Mathematical modelling of phase change in porous media in presence of advection : upscaling technique

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ABSTRACT: This article is devoted to the mathematical modelling of phase change of water into vapor phase. This physical transformation is considered to appear inside the porous medium. In analyzing two-phase flow, the standard method of continuum mechanics is followed. Therefore, a two-phase flow is considered as a field, which is subdivided into single-phase regions with moving boundaries between phases. The standard physical equations hold for each region with appropriate boundary and jump conditions at the interfaces. An industrial application of such models, is to understand the complex phenomena occurring during hot paper pressing. In such a unit operation, we have to consider coupled effects of heat and mass transfer. As the description at the microlevel is too complex, we will consider here the macroscopic behavior. It is obtained from the microscopic scale by an upscaling technique, namely the method of homogenization for periodic structures. It permits to obtain a catalogue of macroscopic models. The domain of validity of each model is defined by means of orders of magnitude of dimensionless numbers. For a specific practical problem (i.e. a given process and a given material), the corresponding dimensionless numbers can easily be estimated by selecting the appropriate characteristic quantities. The suitable model for describing the process under consideration can be selected throughout the catalogue.

1 INTRODUCTION

Nowadays, industrial applications increasingly need improved technical and scientific understanding so as to optimize production and competitiveness. Therefore, developing empirical, numerical or theoretical models has become crucial. Derivation of mathematical models consists in determining behavior laws and the corresponding effective parameters. The knowledge of the domains of validity of these models is also important. For example, paper industry, among other, would draw a great benefit from the improved understanding of physical processes provided by such theoretical investigations. In this example, deriving knowledge models of physical processes involved in new technology of paper pressing at high temperature will allow enhancement of both paper quality and production rate. Indeed, during hot paper pressing, high temperature gradients lead to high-pressure gradients that may give rise to violent phase change of water into vapor. This modification may damage the fibrous structure of the paper. The knowledge of the conditions under which phase change may occur would allow a better control of the destruction of the fibrous network. For this purpose, rigorous mathematical modeling of phase change in porous media is required. In this paper, we use an upscaling technique for determining the macroscopic behavior of water-air flow in porous media with phase change of water into vapor. The upscaling technique is the method of homogenization for periodic structures that has initially been introduced by Bensoussan et al. [1978] and Sanchez-Palancia [1980]. In this study, we use the approach suggested by Auriault [1991]. It permits to obtain macroscopic laws, their domain of validity, and also their effective parameters without any macroscopic pre-requisite. This formulation of the method is on the basis of the analysis of the dimensionless numbers arising from the local description under consideration. This fundamental step is called the normalization and is aimed at specifying all cases that may be homogenized.

In this paper, attention will essentially be focused on the normalized local description. Then the macroscopic models obtained by homogenizing this local description will be presented. We will expose in

Section 2, how the initial local description may be obtained from Ishii analyze [1978] concerning the physical description of phase change. The importance of the description of the interface between water and gas, is underlined. This description is different than considering a source term in the continuity equation. Furthermore, the source term means that the phase change may occur anywhere in the medium at the microlevel. Considering the interface as a front, the description involving the source term is not possible. The dimensionless pore-scale description of water-air flow in porous media with phase change of water into vapor is presented in details in Section 3. The mass, momentum and energy balances in each component domain are completed by both continuity and jump conditions in order the problem to be solved. Homogenization of the corresponding local description will lead to the mechanical macroscopic behavior. For the thermal problem, two independent dimensionless parameters can not be determined: they constitute the so-called free parameters of the problem under consideration. Several orders of magnitude will be considered for these two dimensionless parameters which will lead to several macroscopic behaviors for the thermal problem. These macroscopic behaviors obtained by homogenization are presented in Section 4.

2 LOCAL DESCRIPTION OF THE CONSIDERED PHYSICAL PHENOMENA

2.1 *Physical problem description*

A periodic porous medium is considered. Its period Ω is of the order of magnitude of the microscopic scale l, characterizing the pore scale. We assume that the microscopic and macroscopic scales are separated. In other words, the characteristic macroscopic length L is such that $l/L = \varepsilon \ll 1$. Within the period, the solid space is filled up by two fluids, water (wetting phase) and vapor (non-wetting phase) that occupy domains Ω_w and Ω_a, respectively. We assume that phase change may occur at the water-vapor interface (Γ_{ww}) and that the vapor-phase has no contact with the solid. The water–solid interface is denoted by (Γ_{ws}). This assumption of the existence of a front will lead to a more complicated physical description, as it does not allow introducing simply a source term in the continuity equation in the microscopic description. Therefore physical properties of the vapor–liquid interface has to be introduced. The different equations are presented in the following paragraphs.

