CONVECTIVE AND CONDUCTIVE THERMAL HOMOGENIZATION FOR NON-SATURATED POROUS BUILDING MATERIALS
Application on the Thermal Conductivity Tensor

by

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Porous materials possess a complex structure on a microscopic scale and present strong heterogeneities, which makes their precise study extremely complex. In fact, the macroscopic behavior of these materials is strongly dependent on mechanisms that act to the scale of their components. The present work focus on the development of a macroscopic conductive and convective fluid heat transfer model, with a heat source in the unsaturated porous materials. This model is established by periodic homogenization of energy conservation equations written on a microscopic scale in each phase (solid, liquid and gas). The resulting input parameters formulations of the submodel were explicitly identified. Numerical calculations of the homogenized thermal conductivity tensor are performed on a representative 3-D elementary cell of the porous medium. Finally, a sensitivity study of this tensor depending of the variation of the water content and porosity of the concerned elementary cell has been performed. This sensitivity is required to be considered in simulations to better understand the behavior of building materials and improve the prediction of energy performance.

Key words: *porous media, heat transfer, periodic homogenization, elementary cell*

Introduction

In order to reduce energy costs and environmental impacts related to buildings, several organizations and research laboratories have focused on the physical study of the building and its energy behavior [1]. The building envelope is in constant interaction with the outside environment and the inside air, that we wish maintain on restricted range of temperature. Walls are the seat of various hygrothermal transfers that determine the internal climate of building materials that are mostly porous media with a complex structure and exhibit strong heterogeneities on the microscopic scale. Moreover, most of the phenomena involved at the microscopic scale are the origin of the phenomena presented on the macroscopic scale. The macroscopic behavior of material is strongly dependent mechanisms acting at the scale of these constituents. It is then

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necessary to dispose of macroscopic laws that allow to take into account the heterogeneity and complexity of porous media and describe their overall behavior on a large scale.

One possible solution to describe these highly heterogeneous on the pore scale is to assimilate them to the equivalent continuous media on a macroscopic scale, with the same average behavior, using homogenization methods, also called scaling method or micro-macro transition. The effective medium is then characterized by effective transport properties, or macroscopic coefficients reflecting physics at the pore scale.

Early works, based on scaling method were conducted by Whitaker [2] to homogenize the heat transfer equations in porous media using the method of volume averaging [3]. Thermals transfers were also discussed to identify the homogenized thermal conductivity tensor [4, 5]. With the same method, Quintard and Whitaker [6] have examined the process of transient heat conduction for a two-phase system.

The averaging volume technique requires making certain hypotheses in the calculations to obtain the homogenized macroscopic sought model. On the other hand in the non-linear equations, or when having an average of the product of two quantities, the dispersion terms are generally neglected [7].

That is why, the recourse to a global and pertinent homogenization approach called *periodic homogenization method* that is generally used for evaluating the porous structures properties.

The periodic homogenization method [8-10] is among the most well-known and rigorous scaling methods available in literature allowing obtaining pertinent models. It is mainly based on the method of asymptotic expansions [11]. This method assumes that the microstructure of the macroscopic medium is constituted of a periodic repetition of basic elementary cells. It is based on dimensional analysis of the transfer equations at the microscopic scale, making naturally appear dimensionless numbers characterizing the problem [12]. Regarding literature, several works using periodic homogenization on different multiphysics phenomena in porous media can be found. The homogenization of conduction heat transfer equations in two-phase medium [13-15]. Lewandowska and Laurent [16], Mchirgui *et al.* [17] applied this method to moisture transfer, they presented moisture transfer equations in macroscopic heterogeneous partially saturated porous media. Other researchers field can be found, it concern principally. The high velocity flow in porous heterogeneous media [18], the reactive flows [19], the transport of pollutants in groundwater [20], the ionic diffusion of chlorides ions in saturated porous media, with consideration of ions electrocapillary interactions with the solid matrix [21], and the solutes diffusion [22].

Here, a rigorous and systematic homogenization technique is used to upscale a heat transfer process, because most of authors consider often that both liquid and gas phase as homogeneous representing one phase, called fluid. Moreover there are few studies in the literature on the homogenization of conduction, convection, and phase change equations in the porous media. Thus, in this work, we propose to establish the periodic homogenization of heat transport equations on the microscopic scale for the different phases of the real porous media, the recourse to the periodic homogenization well known by its reliability to achieve relevant and pertinent macroscopic models. Then, numerical simulations on a representative elementary cell of the microstructure of the studied porous medium are investigated, in order to calculate the homogenized tensor of thermal conductivity.

Microstructural description of periodic medium

The internal elements of the material structure constitute the microstructure that affects significantly the properties of its macroscopic behavior. At the macroscopic scale, many

materials present a homogeneous geometry but they are in reality highly heterogeneous, especially when considering the cementitious material. Figure 1 shows an example of an X-ray tomography image of cementitious material representing the heterogeneity of such building material, it contains aggregates in gray, cement and sand in black and voids in white.

Considering a porous medium having a microstructure constituted of periodical repetition of an elementary cells, see fig. 2. Each cell is composed of a solid phase Ω_s^*, a liquid phase Ω_l^* and a gaseous phase Ω_g^*. The interfaces between these various phases are Γ_{lg}^*, Γ_{sg}^*, and Γ_{ls}^*, they represent the gas-liquid, gas-solid, and liquid-solid interfaces, respectively.

