Homogenization of moisture transfer in unsaturated porous media - Highlighting of capillary condensation phenomenon

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Résumé:
Dans cette communication, nous proposons d’établir l’équation de Richards [3], décrivant le transfert d’humidité dans un milieu poreux partiellement saturé, en utilisant la technique d’homogénéisation périodique [4]. L’analyse dimensionnelle des équations de transfert de l’eau liquide et de la vapeur d’eau écrites à l’échelle microscopique fait apparaître des nombres sans dimension caractérisant le phénomène de transfert hydrique [1][2]. Le développement asymptotique des équations permet de retrouver, sans hypothèse a priori, l’équation de Richards macroscopique homogénéisée. De plus, on obtient avec cette approche, une définition mathématique précise du tenseur de diffusion homogénéisé, prenant en compte les propriétés géométriques de la microstructure. Le calcul du tenseur de diffusion hydrique homogénéisé sur un exemple 2D fait apparaître un comportement différent entre les régions hygroscopiques (pour des humidités relatives faibles) et super-hygroscopiques (pour des humidités relatives élevées). En particulier, un phénomène de condensation capillaire est mis en évidence dans la région super-hygroscopique.

Abstract:
In this communication, the classical Richards equation [3] for moisture transport is established in unsaturated porous media using periodic homogenization [4]. The dimensional analysis of transport equations naturally lets appear dimensionless numbers characterizing the moisture transfer in partially saturated porous media [1][2]. Application of the asymptotic homogenization leads to the macroscopic Richards equation which is justified rigorously this way. An accurate definition of the homogenized diffusion tensor of moisture is obtained, involving the geometric properties of the microstructure. The 2D resolution of this latter reveals a different behavior for the transport of water vapor between hygroscopic and super-hygroscopic regions. In particular, capillary condensation phenomenon is highlighted in the super hygroscopic region for high relative humidity.

Mots clés : Milieux poreux partiellement saturés, homogénéisation périodique, équation de Richards.

1. Microscopic equations in unsaturated porous media

Let us consider at the macroscopic scale that the material studied occupies the domain $S^*$ of the three-dimensional space $\mathbb{R}^3$ whose characteristic length is $L$. At the macroscopic level, a current point of $S^*$ will be noted $x^* = (x_1^*, x_2^*, x_3^*)$. We assume that the material $S^*$ has a periodic microstructure, or equivalently is constituted of the periodic repetition of an elementary cell $\Omega^* = \Omega_l^* \cup \Omega_g^* \cup \Omega_s^*$, where $\Omega_l^*$ denotes the liquid phase, $\Omega_g^*$ the gaseous phase, and $\Omega_s^*$ the solid phase (Fig. 1). The boundary $\Gamma^*_l$ of $\Omega_l^*$ is composed of the boundary $\Gamma_{ls}^*$ between the liquid and the solid phases, of the boundary $\Gamma_{lg}^*$ between the liquid and the gaseous phases, and of the part $\Gamma_{lg}^*$ between the liquid phases of two neighboring elementary cells. The same notations are used for the boundary $\Gamma_g^* = \Gamma_{gs}^* \cup \Gamma_{lg}^* \cup \Gamma_{gg}^*$. At the microscopic level, a current point of the elementary cell $\Omega^*$ is noted $y^* = (y_1^*, y_2^*, y_3^*)$. Moreover, the size $l$ of the elementary
cell $\Omega^*$ 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 $\varepsilon << 1$.

The continuity equations for the liquid water and for the water vapor at the local scale classically write:

$$\frac{\partial \rho^*_l}{\partial t} + \text{div}(\rho^*_l V^*_l) = 0 \quad \text{in} \quad \Omega_l^*$$ (1)

$$\frac{\partial \rho^*_v}{\partial t} - \text{div}(D^*_v \text{grad} \rho^*_v) = 0 \quad \text{in} \quad \Omega_v^*$$ (2)

with the associated boundary conditions on $\Gamma_{li}$ and $\Gamma_{gv}$:

$$V^*_l n^*_{li} = 0 \quad \text{on} \quad \Gamma_{li}$$ (3)

$$D^*_v \text{grad} \rho^*_v n^*_{gv} = 0 \quad \text{on} \quad \Gamma_{gv}$$ (4)