The main characteristic of a mixture of two immiscible fluids is the presence of at least one interface separating the phases or components. As we will consider annular regimes for simplicity, we will have to consider both water–solid and water–vapor interfaces. We will follow the standard description involved in continuum mechanics. Therefore, a two-phase flow is considered here as a field which is subdivided into single phase regions with moving boundaries between phases. The standard balance equations hold for each subregion with appropriate jump and boundary conditions at the interfaces. Since an interface is a singular case of the continuous field, we have two different conditions at the interface. *The balance at an interface which corresponds to the field equation is called a jump condition. Whereas any additional information corresponding to the constitutive laws in space which are also necessary at interface, is called an interfacial boundary condition.*

The balance equation may be written in the following form:

$$\frac{\partial \rho_k \Psi_k}{\partial t} + \nabla \cdot (\vec{V}_k \rho_k \Psi_k) = -\nabla \cdot J_k + \rho_k \Phi_k \qquad (1)$$

where ρ_k represents the density and $\vec{V}_k$ the velocity. The first term of the above equation is the time rate of change of the quantity per unit volume, whereas the second term is the rate of convection per unit volume. The right hand side terms represent the surface flux and the volume source.

We may express the conservation equations (continuity, momentum and energy) as follows:

- Continuity equation in the domain Ω_k: $\Psi_k = 1$, $\Phi_k = 0, J_k = 0$. This leads to the following equation:

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\vec{V}_k \rho_k) = 0 \qquad (2)$$

- Momentum equation in the domain Ω_k considering no body force: $\Psi_k = \vec{V}_k, \Phi_k = 0, J_k = -\sigma_k$, where σ_k represents the stress tensor. This quantity may be rewritten as $\sigma_k = -p_k + \tau_k$ splitting the stress tensor into the pressure term and the viscous stress, respectively. Therefore, it leads to the equation:

$$\frac{\partial \rho_k \vec{V}_k}{\partial t} + \nabla \cdot (\vec{V}_k \rho_k \vec{V}_k) = -\nabla p_k + \nabla \cdot \tau_k \qquad (3)$$

- Conservation of energy in the domain Ω_k: We consider here the total energy of the fluid. Therefore, we have: $\Psi_k = u_k + \vec{V}_k^2/2, \Phi_k = Q_k/\rho_k, J_k = -\vec{g}_k - \sigma_k \cdot \vec{V}_k$ where $u_k, \vec{g}_k$ and Q_k represent the internal energy, heat flux and body heating, respectively. We obtain the following equation:

$$\frac{\partial \rho_k (u_k + \vec{V}_k^2/2)}{\partial t} + \nabla \cdot [\rho_k \vec{V}_k (u_k + \vec{V}_k^2/2)] = -\nabla \vec{g}_k + \nabla \cdot (\sigma_k \cdot \vec{V}_k) + Q_k \qquad (4)$$

These Equations express the basic physical laws of the conservation of mass, momentum and energy. In order to solve these equations, it is necessary to specify the

fluxes and the body source, as well as the fundamental equation of state. Furthermore, we may introduce here the decomposition of the total energy between the mechanical and internal energies. Indeed, multiplying the equation of motion by the velocity, we obtain the mechanical energy equation:

$$\frac{\partial \rho_k \vec{V}_k^2/2}{\partial t} + \nabla \cdot (\rho_k \vec{V}_k \vec{V}_k^2/2) = -\vec{V}_k \nabla \cdot p_k - \vec{V}_k \cdot (\nabla \cdot \tau_k) \quad (5)$$

By subtracting the mechanical energy equation from the total energy equation, the internal energy equation is obtained:

$$\frac{\partial(\rho_k u_k)}{\partial t} + \nabla \cdot [\rho_k \vec{V}_k (u_k)] = -\nabla \vec{g}_k - p_k \nabla \cdot \vec{V}_k + \tau_k : \nabla \cdot \vec{V}_k + Q_k \quad (6)$$