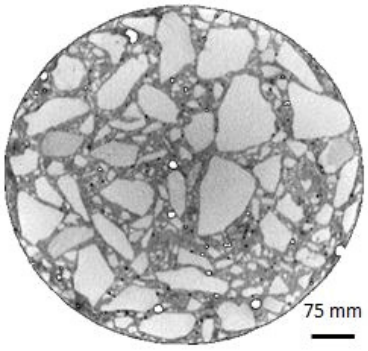

Figure 1. Tomographic image obtained by X-rays of concrete (resolution 75 µm) [23]

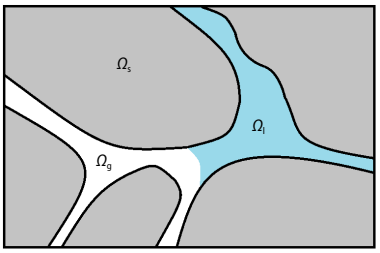

Figure 2. Example of a periodic microstructure partially saturated

The heat transfer in the liquid (l) and gas (s) phases is governed by conduction and convection. However, in the solid phase the heat transfer is only governed by conduction and the conservation of energy equations [4] in each phase can be written, respectively:

$$\rho_s^* c_s^* \frac{\partial^* T_s^*}{\partial t^*} - \mathrm{div}^*\left(\lambda_s^* \mathrm{grad}^* T_s^*\right) = 0 \quad \text{in} \quad \Omega_s^* \tag{1}$$

$$\rho_l^* c_l^* \frac{\partial^* T_l^*}{\partial t^*} - \mathrm{div}^*\left(\lambda_l^* \mathrm{grad}^* T_l^*\right) + \left(\rho_l^* c_l^*\right) v_l^* \mathrm{grad}^* T_l^* = 0 \quad \text{in} \quad \Omega_l^* \tag{2}$$

$$\rho_g^* c_g^* \frac{\partial^* T_g^*}{\partial t^*} - \mathrm{div}^*\left(\lambda_g^* \mathrm{grad}^* T_g^*\right) + \left(\rho_g^* c_g^*\right) v_g^* \mathrm{grad}^* T_g^* = 0 \quad \text{in} \quad \Omega_g^* \tag{3}$$

The boundary conditions at the various interfaces are given by assuming the temperature continuity phase, eqs. (4), (6), and (8), and by the heat flux verifies, eqs. (5), (7), and (9):

– gas-liquid

$$T_g^* = T_l^* \quad \text{on} \quad \Gamma_{gl}^* \tag{4}$$

$$-\lambda_g^* \frac{\partial^* T_g^*}{\partial y^*} n_{gl}^* = -\lambda_l^* \frac{\partial^* T_l^*}{\partial y^*} n_{gl}^* + q_{gl}^* n_{gl}^* \quad \text{on} \quad \Gamma_{gl}^* \tag{5}$$

– gas-solid

$$T_g^* = T_s^* \quad \text{on} \quad \Gamma_{gs}^* \tag{6}$$

$$\lambda_g^* \frac{\partial^* T_g^*}{\partial y^*} n_{gs}^* = \lambda_s^* \frac{\partial^* T_s^*}{\partial y^*} n_{gs}^* \quad \text{on} \quad \Gamma_{gs}^* \tag{7}$$

– liquid-solid

$$T_{\mathrm{l}}^{*} = T_{\mathrm{s}}^{*} \quad \text{on} \quad \Gamma_{\mathrm{ls}}^{*} \tag{8}$$

$$\lambda_{\mathrm{l}}^{*} \frac{\partial^{*} T_{\mathrm{l}}^{*}}{\partial y^{*}} n_{\mathrm{ls}}^{*} = \lambda_{\mathrm{s}}^{*} \frac{\partial^{*} T_{\mathrm{s}}^{*}}{\partial y^{*}} n_{\mathrm{ls}}^{*} \quad \text{on} \quad \Gamma_{\mathrm{ls}}^{*} \tag{9}$$

These terms, eqs. (4)-(9), represent the continuity of temperatures and heat flows on the interfaces Γ_{gl}^{*}, Γ_{gs}^{*}, and Γ_{ls}^{*} for a medium in local thermodynamic equilibrium. In addition to the conduction and convection terms, the consumption or energy production (term source or sink) due to the phase change are added to the balance energy. In the present case this term q_{gl}^{*} is a heterogeneous source of heat [15, 24] at the liquid-gas interface:

$$q_{\mathrm{gl}}^{*} = \rho_{\mathrm{g}}^{*} h_{\mathrm{lv}}^{*} (v_{\mathrm{g}}^{*} - \omega_{\mathrm{lg}}^{*}) \tag{10}$$

On the other hand, the time average of each balance equation term in the phase *i* is given by:

$$\left\langle \frac{\partial^{*} T_{\alpha}^{*}}{\partial t^{*}} \right\rangle_{i} = \frac{\partial^{*}}{\partial t^{*}} \left\langle T_{\alpha}^{*} \right\rangle_{i} - \frac{1}{\left|\Omega\right|^{*}} \int T_{\alpha}^{*} \omega_{\mathrm{lg}}^{*} n_{\mathrm{lg}}^{*} \mathrm{d}\Gamma^{*} \tag{11}$$

where $\alpha = \mathrm{s,l,}$ and g.