They must be completed by the boundary condition on $\Gamma_{lg}$:

$$- D^*_v \text{grad} \rho^*_v = \rho^*_v V^*_v \quad \text{in hygroscopic region}$$ (5)

$$\rho^*_v = \rho^*_{eq} \quad \text{in super-hygroscopic region}$$ (6)

Moreover for both regions (hygroscopic and super-hygroscopic), the flux continuity condition at the interface stands:

$$\rho^*_l (V^*_l - \omega^*_l) n^*_{lg} = \rho^*_v (V^*_v - \omega^*_v) n^*_{lg} \quad \text{on} \quad \Gamma_{lg}^*$$ (7)

where $\rho^*_l$ and $\rho^*_v$ denote the mass of liquid water and of water vapor per unit volume, $\rho^*_{eq}$ the water vapor density at equilibrium, $V^*_l$ and $V^*_v$ the convection velocity of the liquid water and of the water vapor, $D^*_v$ the self-diffusion coefficient of water vapor in the gaseous phase. $\omega^*_l$ (respectively $\omega^*_v$) denotes the liquid-gas interface velocity (respectively the gas-liquid interface velocity).

2. The periodic homogenization procedure

The essential assumption of the periodic homogenization method is the periodicity of the material, that is to say that there exists an "elementary cell" or "representative element volume" (R.E.V), which by periodicity produces the whole structure. Obviously it is supposed to contain a very large number of heterogeneities.

For the problem to be well-posed, the fields involved (the volumetric mass of liquid water and of water vapor, the velocity of the liquid water and of the water vapor,...) must be considered as periodical on the cell boundary.

![FIG.1-Example of elementary cell constituting the periodic microstructure.](image)

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1 Classically, the hygroscopic regions correspond to a relative humidity RH ≤ 95% and the super-hygroscopic regions correspond to RH > 95%.
3. Dimensional analysis of equations

The dimensional analysis of equations (1)-(7) is similar to that developed in the saturated case in [1][2]. We define dimensionless physical data and dimensionless unknowns of the problem:

\[
y = \frac{y^*}{l}, \quad x = \frac{x^*}{L}, \quad t = \frac{t^*}{T^*}, \quad \rho_l = \frac{\rho_l^*}{\rho_l^r}, \quad \rho_v = \frac{\rho_v^*}{\rho_v^r},
\]

\[
D_v = \frac{D_v^*}{D_v^r}, \quad V_l = \frac{V_l^*}{V_l^r}, \quad V_v = \frac{V_v^*}{V_v^r}, \quad \omega_{lg} = \frac{\omega_{lg}^*}{\omega_{lg}^r}.
\]

where the variables indexed by "r" are the reference ones, and those without a star are dimensionless. Introducing the dimensionless variables (8) into equations (1)-(7), we obtain the following dimensionless equations of transport of liquid water posed in \( \Omega_l \):

\[
\tau_l \frac{\partial \rho_l}{\partial t} + \text{div}(\rho_l V_l) = 0 \quad \text{in} \quad \Omega_l
\]

and that of transport of water vapor posed in \( \Omega_g \)

\[
\tau_v \frac{\partial \rho_v}{\partial t} - \text{div}(D_v \text{grad} \rho_v) = 0 \quad \text{in} \quad \Omega_g
\]

with the associated boundary conditions on \( \Gamma_{ls} \) and \( \Gamma_{gs} \):

\[
V_l n_{ls} = 0 \quad \text{on} \quad \Gamma_{ls}
\]

\[
D_v \text{grad} \rho_v n_{gs} = 0 \quad \text{on} \quad \Gamma_{gs}
\]

The boundary condition on \( \Gamma_{lg} \) writes in the hygroscopic region:

\[-D_v \text{grad} \rho_v = \gamma \rho_v V_v\]

while in the super-hygroscopic region, it reduces to:

\[
\rho_v = \rho_v^{eq}
\]