The enthalpy h_k is defined as: $h_k = u_k + p_k/\rho_k$. Therefore, the internal energy equation becomes:

$$\frac{\partial(\rho_k h_k)}{\partial t} + \nabla \cdot (\rho_k \vec{V}_k h_k) = -\nabla \cdot \vec{g}_k + \frac{Dp_k}{Dt} + \tau_k : \nabla \cdot \vec{V}_k + Q_k \quad (7)$$

Hence, we obtain the following expressions of the continuity, momentum (considering no body force) and internal energy equations in the domain Ω_k:

$$\frac{\partial \rho_k}{\partial t} + \nabla \cdot (\rho_k \vec{V}_k) = -\nabla \vec{g}_k - p_k \nabla \cdot \vec{V}_k + \tau_k : \nabla \cdot \vec{V}_k + Q_k \quad (8)$$

$$\frac{\partial \rho_k \vec{V}_k}{\partial t} + \nabla \cdot (\vec{V}_k \rho_k \vec{V}_k) = -\nabla p_k + \nabla \cdot \tau_k \quad (9)$$

$$\frac{\partial(\rho_k h_k)}{\partial t} + \nabla \cdot (\rho_k \vec{V}_k h_k) = -\nabla \vec{g}_k + \frac{Dp_k}{Dt} + \tau_k : \nabla \cdot \vec{V}_k + Q_k \quad (10)$$

2.2 *Equations at the interfaces*

We now have to consider the different interfaces involving the water, gas and solid phases.

2.2.1 *Water solid interface* Γ_{ws}

First, we analyse the interface water/solid.

Continuity of velocities

$$\vec{V}_w = \dot{u}_s \quad (11)$$

where $\vec{V}_w$ is the velocity of the water phase and $\dot{u}_s$ represents the time derivative of the solid displacement.

Continuity of temperatures

$$T_w = T_s \quad (12)$$

Continuity of heat fluxes

$$(\lambda_w \vec{\nabla} T_w) \cdot \vec{N}_{ws} = (\lambda_s \vec{\nabla} T_s) \cdot \vec{N}_{ws} \quad (13)$$

where $\vec{N}_{ws}$ is the outer normal unit vector of Γ_{ws} and where λ_w and λ_s are the thermal conductivities of the water and of the solid phase, respectively.

2.2.2 *Water gas interface* Γ_{wa}

2.2.2.1 Interfacial balance

The description of the interface Γ_{wa} is the delicate part of the physical description. The presented modelisation is based on the work of Ishii (1975). The main steps of this description are the consideration of the mass, momentum and energy conservation. The balance equations derived previously (equations 8, 9, 10), may be applied to each phase up to an interface, but not across it. A particular form of the balance equation should be used at an interface in order to take into account the singular characteristics (discontinuities) in various variables. Special conditions, on fluid density, energy and velocity, constitute the jump conditions

(a) Interfacial mass balance: Continuity of mass fluxes

$$\rho_a(\vec{V}_a - \vec{V}_i) \cdot \vec{N}_a + \rho_w(\vec{V}_w - \vec{V}_i) \cdot \vec{N}_w = 0 \quad (14)$$

where $\vec{V}_i$ is the velocity of the interface. We may also introduce the notation: $\dot{m}_k = \rho_k(\vec{V}_k - \vec{V}_i) \cdot \vec{N}_k$

(b) Interfacial Momentum balance and Interfacial Energy balance

- We first consider the momentum balance:

$$[\rho_a(\vec{V}_a - \vec{V}_i) \cdot \vec{N}_a]\vec{v}_a - (-p_a \underline{I} + \tau_a) \cdot \vec{N}_a + [\rho_w(\vec{V}_w - \vec{V}_i) \cdot \vec{N}_w]\vec{v}_w - (-p_w \underline{I} + \underline{\tau_w}) \cdot \vec{N}_w = 0 \quad (15)$$