Dimensional analysis of equations

The dimensionless physical data are defined by dividing each variable by its characteristic value. These variables are estimated in terms of the parameter ε which represents the ratio between the characteristic microscopic length, *l*, and the characteristic macroscopic length, *L*. The perturbation parameter, ε, verifies the scale separation condition and the existence of an equivalent medium:

$$\varepsilon = \frac{l}{L} \ll 1 \tag{12}$$

By introducing in the previous eqs. (1)-(11) the dimensionless variables following:

$$y = \frac{y^{*}}{l} \quad x = \frac{x^{*}}{L} \quad t = \frac{t^{*}}{t^{r}} \quad \omega_{lg} = \frac{\omega_{lg}^{*}}{\omega_{lg}^{r}} \quad \rho_{\alpha} = \frac{\rho_{\alpha}^{*}}{\rho_{\alpha}^{r}}$$

$$v_{\beta} = \frac{v_{\alpha}^{*}}{v_{\alpha}^{r}} \quad T_{\alpha} = \frac{T_{\alpha}^{*}}{T_{\alpha}^{r}} \quad C_{\alpha} = \frac{C_{\alpha}^{*}}{C_{\alpha}^{r}} \quad \lambda_{\alpha} = \frac{\lambda_{\alpha}^{*}}{\lambda_{\alpha}^{r}} \quad q_{lg} = \frac{q_{lg}^{*}}{q_{lg}^{r}}$$

where *y* represents the microscopic space variable and *x* the macroscopic space variable. The variables indexed by ^{r} are the reference ones, supposed known. The sign * denotes the dimensional variables, and the new variables appeared without star $(^{*})$ are dimensionless. Replacing the dimensionless variables defined into the previous equations of transport, eqs. (1)-(11), we obtain new dimensionless energy conservation equations:

$$\mathrm{Fo}\, C_{\mathrm{s}} \frac{\partial T_{\mathrm{s}}}{\partial t} - \mathrm{div}\left(\lambda_{\mathrm{s}} \mathrm{grad} T_{\mathrm{s}}\right) = 0 \quad \text{in} \quad \Omega_{\mathrm{s}} \tag{13}$$

$$\mathrm{Fo}\, C_{\mathrm{l}} C_{\mathrm{l}} \frac{\partial T_{\mathrm{l}}}{\partial t} - \lambda_{\mathrm{l}} \mathrm{div}\left(\lambda_{\mathrm{l}} \mathrm{grad} T_{\mathrm{l}}\right) + \mathrm{Pe}\, C_{\mathrm{l}} v_{\mathrm{l}} \mathrm{grad} T_{\mathrm{l}} = 0 \quad \text{in} \quad \Omega_{\mathrm{l}} \tag{14}$$

$$\mathrm{Fo}\,C_2 C_\mathrm{g}\frac{\partial T_\mathrm{g}}{\partial t}-\lambda_2\mathrm{div}\left(\lambda_\mathrm{g}\mathrm{grad}T_\mathrm{g}\right)+\mathrm{Pe}\,C_3 v_\mathrm{l} C_\mathrm{g} v_\mathrm{g}\mathrm{grad}T_\mathrm{g}=0 \quad \text{in} \quad \Omega_\mathrm{g} \tag{15}$$

with $C_\alpha=\rho_\alpha c_\alpha$, and $\alpha=\mathrm{s,l,}$ and g.

The dimensionless boundary conditions on the various interfaces become:

– gas-liquid

$$T_\mathrm{g}=T_\mathrm{l} \quad \text{on} \quad \Gamma_\mathrm{gl} \tag{16}$$

$$\lambda_3\lambda_\mathrm{g}\frac{\partial T_\mathrm{g}}{\partial y}\boldsymbol{n}_{\mathbf{gl}}=\lambda_l\frac{\partial T_\mathrm{l}}{\partial y}\boldsymbol{n}_{\mathbf{gl}}+N_\mathrm{lv}q_\mathrm{gl}\boldsymbol{n}_{\mathbf{gl}} \quad \text{on} \quad \Gamma_\mathrm{gl} \tag{17}$$

– gas-solid

$$T_\mathrm{g}=T_\mathrm{s} \quad \text{on} \quad \Gamma_\mathrm{gs} \tag{18}$$

$$\lambda_2\lambda_\mathrm{g}\frac{\partial T_\mathrm{g}}{\partial y}\boldsymbol{n}_{\mathbf{gs}}=\lambda_\mathrm{s}\frac{\partial T_\mathrm{s}}{\partial y}\boldsymbol{n}_{\mathbf{gs}} \quad \text{on} \quad \Gamma_\mathrm{gs} \tag{19}$$

– liquid-solid

$$T_\mathrm{l}=T_\mathrm{s} \quad \text{on} \quad \Gamma_\mathrm{ls} \tag{20}$$

$$\lambda_1\lambda_\mathrm{l}\frac{\partial T_\mathrm{l}}{\partial y}\boldsymbol{n}_{\mathbf{ls}}=\lambda_\mathrm{s}\frac{\partial T_\mathrm{s}}{\partial y}\boldsymbol{n}_{\mathbf{ls}} \quad \text{on} \quad \Gamma_\mathrm{ls} \tag{21}$$

The average time derivative of each equation then becomes:

$$\left\langle C_\alpha\frac{\partial T_\alpha}{\partial t}\right\rangle=C_\alpha\frac{\partial}{\partial t}\left\langle T_\alpha\right\rangle-\frac{\mathcal{R}_T}{|\Omega|}\int_{\Gamma_{lg}}T_\alpha\omega_\mathrm{lg}\boldsymbol{n}_{\mathbf{lg}}\mathrm{d}\Gamma \tag{22}$$