To these boundary conditions can be added the following one coming from the dimensional analysis of the flux continuity condition (7) on \( \Gamma_{lg} \):

\[
\rho_l (\lambda V_l \frac{\partial \rho_v}{\partial n_{lg}}) n_{lg} = (D_v \text{grad} \rho_v - \delta \rho_v \omega_{lg}) n_{lg} \quad \text{on} \quad \Gamma_{lg}
\]

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

\[
\tau_l = \frac{t_{l,\text{conv}}}{T_l}, \quad \tau_v = \frac{t_{v,\text{diff}}}{T_v}, \quad \lambda = \frac{\lambda_{l,\text{conv}}}{\lambda_{v,\text{diff}}}, \quad \xi = \frac{\omega_{lg}^r}{V_l}, \quad \zeta = \frac{\omega_{lg}^r}{\rho_l^r}, \quad \gamma = \frac{V_v}{\omega_{lg}^r}\]

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, \( \varepsilon \) is chosen as the reference perturbation parameter and the other dimensionless numbers are linked to \( \varepsilon \).

For a moderate convection of the liquid water and water vapor, we obtain the following order of magnitude of the dimensionless numbers based on physical considerations:

\[
\tau_l = o(\varepsilon), \quad \tau_v = o(\varepsilon^3), \quad \lambda = o(\varepsilon), \quad \xi = o(\varepsilon), \quad \delta = o(\varepsilon^3), \quad \gamma = o(\varepsilon^2)
\]
4. Homogenized Richards equation

The classical procedure of periodic homogenization [4] leads to search the unknowns \( \rho_l, \rho_v, V_l, V_v \) and \( \omega_{lg} \) 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 unknowns \( \rho_l, \rho_v, V_l, V_v \) and \( \omega_{lg} \) of the problem are postulated to admit a formal expansion with respect to \( \varepsilon \) [4] :

\[
\begin{align*}
\rho_l &= \rho_l^0(x,y,t) + \varepsilon \rho_l^1(x,y,t) + \varepsilon^2 \rho_l^2(x,y,t) + \ldots \\
\rho_v &= \rho_v^0(x,y,t) + \varepsilon \rho_v^1(x,y,t) + \varepsilon^2 \rho_v^2(x,y,t) + \ldots \\
V_l &= V_l^0(x,y,t) + \varepsilon V_l^1(x,y,t) + \varepsilon^2 V_l^2(x,y,t) + \ldots \\
V_v &= V_v^0(x,y,t) + \varepsilon V_v^1(x,y,t) + \varepsilon^2 V_v^2(x,y,t) + \ldots \\
\omega_{lg} &= \omega_{lg}^0(x,y,t) + \varepsilon \omega_{lg}^1(x,y,t) + \varepsilon^2 \omega_{lg}^2(x,y,t) + \ldots
\end{align*}
\] (18)

Replacing \( \rho_l, \rho_v, V_l, V_v \) and \( \omega_{lg} \) by their expansions (18) in the dimensionless equilibrium equations, and equating to zero the factors of successive powers of \( \varepsilon \), we obtain the coupled problems \( P_0, P_1, \ldots \) corresponding respectively to the cancellation of the factors of \( \varepsilon^0, \varepsilon^1, \ldots \). Their resolution leads to the following result.

**Result:** The water content \( \theta_l = \frac{\Omega_l}{\Omega} \) is solution of the macroscopic homogenized Richards equation:

\[
\frac{\partial \theta_l}{\partial t} - \text{div} (D_{\theta}^{\text{hom}} \text{grad} \theta_l) = 0
\] (19)

where

\[
D_{\theta}^{\text{hom}} = -\Lambda_{\theta} \frac{\partial P_c}{\partial \theta_l} + \frac{1}{\rho_l^0} D_v^{\text{hom}} \frac{\partial \rho_v}{\partial \theta_l}
\] (20)

denotes the homogenized diffusion tensor of moisture when \( \rho_l^0 \) is assumed to be constant. \( \Lambda_{\theta} \) is the Darcy tensor, \( P_c \) the macroscopic capillary pressure, and \( D_v^{\text{hom}} \) the homogenized diffusion tensor of water vapor given by :

\[
D_v^{\text{hom}} = \frac{1}{\Omega} \int_{\Omega} D_v (I + \frac{\partial \chi}{\partial y}) dy
\] (21)