- The internal energy may be written:

$$(\rho_a(\vec{V}_a - \vec{V}_i) \cdot \vec{N}_a)\left(u_a + \frac{1}{2}\vec{v}_a^2\right) + (\rho_w(\vec{V}_w - \vec{V}_i) \cdot \vec{N}_w)\left(u_w + \frac{1}{2}\vec{v}_w^2\right) + \vec{N}_w \cdot (-\Pi_w \vec{V}_w + \vec{g}_w) + \vec{N}_a \cdot (-\Pi_a \vec{V}_a + \vec{g}_a) = 0 \quad (16)$$

where Π_k is the total stress: $\Pi_w = -p_k \underline{I} + \underline{\tau_k}$

2.2.2.2 Boundary conditions at interface

In order to state the second law of thermodynamics, it is necessary to introduce the concept of a temperature T_k and the specific entropy s_k. The second law may be

written as:

$$\frac{\partial(\rho_k s_k)}{\partial t} + \nabla \cdot (\rho_k \vec{V}_k s_k) + \nabla \cdot \left(\frac{\vec{g}k}{T_k}\right) - \frac{Q_k}{T_k} = \Delta_k \tag{17}$$

where Δ_k is the rate of entropy production per unit volume.

Constitutive Equations

To this extent, the number of dependent variables exceed that of the field equations. Consequently, it is necessary to supplement them with constitutive equations which define the behavior of the considered medium. From their physical significances, it is possible to classify the different constitutive equations into three groups: Mechanical Constitutive equations, Energetic constitutive equations, Constitutive equation of state. The first group specifies the stress tensor and the body force, if any, whereas the second group supplies the heat flux and the body heating. The last equation gives a relation between entropy, the internal energy.

(a) Mechanical Constitutive Equation.

The rheological constitutive equations may have different forms related to the various mechanical behaviors. Usually, a linear relationship is used which involves the viscosity μ.

(b) Energetic Constitutive Equation.

We may consider here the Fourier Law, that is checked by most fluids: $\vec{g}_k = \lambda_k . \nabla T_k$ in which λ_k is a second order tensor of conductivity.

(c) Fundamental Equation of state.

This relation is often given under the form both for the fluid and the gas: $p_k = p_k(\rho_k, T_k)$. As in the field domain, the surface balance equations should be supplemented by various constitutive laws. In order to establish these conditions, we may introduce the concept of interfacial entropy (Δ_a) inequality at the interface that may be written (Ishii 1978, Delhaye 1974):

$$T_i \Delta_a = \sum_{k=w}^{a} \left\{ \dot{m}_k \left[u_k - s_k T_i + \frac{|\vec{V}_k - \vec{V}_i|^2}{2} + \frac{p_k}{\rho_k} \right] - \vec{n}_k \cdot \tau_k \cdot (\vec{V}_k - \vec{V}_i) + \vec{n}_k \cdot \vec{g}_k \left(1 - \frac{T_i}{T_k}\right) \right\} \geq 0 \tag{18}$$

where T_i and $\vec{n}_k$ are the interfacial (or surface) temperature and the normal unit vector, respectively.

For sake of simplicity, we will consider only here a limiting case when entropy production of the interface Δ_a is set to zero, which means that the transfer is considered as reversible. In other word, each term of the entropy is assumed to equal to 0. This means that there is no resistances to interfacial transfer of quantities. This also means that the exchanges between the two phases are governed by the conditions of the bulk fluids at each side, and not by the interface itself. By assuming that the source is zero, we also assume that each term is independently equal to zero. This leads to 3 conditions.

(a) Thermal Boundary Conditions.

From the last term, we obtain the thermal equilibrium at the interface: $T_a = T_w = T_i$

This condition set the energy level of the interface, contrary to the energy jump equation which specifies the relation between the energy transfers to the interface.

(b) Mechanical condition, No slip conditions.

It may be shown that the tangential components of the fluid velocities are equal. This assumption means that there is no slip at the interface. The equation may be written (Ishii, 1975, p.35, Eq. II 2–44):

$$\vec{N}_w \frac{\dot{m}_w^2}{\rho_w} + \vec{N}_w p_w + \vec{N}_a \frac{\dot{m}_a^2}{\rho_a} + \vec{N}_a p_a = -2H_{wa}\gamma \vec{N}_w \tag{19}$$

(c) Chemical (Phase change) Boundary conditions.

This relation is obtained from the first term of the entropy equation.

$$\begin{aligned} g_w - g_a &= \left\{ \frac{|\vec{V}_a - \vec{V}_i|^2}{2} - \frac{|\vec{V}_a - \vec{V}_i|^2}{2} \right\} - \left\{ \frac{\tau_{nn_a}}{\rho_a} - \frac{\tau_{nn_w}}{\rho_w} \right\} \\ &= -\frac{\dot{m}_w}{2} \left(\frac{1}{\rho_w^2} - \frac{1}{\rho_a^2} \right) + \left(\frac{\tau_{nn_a}}{\rho_w} - \frac{\tau_{nn_a}}{\rho_w} \right) \end{aligned} \tag{20}$$

where g_k is the Gibbs free energy defined as follows:

$$g_k = u_k - T_k s_k + p_k/\rho_k$$

and τ_{nn} is defined as a normal viscous stress: $\vec{n}_k \cdot \tau_k = \tau_{nk} + \tau_{tk} = \vec{n}_k \cdot \tau_{nn_k} + \tau_{tk}$.