The following dimensionless numbers characterizing the various transfers appear naturally after the dimensional analysis of the microscopic transfer equations:

$$\mathrm{Fo}=\frac{C_\alpha^r l^2}{\lambda_\mathrm{s}^r t^r} \quad \mathrm{Pe}=\frac{C_\mathrm{l}^r v_\mathrm{l}^r l}{\lambda_\mathrm{s}^r} \quad C_1=\frac{C_\mathrm{l}^r}{C_\mathrm{s}^r} \quad C_2=\frac{C_\mathrm{g}^r}{C_\mathrm{s}^r} \quad C_3=\frac{C_\mathrm{g}^r}{C_\mathrm{l}^r} \quad \lambda_\mathrm{l}=\frac{\lambda_\mathrm{l}^r}{\lambda_\mathrm{s}^r}$$

$$\lambda_2=\frac{\lambda_\mathrm{g}^r}{\lambda_\mathrm{s}^r} \quad \lambda_3=\frac{\lambda_\mathrm{g}^r}{\lambda_\mathrm{l}^r} \quad v_\mathrm{l}=\frac{v_\mathrm{g}^r}{v_\mathrm{l}^r} \quad N_{lv}=\frac{l}{\lambda_\mathrm{l}^r}q_\mathrm{gl}^r \quad \mathcal{R}_T=\frac{t^r\omega_\mathrm{lg}^r}{l}$$

All these appeared parameters characterizing the various transfers considered in porous media are dimensionless number, as examples: the inverse of the Fourier number, Fo, the Peclet number, Pe, the ratio of thermal conductivities λ_l, λ_2, and λ_3, the ratio of thermal capacities C_l, C_2, and C_3. To be reduced to a dimensionless one scale problem, we express the dimensionless numbers depending on the perturbation parameter, ε. Taking into account the characteristic values and different physical phenomena and for homogenisables problems. The orders of magnitude of dimensionless numbers corresponding are then given by:

$$\mathrm{Fo}=\mathcal{O}(\varepsilon^2) \quad \mathrm{Pe}=\mathcal{O}(\varepsilon) \quad C_1=\mathcal{O}(1) \quad C_2=\mathcal{O}(\varepsilon) \quad C_3=\mathcal{O}(\varepsilon) \quad \lambda_\mathrm{l}=\mathcal{O}(1)$$

$$\lambda_2=\mathcal{O}(\varepsilon) \quad \lambda_3=\mathcal{O}(\varepsilon) \quad v_\mathrm{l}=\mathcal{O}(\varepsilon) \quad N_{lv}=\mathcal{O}(\varepsilon^2) \quad \mathcal{R}_T=\mathcal{O}(\varepsilon)$$

Macroscopic model

The classical periodic homogenization procedure consists to replace the orders of magnitude of the dimensionless numbers in the dimensionless eqs. (13)-(22). Then, the unknowns variables of the problem are searched in the form of an asymptotic development depending on the perturbation parameter, ε, as following:

$$T_\alpha(x,y) = T_\alpha^{(0)}(x,y) + \varepsilon T_\alpha^{(1)}(x,y) + \varepsilon^2 T_\alpha^{(2)}(x,y) + \ldots \tag{23}$$

Note that all the terms T_α^i in eq. 23 are y-periodic. The variables x and y are linked by $x = \varepsilon y$.

The derivation operators grad and div are written:

$$\text{grad} = \text{grad}_y + \varepsilon \text{grad}_x = \frac{\partial}{\partial y} + \varepsilon \frac{\partial}{\partial x} \tag{24}$$

$$\text{div} = \text{div}_y + \varepsilon \text{div}_x \tag{25}$$

The liquid flow is governed by the Darcy law [25] at the macroscopic scale which will be used thereafter:

$$v_l = -\mathbf{\Lambda}_{ll} \nabla \left(P - P_c \right) \tag{26}$$

where $\mathbf{\Lambda}_{ll}$ represents the Darcy tensor defined by the expression:

$$\mathbf{\Lambda}_{ll} = \frac{K_{rl} K_l}{\mu_l} \tag{27}$$

where K_{rl} is the relative permeability of the liquid phase, K_l – the intrinsic permeability of the material, and μ_1 – the fluid viscosity.

The total pressure of the gas phase, resulting from eq. (26), is considered constant, and the capillary pressure, P_c, is a characteristic of the porous medium, dependent on temperature, which allows us to write:

$$\nabla P_c = \left(\frac{\partial P_c}{\partial T} \right) \nabla T \tag{28}$$

By equating to zero the factors of successive powers of ε in the eqs. (13)-(22), we obtain the coupled problems $\mathcal{P}_0, \mathcal{P}_1$, and $\mathcal{P}_2$. The homogenized equation of heat transfer in porous media at the macroscopic scale is given by:

$$\left(n_\text{s} C_\text{s} + n_\text{l} C_\text{l} \right) \frac{\partial T}{\partial t} - \text{div}_x \left(\lambda_\text{s}^\text{hom} + \lambda_\text{l}^\text{hom} \right) \nabla T + \rho_\text{l} h_\text{l} \text{div}_x \mathbf{\Lambda}_{ll}^\text{hom} \left(\frac{\partial P_c}{\partial T} \right) \nabla T - h_{lv} m_\text{g} = 0 \tag{29}$$

where h_l is the specific enthalpy of liquid, $h_{lv} m_g$ – the macroscopic phase change rate, and h_{lv} – the specific enthalpy of vaporization. The n_s and n_l are the volume fractions of the solid and liquid phases:

$$n_s = \frac{\left| \Omega_\text{s} \right|}{\left| \Omega \right|} \text{ and } n_\text{l} = \frac{\left| \Omega_\text{l} \right|}{\left| \Omega \right|}$$