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

\[
\begin{cases}
\text{div}_y (D_v (I + \frac{\partial \chi}{\partial y})) = 0 & \text{in } \Omega_g \\
D_v (I + \frac{\partial \chi}{\partial y}) n_{gl} = 0 & \text{on } \Gamma_{gl}
\end{cases}
\] (22)

(23)

with a Neumann condition on \( \Gamma_{gl} \) in the hygroscopic region:

\[
D_v (I + \frac{\partial \chi}{\partial y}) n_{gl} = 0
\] (24)

and a Dirichlet condition on \( \Gamma_{gl} \) in the super-hygroscopic region:

\[
\chi = 0
\] (25)
5. **Homogenized diffusion tensor of water vapor**

We propose in this section to determine the homogenized diffusion tensor of water vapor $D_{v}^{\text{hom}}$ in the hygroscopic and super-hygroscopic regions by solving the Neumann local problem (22)-(24) for $\text{RH} \leq 95\%$ and the Dirichlet local problem (22)-(23) and (25) for $\text{RH} > 95\%$, and to compare the results obtained. Let us consider a porous medium whose microstructure (Fig. 3) consists in a periodic repetition of a two-dimensional unit cell of size $l \times l$ containing a square inclusion of size $a \times a$ representing the liquid and vapor phases $\Omega_f = \Omega_l \cup \Omega_v$ (Fig. 2).

**5.1 Resolution in the hygroscopic region**

We consider that the square inclusion of size $a \times a$ is half filled with liquid water, the other part contains the gaseous phase in which the water vapor diffuses (Fig. 4). It is assumed that there is no significant convection of the liquid water and that the solid is not deformable.

Once the Neumann local problem (22)-(24) solved, we obtain classically:

$$D_{v}^{\text{hom}} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \theta_D v \end{pmatrix}$$

Expression (25) means that water vapor diffusion only occurs in $y_3$ direction.

**5.2 Resolution in the super-hygroscopic region**

We recall that in the super-hygroscopic region, the liquid water (assumed to be without moving) occupies the major part leaving only a small space where the water vapor can diffuse. For the sake of simplicity, we assume this small space to be a rectangular inclusion of size $a \times b$ with $a \gg b$ (Fig. 5).
FIG. 5- Example of fluid distribution in the super-hygroscopic region

Once the Dirichlet local problem (22)-(23) and (24) solved, we obtain:

$$D^\hom = \begin{pmatrix}
\theta_s D_y - \frac{D_y}{|\Omega|} \sum_{n=0}^{\infty} b p_n \frac{\cosh(p_n a) - 1}{\sinh(p_n a)} & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & \theta_s D_x 
\end{pmatrix}$$

(27)

It is clear that water vapor diffuses completely in $y_3$ direction and partially in $y_1$ direction, whereas it is stopped in $y_2$ direction. This is obviously due to the geometry of the cell considered (Fig. 5). The variations of the local tortuosity tensor, defined by $\Phi = (I + \frac{\partial X}{\partial y})$ on a square inclusion in the super-hygroscopic region, are represented in Fig. 6. They highlight the phenomenon of capillary condensation that occurs.

FIG. 6- Numeric solution for $\Phi$

6. Conclusion

The periodic homogenization technique applied to transport equations 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 geometrical and known transport properties of the unsaturated porous material. Moreover, the mathematical local problem defining the homogenized moisture tensor is different in the hygroscopic and super-hygroscopic regions. Analytical and numerical solutions for 2D square inclusions modeling the microstructure of the porous media, revealed that the condensation of the water vapor occurs only in the super-hygroscopic region, which seems to be consistent with the condensation phenomenon generally observed experimentally [5].

7. References