liquid water at the micro-scale to the characteristic time T_L^r of convection of the liquid water at the macro-scale.
- τ_v represents the ratio of the characteristic time of diffusion $t_v^{diff} = \frac{l^2}{D_v^r}$ of the water vapor at the micro-scale to the characteristic time T_V^r of diffusion of the water vapor at the macro-scale.
- λ is the ratio of the flux of the liquid water $\lambda_l^{conv} = \rho_l^r V_l^r$ to the flux of the water vapor $\lambda_v^{diff} = \frac{\rho_v^r D_v^r}{l}$.

The other dimensionless numbers are directly linked to λ. To apply the periodic homogenization procedure to the problem of moisture transport considered, we must first reduce our dimensionless problem to a one scale problem. To do this, $\varepsilon = \frac{l}{L}$ is chosen as the reference perturbation parameter and the other dimensionless numbers are linked to ε.

For a moderate convection of the liquid water, a strong diffusivity of the water vapor, and a moderate drying/wetting phenomenon, we obtain the following order of magnitude of the dimensionless numbers based on physical considerations:

$$\begin{aligned} \tau_l &= \mathcal{O}(\varepsilon)\,, \qquad \tau_v = \mathcal{O}(\varepsilon^3)\,, \\ \delta &= \mathcal{O}(\varepsilon^2), \qquad \gamma = \mathcal{O}(\varepsilon^2), \\ \lambda = \mathcal{O}(\varepsilon)\,, &\qquad \zeta = \mathcal{O}(\varepsilon) \end{aligned} \tag{15}$$

5. MACROSCOPIC MODEL FOR MOISTURE TRANSPORT

The classical procedure of periodic homogenization [6] leads to search the unknowns ρ_l, ρ_v, V_l , V_v and ω_{lg} of the problem as functions depending on the macroscopic variable *x*, on the microscopic variable *y*, and on the time *t*, considered as separate variables. This is justified because of the separation of scales ($\varepsilon \ll 1$). Moreover, the solutions ρ_l, ρ_v, V_l, V_v and ω_{lg} of the problem is postulated to admit a formal expansion with respect to ε [6]:

$$\begin{aligned} \rho_l &= \rho_l^0(x,y,t) + \varepsilon\, \rho_l^1(x,y,t) + \varepsilon^2\, \rho_l^2(x,y,t) + \ldots \\ \rho_v &= \rho_v^0(x,y,t) + \varepsilon\, \rho_v^1(x,y,t) + \varepsilon^2\, \rho_v^2(x,y,t) + \ldots \\ V_l &= V_l^0(x,y,t) + \varepsilon\, V_l^1(x,y,t) + \varepsilon^2\, V_l^2(x,y,t) + \ldots \\ V_v &= V_v^0(x,y,t) + \varepsilon\, V_v^1(x,y,t) + \varepsilon^2\, V_v^2(x,y,t) + \ldots \\ \omega_{lg} &= \omega_{lg}^0(x,y,t) + \varepsilon\, \omega_{lg}^1(x,y,t) + \varepsilon^2\, \omega_{lg}^2(x,y,t) + \ldots \end{aligned} \tag{16}$$

Replacing ρ_l, ρ_v, V_l, V_v and ω_{lg} by their expansions (16) in the dimensionless equilibrium equations, and equating to zero the factors of successive powers of ε, we obtain the coupled problems $P_0, P_1, \ldots$ corresponding respectively to the cancellation of the factors of ε^0, ε^1,… Their resolution leads to the following result.

Result: *The water content* $\theta_l = \frac{|\Omega_l|}{|\Omega|}$ *is solution of a macroscopic homogenized equation:*

$$\frac{\partial\ \theta_l}{\partial t} - div_x(\boldsymbol{D}_\theta^{hom}\ \frac{\partial \theta_l}{\partial x}) = 0 \tag{17}$$

where

$$\boldsymbol{D}_\theta^{hom} = -\ \Lambda_{ll}\ \frac{\partial P_c^0}{\partial \theta_l} + \frac{1}{\rho_l^0}\boldsymbol{D}_v^{hom}\frac{\partial \rho_v^0}{\partial \theta_l} \tag{18}$$

denotes the homogenized diffusion tensor of moisture when ρ_l^0 *is assumed to be constant.* Λ_{ll} *is the Darcy tensor of permeability,* P_c^0 *the macroscopic capillary pressure,* D_v^{hom} *the homogenized diffusion tensor of water vapor given by :*

$$\boldsymbol{D}_v^{hom} = \frac{1}{|\ \Omega\ |}\int_{\Omega_g} D_v(I + \overline{\frac{\partial \chi}{\partial y}})dy \tag{19}$$

The vector $\chi(y)$ *is periodic, of zero average on* Ω_g*, and solution of the local boundary problem:*

$$\begin{cases} div_y(D_v\ (I + \overline{\frac{\partial \chi}{\partial y}})) = 0 & \text{in} \quad \Omega_g \\ D_v\ (I + \frac{\partial \chi}{\partial y}).n = 0 & \text{on} \quad \Gamma_{gs} \\ D_v\ (I + \frac{\partial \chi}{\partial y}).n = 0 & \text{on} \quad \Gamma_{gl} \end{cases} \tag{20}$$

Note that the density of liquid water ρ_l was supposed to be constant.