Then

$$C^\text{hom} \frac{\partial T^0}{\partial t} - \text{div}_x \left(a_t \nabla T \right) - h_{lv} m_\text{g} = 0 \tag{30}$$

Thus

$$C^{\hom} = \left(n_{\mathrm{s}} C_{\mathrm{s}} + n_{\mathrm{l}} C_{\mathrm{l}}\right) \tag{31}$$

$$a_t = \boldsymbol{\lambda}^{\hom} - h_{\mathrm{l}} \rho_{\mathrm{l}} \boldsymbol{\Lambda}_{ll}^{\hom} \left(\frac{\partial P_c}{\partial T}\right) \tag{32}$$

$$m_{\mathrm{g}} = \frac{1}{|\Omega|} \int \rho_{\mathrm{g}} (v_{\mathrm{g}} - \omega_{\mathrm{lg}}) n_{\mathrm{lg}} \mathrm{d}\Gamma \tag{33}$$

where $C^{\hom}$ is the macroscopic heat capacity, a_t – the corrected thermal conductivity, and m_{g} represents the mass evaporation rate. It is to notice that the term of phase change is a function of the velocity of the gas-liquid interface, ω_{lg}. If this parameter decreases, the available interface liquid-gas for the phase change also decreases.

$$\boldsymbol{\Lambda}_{ll}^{\hom} = \frac{1}{|\Omega|} \int \boldsymbol{\Lambda}_{ll} \left(\frac{\partial \chi_{\mathrm{l}}}{\partial y} + [\mathrm{I}]\right) \mathrm{d}\Omega \tag{34}$$

$$\boldsymbol{\lambda}^{\hom} = \frac{1}{|\Omega|} \int \lambda_{\mathrm{s}} \left(\frac{\partial \chi_{\mathrm{s}}}{\partial y} + [\mathrm{I}]\right) \mathrm{d}\Omega + \frac{1}{|\Omega|} \int \lambda_{\mathrm{l}} \left(\frac{\partial \chi_{\mathrm{l}}}{\partial y} + [\mathrm{I}]\right) \mathrm{d}\Omega \tag{35}$$

The homogenized thermal conductivity tensor is strongly dependent on the porous structure through local variables χ_{s} and χ_{l}, determined by solving the local boundary value problem in the porous medium.

Here χ_{s} is periodic, of zero average on Ω_{s}, and χ_{l} is periodic, of zero average on Ω_{l}. The solutions are obtained by solving on the period, the local boundary value problem is:

$$\begin{aligned}
&\mathrm{div}_y \left[\lambda_{\mathrm{s}} \left(\frac{\partial \chi_{\mathrm{s}}}{\partial y} + [\mathrm{I}]\right)\right] = 0 \quad \text{in} \quad \Omega_{\mathrm{s}} \\
&\mathrm{div}_y \left[\lambda_{\mathrm{l}} \left(\frac{\partial \chi_{\mathrm{l}}}{\partial y} + [\mathrm{I}]\right)\right] = 0 \quad \text{in} \quad \Omega_{\mathrm{l}} \\
&\lambda_{\mathrm{s}} \left(\frac{\partial \chi_{\mathrm{s}}}{\partial y} + [\mathrm{I}]\right) n_{\mathrm{gs}} = 0 \quad \text{on} \quad \Gamma_{\mathrm{gs}} \\
&\lambda_{\mathrm{l}} \left(\frac{\partial \chi_{\mathrm{l}}}{\partial y} + [\mathrm{I}]\right) n_{\mathrm{gl}} = 0 \quad \text{on} \quad \Gamma_{\mathrm{gl}} \\
&\lambda_{\mathrm{l}} \left(\frac{\partial \chi_{\mathrm{l}}}{\partial y} + [\mathrm{I}]\right) \boldsymbol{n}_{\boldsymbol{ls}} = \lambda_{\mathrm{s}} \left(\frac{\partial \chi_{\mathrm{s}}}{\partial y} + [\mathrm{I}]\right) \boldsymbol{n}_{\mathbf{ls}} \quad \text{on} \quad \Gamma_{\mathrm{ls}} \\
&\chi_{\mathrm{l}} = \chi_{\mathrm{s}} \quad \text{on} \quad \Gamma_{\mathrm{ls}} \\
&\langle \chi_{\mathrm{s}} \rangle = 0 \quad \langle \chi_{\mathrm{l}} \rangle = 0
\end{aligned} \tag{36}$$

Numerical application

In this part, we concentrate on the main input parameter of the heat transfer model which is the thermal conductivity. Regarding the obtained model, this macroscopic parameter depends on the microstructure of the considered porous medium via the thermal conductivity,

$\boldsymbol{\lambda}^{\text{hom}}$, tensors calculated in the previous section, eq. (35). Here, we calculate this obtained parameter by the periodic homogenization method. The use of digital simulation aims to study this parameter correctly while studying a representative unit cell of the material.

Thermal conductivity homogenized tensor

Let us consider a porous medium whose microstructure consists in a periodic repetition of a 3-D unit cell, fig. 3. Where the liquid, solid and gas interfaces are presented.

The studied consists of two spheres of radius $r_{c1} = 0.3858$ and $r_{c2} = 0.4045$ located in the center of the unit cell, and eighths of spheres of radius $r_s = 0.36$ located at the corners of the cell, and quarters of spheres of the same radius, located on each side of the cell. The domain in green represents the liquid phase. This water layer adsorbed on the solid phase is of very small thickness ($e_l = 0.0187$), which lays to a water content of 3.0%, that corresponds to a constant relative humidity in the hygroscopic region. These dimensions are selected to obtain low porosity corresponding to porosity of the cementitious materials, such as concrete.