The stress (τ_{nn}) are now considered as negligible. Therefore, this condition may be written:

$$g_w - g_a = \frac{|\vec{v}_a - \vec{v}_i|}{2} - \frac{|\vec{v}_w - \vec{v}_i|}{2} \tag{21}$$

The phase change is not here considered to be due to force equilibrium but rather as a state transformation. Assuming more over that the normal stresses are negligible in respect of the pressure, it can be

shown that:

$$p_w - p_{sat}(T_i) = -2H_{wa}\gamma\left(\frac{\rho_w}{\rho_w - \rho_a}\right) + \frac{1}{2}(\rho_w \cdot \vec{N}_k[\vec{V}_w - \vec{V}_k]^2) \times \left(\frac{1}{\rho_a} - \frac{1}{\rho_w}\right) \quad (22)$$

$$p_a - p_{sat}(T_i) = -2H_{wa}\gamma\left(\frac{\rho_a}{\rho_w - \rho_a}\right) + \frac{1}{2}(\rho_w \cdot \vec{N}_k[\vec{V}_w - \vec{V}_k]^2) \times \left(\frac{1}{\rho_w} - \frac{1}{\rho_a}\right) \quad (23)$$

where T_i is the interface temperature, H_{wa} and γ represent the mean interface curvature and the surface tension, respectively.

We may notice that we find the Laplace law if the phase change is considered as equal to 0.

2.3 *Characteristic values and dimensionless quantities*

Considering a given physical quantity, denoted by Ψ_w for the water-phase and by Ψ_a for the vapor-phase, their characteristic values Ψ_{w_R} and Ψ_{a_R} are assumed to be known. We define the two following dimensionless quantities associated to Ψ_w and Ψ_a, respectively $\Psi_w^* = \Psi_w/\Psi_{w_R}$ and $\Psi_a^* = \Psi_a/\Psi_{a_R}$. The characteristic values for all physical quantities are shown on Table 1.

Where μ, ρ t, v, T, λ, C_p, γ and A represent the viscosity, density, time, pressure, velocity, temperature, thermal conductivity, specific heat, interfacial tension and compressibility, respectively.

Let us denote by N the measure of the ratio of Ψ_w to Ψ_a: $N = |\Psi_w|/|\Psi_a| = (\Psi_w^*/\Psi_a^*) \times (\Psi_{w_R}/\Psi_{a_R}) = O(\Psi_{w_R}/\Psi_{a_R})$.

Assume for example that $\varepsilon = O(10^{-2})$. Since Ψ_R and Φ_R are given (Table 1), we are therefore able to estimate N with respect to ε: $N = O(\varepsilon^p)$. Thus, from the characteristic values on Table 1 and the estimate $\varepsilon = O(10^{-2})$, we deduce the orders of magnitude of any physical properties presented on the following table.

2.4 *Normalised local description*

At the pore-scale the flow of both fluids and the phase change of water into vapour is described by balance equations in Ω_w and Ω_a and appropriate continuity and energy balance conditions on Γ_{wa} and Γ_{ws}. The studied process is time dependent. However, when written in Eulerian coordinates, the equations that describe the process are steady-state. Therefore, we choose the Eulerian representation for writing the local description. All the equations below are cast in a dimensionless form, but for the sake of simplicity symbols *, in the dimensionless equations, and $_R$, in the expressions of the dimensionless numbers, are omitted.

2.4.1 *Balance equations in Ω_w and Ω_a*

Mass balance

For compressible fluids, the dimensionless mass-balance equations in Eulerian coordinates are the following:

$$\vec{\nabla} \cdot (\rho_k \vec{v}_k) = 0, \quad k = w, a \quad (24)$$

in which ρ_k and $\vec{v}_k$ are the density and the velocity of the k-component, respectively.

Momentum balance

For both fluids, the momentum balance is expressed by Navier-Stokes equation. In Eulerian coordinates the

Table 1. Characteristic values of physical properties.