6. APPLICATION

We propose in this section an analytic solution for the calculation of D_v^{hom} in the case of the layered medium considered in Fig. 2 (at the macro-scale):

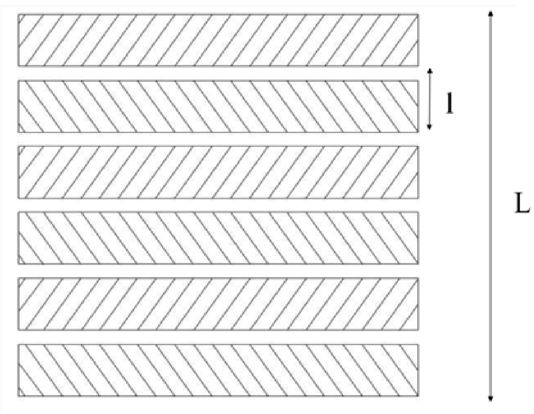

Figure 2: The layered medium considered

It is composed of horizontal impermeable layers, infinite in directions y_1 and y_3, half-filled with liquid water. The other part is filled with the gaseous phase in which the water vapor diffuses at the microscale (Fig.3). It is assumed that there is no significant convection of the liquid water and that the solid is undeformable.

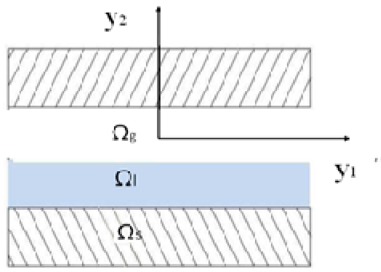

Figure 3: The associated periodic cell

The solution of problem (20) is given by:

$$\begin{cases} \chi_1(y_2) = \alpha_1 \\ \chi_2(y_2) = -y_2 + \alpha_2 \\ \chi_3(y_2) = \alpha_3 \end{cases} \tag{21}$$

where α_1, α_2, α_3 are real constants. The equivalent macroscopic tensor of water vapor deduced from (19) stands:

$$\mathbf{D}_{\mathbf{v}}^{\mathbf{hom}} = \begin{pmatrix} \theta_g D_v & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \theta_g D_v \end{pmatrix} \tag{22}$$

which means that water vapor diffusion only occurs in directions y_1 and y_3. Obviously, in this simple case, the tensor D_v^{hom} should easily be predicted without using the homogenization technique. Nevertheless, this example enables to validate the theoretical development presented.

7. CONCLUSION

The periodic homogenization technique, applied to transport equation for both liquid water and water vapor, enabled to obtain a macroscopic equation similar to the classical Richards one, where the expression of the homogenized tensor of moisture is directly linked to the geometric properties of the microstructure and to known transport properties of the unsaturated porous medium. Moreover, the domain of validity of Richards equation is clearly specified through the dimensionless numbers introduced.

8. REFERENCES

1. Auriault J.L., Lewandowska J., Diffusion / adsorption / advection macrotransport in soils. Eur. J. Mech. A / Solids, 15(4), pages 681-704 (1996).
2. Millet O., Ait-Mokhtar A., Amiri O., Determination of the macroscopic chloride diffusivity in cementitious porous materials by coupling periodic homogenization of Nernst-Planck equation with experimental protocol. International Journal of Multiphysics, 2(1), pages 129-145 (2008).
3. Moyne C., Murad M., A two-scale model for coupled electro-chemo-mechanical phenomena and onsager's reciprocity relations in expansive clays: I homogenization analysis. Transport in Porous Media, 62(3), pages 333-380 (2006).
4. Richards L.A., Capillary conduction of liquids through porous mediums. Physics, 1, pages 318-333 (1931).
5. Samson E., Marchand J., Snyder K., Beaudoin J. J., Modeling ion and fluid transport in unsaturated cement systems in isothermal conditions, *Cement and Concrete Research* (2005).
6. Sanchez Palencia E, Non homogeneous media and vibration theory. Lecture notes in Physics, springer-Verlag (1980).
7. Sleiman H., Amiri O., Ait-Mokhtar A., Chloride transport in unsaturated cement-based materials : Modeling and simulation in case of a tidal zone, EJECE (2009).
8. Whitaker S., Coupled transport in Multiphase systems : A theory of Drying, Advances in Heat Transfer (1998).
9. Whitaker S., Simultaneous heat, mass, and momentum transfer in porous media : a theory of drying, Heat transf (1977).