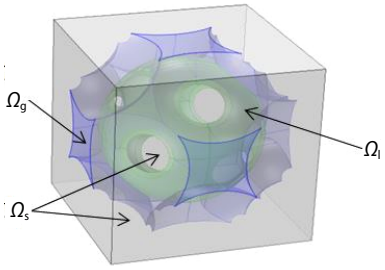

Figure 3. Elementary cell of periodic medium
(*for color image see journal web site*)

By solving the local boundary value, eq. (36), the homogenized thermal conductivity tensors was calculated to determine the variables χ_s and χ_l. These local boundary value problems are solved by the finite element method by using COMSOL Multiphysics [26]. The local boundary value problem to be solved in this case is:

$$
\begin{gathered}
\Delta_y \chi_{s_i} = 0 \quad (i = 1,2,3) \quad \text{in} \quad \Omega_s \\
\frac{\partial \chi_{s_i}}{\partial y} n = n_i \quad \text{on} \quad \Gamma_{sg} \\
\frac{\partial \chi_{s_i}}{\partial y} n = \frac{\lambda_l}{\lambda_s}\left(\frac{\partial \chi_{l_i}}{\partial y}\right) n_i - \left(1 - \frac{\lambda_l}{\lambda_s}\right) n_i \quad \text{on} \quad \Gamma_{ls} \\
\chi_{s_i} = \chi_{l_i} \quad \text{on} \quad \Gamma_{ls} \\
\left\langle \chi_{s_i} \right\rangle_{\Omega_s} = 0
\end{gathered}
\tag{37}
$$

$$
\begin{gathered}
\Delta_y \chi_{l_i} = 0 \quad (i = 1,2,3) \quad \text{in} \quad \Omega_l \\
\frac{\partial \chi_{l_i}}{\partial y} n = n_i \quad \text{on} \quad \Gamma_{lg} \\
\frac{\partial \chi_{l_i}}{\partial y} n = \frac{\lambda_s}{\lambda_l}\left(\frac{\partial \chi_{s_i}}{\partial y}\right) n_i - \left(1 - \frac{\lambda_s}{\lambda_l}\right) n_i \quad \text{on} \quad \Gamma_{ls} \\
\chi_{l_i} = \chi_{s_i} \quad \text{on} \quad \Gamma_{ls} \\
\left\langle \chi_{l_i} \right\rangle_{\Omega_l} = 0
\end{gathered}
\tag{38}
$$

Remind that on the solid-solid and liquid-liquid interfaces, the conditions of periodicity are applied for each component of χ_s and χ_l.

After the numerical resolution, the obtained homogenized thermal conductivity tensor is the following:

$$\boldsymbol{\lambda}^{\text{hom}} = \lambda_s \begin{bmatrix} 0.78217 & 0 & 0 \\ 0 & 0.78217 & 0 \\ 0 & 0 & 0.78217 \end{bmatrix} + \lambda_l \begin{bmatrix} 0.02188 & 0 & 0 \\ 0 & 0.02188 & 0 \\ 0 & 0 & 0.02188 \end{bmatrix}$$

The considered cell is an approximate representation of the real material (concrete), and it also allows us to approach the porosity of concrete. It is clear that the homogenized of thermal conductivity tensor is characterized by the same value in the three main directions, and this is due to the isotropy and symmetry of the considered unit cell.

The thermal homogenized conductivity coefficient is calculated on a 3-D cell to a volumetric water content of 3% corresponding to 20% saturation. We calculate the value of $\boldsymbol{\lambda}^{\text{hom}}$, considering in this case the same porosity material (concrete) with $\lambda_s = 1.46$ W/mK [27] and $\lambda_l = 0.6051$ W/mK. The first components of the homogenized thermal conductivity tensor are presented in the tab. 1 for two different saturations. Subsequently, we propose to compare the values of homogenized thermal conductivity tensor previously obtained with existing experimental values in the literature [27] for the same saturation value.

Table 1. Comparison of the calculated and experimental values of thermal conductivity

Saturation [%]	λ^{exp} [$\text{Wm}^{-1}\text{K}^{-1}$]	$\lambda_{11}^{\text{hom}}$ [$\text{Wm}^{-1}\text{K}^{-1}$]	$\lambda^{\text{exp}}/\lambda_{11}^{\text{hom}}$
10	1.47	1.120	1.31
20	1.51	1.155	1.30

The tab. 1 shows that the calculated values of the of homogenized thermal conductivity coefficient are less than the values measured experimentally, and the maximum ratio between the experimental and calculated values is 1.31. The considered cell is an approximate representation of the real material (concrete), the differences between the values may be due to the fact that certain physical phenomena intervening on a microscopic scale in the cementitious materials were neglected, namely the non-connected porosity, the pore size and their connection. On the other hand, note that the experimental determination of the thermal conductivity coefficient can also be discussed, they are global values.

Sensitivity of thermal conductivity tensor homogenized

In reality the water content and the porosity affect the entire thermal transfer parameters [28]. These parameters include the thermal conductivity coefficient. It informs us directly on the kinetics of the transfer within the porous medium, it therefore has a major role in the refine prediction of thermal exchanges. This sensitivity study allows showing the impact of varying the water content or relative humidity, and porosity on the homogenized thermal conductivity tensor calculated in the previous section, eq. (35). In this part, the homogenized thermal conductivity tensor is calculated numerically by varying the water content then the porosity.