Variables	Units	Water	Air	Fibres
μ	$Pa \cdot S$	10^{-3}	19×10^{-6}	
ρ	$kg \cdot m^{-3}$	10^3	1,23	$1,5 \times 10^3$
t	s	10^{-3}	10^{-3}	10^{-3}
p	Pa	10^5 *to* 10^6	10^5 *to* 10^6	10^5 *to* 10^6
$\vec{v}$	$m \cdot s^{-1}$	10^{-2}	10^{-2}	
T	K	293 *to* 373	293 *to* 373	293 *to* 373
λ	$m^{-1} \cdot s^{-1} \cdot K^{-1}$	0.602	0.026	0.33
C_p	$J \cdot kg^{-1} \cdot K^{-1}$	4.18×10^3	10^3	1.33×10^3
γ	$N \cdot m^{-1}$	72.75×10^3 (293)	58.8×10^3 (373)	
A	$kg \cdot m^{-1} \cdot s^{-2}$	2×10^6	8.1×10^4	

equations for (k = w,a), reduce to:

$$\mu_k(\Delta\vec{v}_k + \vec{\nabla}(\vec{\nabla}\cdot\vec{v}_k)) - Q_k\vec{\nabla}p_k = Re_k\rho_k(\vec{v}_k\cdot\vec{\nabla})\vec{v}_k \tag{25}$$

We have introduced here two dimensionless parameters Q_k and Re_k defined classically as follows: $Q_k = O(P_k l/\mu_k V_k)$; $Re_k = O(\rho_k l V_k/\mu_k)$.

It can be shown () by a simple physical reasoning that: $Q_k = O(\varepsilon^{-1})$. Furthermore, there are some restrictions on the order of magnitude of Re (): the situation is homogenizable if $Re \leq O(1)$ and for $Re = O(1)$ non-linearities appear and the drag law becomes non-linear. We therefore consider the case: $Re_k = O(\varepsilon)$.

Energy balance

The total energy is the sum of the mass internal energy and of the mechanical energy. When the viscous dissipation is neglected and when there is no heat source term, the energy-balance equation is written for (k = w,a), as:

$$Pe_k\vec{v}_k\cdot\vec{\nabla}(\rho_k h_k) = -\vec{\nabla}\cdot\vec{g}_k + E_{u_k}Pe_k E_{c_k}(\vec{v}_k\cdot\vec{\nabla}p_k) \tag{26}$$

where $\vec{g}_k$ is the heat flux and h_k is the enthalpy.

We may define the following quantities:

$$\textit{Euler Number}: E_{u_k} = O(P_k)/(\rho_k V_k^2)$$
$$\textit{Eckert Number}: E_{c_k} = O(V_k^2)/(C_{p_k}T_k)$$
$$\textit{Peclet Number}: Pe_k = O(l\rho_k C_{p_k}V_k)/(\lambda_k)$$

It turns out that $E_{u_k} = Q_k/Re_k$. Thus, since $Q_k = O(\varepsilon^{-1})$ and since we consider $Re_k = O(\varepsilon)$, we get: $E_{u_k} = O(\varepsilon^{-2})$. Moreover, it can be shown that for the cases of interest, the Eckert number is always such that: $E_{c_k} \leq O(\varepsilon^4)$. We therefore assume: $E_{c_k} = O(\varepsilon^4)$. Finally, there is no possible estimation for the Peclet numbers Pe_w and Pe_a. However, from the considered values, we deduce: $(Pe_a/Pe_w) = O(1)$. These numbers are the parameters of the modelisation.

Equations of State of the Fluids

We consider linear equations of state:

$$p_k = A_k\rho_k, \quad A_k \text{ is constant}, \quad k = w,a \tag{27}$$

2.4.2 *Conditions on solid/liquid interface* Γ_{ws}

Continuity of velocities

The conditions on the solid/liquid interface γ_{ws} are considered below.

$$\vec{v}_w = \dot{\vec{u}}_s\,(= \vec{0} \text{ if the medium is rigid}) \tag{28}$$

where $\vec{v}_w$ is the velocity of the water phase and $\dot{\vec{u}}_s$ is the time derivative of the solid displacement.