It should be noted that for a cementitious material several parameters may be involved for changing its porosity, such as the dosage of water, cement and aggregates, its vibration during manufacture.The water content for its part evolves depending on the relative humidity of the environment. So these two properties are independent.

The fig. 4 shows the sorption isotherm, of C4 concrete, at 20°C. It represents the change in the volumetric water content as a function of the relative humidity of the material. These tests were conducted as part of the thesis of Issaadi [29].

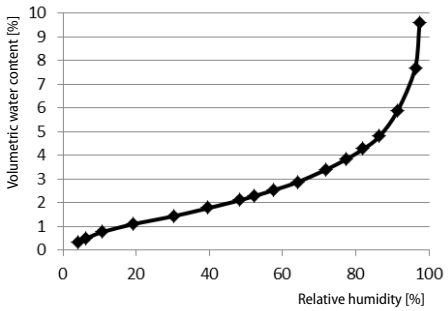

Figure 4. Sorption isotherms of C4 concrete at 20 °C [29]

This curve will allow us to move from the volumetric water content to the relative humidity, in order to represent the variation in the thermal conductivity as a function of the relative humidity of the medium. The thermal conductivity evolutions as a function of the relative humidity and the porosity of the materials are illustrated in the tab. 2.

Table 2 represents the values of homogenized thermal conductivity tensor deduced from numerical simulations based on the relative humidity, and porosity of the representative unit cell. It is shown that when the material is exposed to high relative humidity the water content increases and the water replaces the air, which increases the thermal conductivity of the medium. Concerning porosity, it significantly affects the thermal conductivity of the medium, in effect with increasing in the voids volume, the thermal conductivity decreases. It should be noted that these two parameters (humidity and porosity) are key parameters in calculating the homogenized tensor of thermal conductivity.

Table 2. Evolution of homogenized thermal conductivity

θ_l [%]	φ [%]	$\lambda_{ll}^{hom} = f(\theta_l)$ [$Wm^{-1}K^{-1}$]	ε_p [%]	$\lambda_{ll}^{hom} = f(\varepsilon_p)$ [$Wm^{-1}K^{-1}$]
0.5	6.5	1.0878	11.05	1.2487
1.0	18	1.1036	12.03	1.2223
1.5	32	1.1202	13.08	1.1909
2.0	45	1.1327	14.09	1.1639
2.5	55	1.1430	14.42	1.1552
3.0	67	1.1552	15.02	1.1358
3.5	73	1.1685	15.51	1.1210
4.0	80	1.1771	16.01	1.1067

Conclusion

The implementation of the multiscale homogenization technique, allowed us to elaborate, from the equations written at the pore scale of the porous medium, a pertinent macroscopic model of heat transfers. The homogenization method used is based on dimensional analysis of the conservation energy equations at the microscopic scale. The resulting macroscopic parameters of the developed model are so defined. This method assumes that the microstructure of the porous medium consists of a periodic repetition of a certain elementary cell, called basic cell. A representative elementary cell of concrete was chosen in order to numerically determine the homogenized tensor of thermal conductivity. This latter depend on the geometrical properties of the cell. Finally, a sensitivity analysis has allowed us to highlight the influence of the water content and porosity of the material on the homogenized thermal conductivity tensor. It proved that the homogenized thermal conductivity tensor is sensitive to variations of the water content and porosity of unit cell.

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Nomenclature

c – volumetric heat capacity, [$Jm^{-3}K^{-1}$]
h_l – specific enthalpy of the liquid, [Jkg^{-1}]
h_{lv} – specific enthalpy of vaporization, [Jkg^{-1}]
[I] – identity matrix, [–]

L – characteristic macroscopic length, [m]
l – characteristic microscopic length, [m]
$\boldsymbol{n}_{ij}$ – normal unit vector directed from the domain Ω_i toward the domain Ω_i, [–]
n_i – volume fractions of the materials i, [–]
P_c – capillary pressure, [Pa]
T – temperature, [K]
t – time, [s]
v – velocity, [ms^{-1}]
x – macroscopic dimensionless space variable, [–]
y – microscopic dimensionless space variable, [–]

Greek symbols

Γ – interface between two different phases, [–]
ε – scale separation parameter, [–]
ε_p – porosity, [%]
θ_l – volumetric water content, [%]
λ – thermal conductivity, [Wm^{-1}K^{-1}]
$\boldsymbol{\lambda}^{hom}$ – macroscopic conductivity tensor, [Wm^{-1}K^{-1}]
ρ – density, [kgm^{-3}]
φ – relative humidity, [%]
ω_{lg} – liquid-gas interface velocity, [ms^{-1}]
Ω – period, [–]
Ω_i – part of the period occupied by the pores by mediums i, [m^3]

Subscripts

g – gas
l – water liquid
s – solid

Superscripts

* – dimensional variable
r – reference variable

References

[1] Ferroukhi, M. Y., *et al*., Effect of Coupled Heat, Air and Moisture Transfers Modeling in the Wall on the Hygrothermal Behavior of Buildings, *Energy Procedia*, *78* (2015), Nov., pp. 2584-2589
[2] Whitaker, S., Simultaneous Heat, Mass, and Momentum Transfer in Porous Media: A Theory of Drying. *Advances in Heat Transfer*, *13* (1977), Dec., pp. 119-203
[3] Whitaker, S., Advances in Theory of Fluid Motion in Porous Media, *Industrial & Engineering Chemistry*, *61* (1969), 12, pp. 14-28
[4] Moyne, C., *et al*., Experimental and Theoretical Approach of the Thermal Conductivity of Wet Porous Media – II Theory, *International Journal of Heat and Mass Transfer*, *31* (1988), 11, pp. 2319-2330
[5] Goyeau, B., Macroscopic Conduction Models by Volume Averaging for Two-Phase Systems, in: *Thermal Nanosystems and Nanomaterials*, Springer-Verlag, Berlin, 2009, pp. 95-105
[6] Quintard, M., Whitaker, S., One- and Two-Equation Models for Transient Diffusion Processes in Two-Phase Systems, *Advances in Heat Transfer*, *23* (1993), Dec., pp. 369-464
[7] Bourbatache, M. K., Modeling of the Transfer of Ions Chlorides in Cementitious by Periodic Homogenization Materials, Ph. D. thesis, La Rochelle University, La Rochelle, France, 2009
[8] Sanchez-Palencia, E., *Non-Homogeneous Media and Vibration Theory*, Springer-Verlag, Berlin, 1980
[9] Keller, J. B., Effective Behavior of Heterogeneous Media, in: *Statistical Mechanics and Statistical Methods in Theory and Application*, Springer, Boston, Mass., USA, 1977, pp. 631-644
[10] Auriault, J. L., Adler, P. M., Taylor Dispersion in Porous Media: Analysis by Multiple Scale Expansions, *Advances in Water Resources, 18* (1995), 4, pp. 217-226
[11] Bensoussan, A., *et al*., Asymptotic Analysis for Periodic Structures, Studies in Mathematics and Its Applications, Elsevier North-Holland, Amsterdam, The Netherland, 1978
[12] Bourbatache, K., *et al*., Ionic Transfer in Charged Porous Media, Periodic Homogenization and Parametric Study on 2-D Microstructures*, International Journal of Heat and Mass Transfer, 55* (2012), 21-22, pp. 5979-5991
[13] Auriault, J. L., Ene, H. I., Macroscopic Modelling of Heat Transfer in Composites with Interfacial Thermal Barrier, *International Journal of Heat and Mass Transfer, 37* (1994), 18, pp. 2885-2892
[14] Auriault, J. L., Effective Macroscopic Description for Heat Conduction in Periodic Composites, *International Journal of Heat and Mass Transfer, 26* (1983), 6, pp. 861-869
[15] Moyne, C., Amaral Souto, H. P., Multi-Scale Approach for Conduction Heat Transfer: One- and Two-Equation Models: Part 1: Theory, *Computational and Applied Mathematics*, *33* (2014), 2, pp. 257-274
[16] Lewandowska, J., Laurent, J. P., Humidity Transfer in Unsaturated Heterogeneous Porous Media by Homogenization, *Physics and Chemistry of the Earth, Part A: Solid Earth and Geodesy, 25* (2000), 2, pp. 175-181
[17] Mchirgui, W., *et al*., Modelling Moisture Transport for a Predominant Water Vapour Diffusion in a Partially Saturated Porous Media, *European Journal of Environmental and Civil Engineering, 17* (2013), 3, pp. 202-218

[18] Auriault, J. L., *et al*., Upscaling Forchheimer law, *Transport in Porous Media, 70* (2007), 2, pp. 213-229
[19] Allaire, G., *et al*., Two-Scale Expansion with Drift Approach to the Taylor Dispersion for Reactive Transport through Porous Media, *Chemical Engineering Science, 65* (2010), 7, pp. 2292-2300
[20] Attinger, S., *et al*., Homogenization of the Transport Behavior of Nonlinearly Adsorbing Pollutants in Physically and Chemically Heterogeneous Aquifers, *Advances in Water Resources, 32* (2009), 5, pp. 767-777
[21] Bourbatache, K., *et al*., Modeling the Chlorides Transport in Cementitious Materials by Periodic Homogenization, *Transport in Porous Media, 94* (2012), 1, pp. 437-459
[22] Auriault, J. L., Lewandowska, J., Non-Linear Diffusion in Porous Media, *Comptes Rendus de l'Académie des Sciences, Series IIB., Mechanics-Physics-Chemistry-Astronomy*, *324* (1997), 5, pp. 293-298
[23] Darquennes, A., *et al*., Monitoring Internal Sulphate Reactions by X-ray Tomography, *Proceedings*,15th Euroseminar on Microscopy Applied to Building Materials, Delft, The Netherlands, 2015
[24] Duval, F., Modeling of the Renoyage of a Bed of Particles: Contribution to the Estimation of Macroscopic Transport Properties, Ph. D. thesis, INPT Toulouse, Toulouse, France, 2002
[25] Abahri, K., Modeling of Transfers Combinet Heat, Air and Moisture in Porous Construcyon Materials, Ph. D. thesis, La Rochelle University, La Rochelle, France, 2012
[26] ***, COMSOL, COMSOL Multiphysics User's Guide, Version 4.3, 2012
[27] Zhang, W., *et al*., Mesoscale Model for Thermal Conductivity of Concrete, *Construction and Building Materials, 98* (2015), 15, pp. 8-16
[28] Trabelsi, A., Numerical and Experimental Studies of Moisture Transfer in Porous Construction Materials, Ph. D. thesis, La Rochelle University, La Rochelle, France, 2010
[29] Issaadi, N., Influence of Variability of Cement Based Materials Properties on the Moisture Transport: Development of Probality approach, Ph. D. thesis, La Rochelle University, FR, 2015

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