Continuity of temperatures

$$T_w = T_s \tag{29}$$

Continuity of heat fluxes

$$C_{ws}(\lambda_w\vec{\nabla}T_w)\cdot\vec{N}_{ws} = (\lambda_s\vec{\nabla}T_s)\cdot\vec{N}_{ws} \tag{30}$$

where $\vec{N}_{ws}$ is the outer normal unit vector of Γ_{ws} and where λ_w and λ_s are the thermal conductivities of the water phase and of the solid, respectively. Thus we have: $C_{ws} = O(\lambda_w/\lambda_s) = O(1)$.

2.4.3 *Conditions on liquid/vapour interface* Γ_{wa}

The analysis of the physics at the liquid/vapour interface is taken from ().

Continuity of mass fluxes

$$N_\rho\rho_a(\vec{v}_a - \vec{v}_i)\cdot\vec{N}_a + \rho_w(\vec{v}_w - \vec{v}_i)\cdot\vec{N}_w = 0 \tag{31}$$

Where $\vec{v}_i$ is the velocity of the interface. $N_\rho = O(\rho_a/\rho_w) = O(\varepsilon)$.

Capillary equilibrium conditions

$$\frac{1}{N_\gamma}(p_w - p_{sat}(T_i)) = -2H_{wa}\gamma\left(\frac{\rho_w}{\rho_w - N_\rho\rho_a}\right) + \frac{1}{2}CL_{wa4}[\rho_w\vec{N}_w\cdot(\vec{v}_w - \vec{v}_i)^2] \times\left(\frac{1}{N_\rho\rho_a} - \frac{1}{\rho_w}\right) \tag{32}$$

$$\frac{1}{N_\gamma}(p_a - p_{sat}(T_i)) = -2H_{wa}\gamma\left(\frac{\rho_w}{\frac{\rho_w}{N_\rho} - \rho_a}\right) + \frac{1}{2}CL_{wa4}[\rho_w\vec{N}_w\cdot(\vec{v}_w - \vec{v}_i)^2] \times\left(\frac{1}{\rho_w} - \frac{1}{N_\rho\rho_a}\right) \tag{33}$$

We have introduced here the following parameters: $N_\rho = O(\rho_a/\rho_w)$; $N_\gamma = |H_{wa}\gamma|/|p_w - p_{sat}|$; $CL_{wa4} = |(\dot{m}_w)^2|/|H_{wa}\gamma\rho_w|$. Here, we get: $N_\rho = O(1)$. It can be shown () that for $N_\gamma < 1$, there is no capillary effect. We therefore consider $N_\gamma = O(1)$. There is no possible estimation for the phase change number.

Enthalpy

$$0 = \dot{m}_w\left[(C_{p_w}T_w - C_{p_a}T_a) + E_c\left\{\left(\frac{1}{2}\vec{v}_w^2 - \vec{v}_w\cdot\vec{v}_\rho\right) - \left(\frac{1}{2}\vec{v}_a^2 - \vec{v}_a\cdot\vec{v}_\rho\right)\right\}\right] + CL_{wa_3}(\vec{v}_w\cdot\vec{g}_w + N_\gamma\vec{v}_a\cdot\vec{g}_a) \tag{34}$$

where $\vec{v}_\rho = (\vec{v}_i\cdot\vec{N}_{wa})\vec{N}_{wa} + \vec{v}_i^t$, $\dot{m}_{w_k} = \rho_k(\vec{v}_k - \vec{v}_i)\cdot\vec{N}_k$, C_{p_w} and C_{p_a} are the specific heat coefficients for both

phases. Therefore we have : $N_\lambda = O\left(\frac{\lambda_g}{\lambda_w}\right) = O(\varepsilon)$; and $CL_{wa_3} = O\left(\frac{\lambda_w}{l\rho_w V_w C_{pw}}\right) = O(Pe_w^{-1})$.

Continuity of temperatures

$$T_{wi} = T_{ai} = T_i \tag{35}$$

2.5 *Cases of interest*

Note that for the mechanical problem, defined by equations (24), (25), (27), (28), (31), (32) and (33), all dimensionless numbers have been estimated. As a result, only one mechanical macroscopic behaviour will be obtained. For the thermal problem, which is defined by equations (26), (29), (30), (34) and (35), two independent dimensionless numbers are remaining: the phase change number CL_{wa_4} and the waterphase Peclet number Pe_w. We will consider the following cases: $CL_{wa_4} = O(\varepsilon^p)(p = 0, 1, 2, 3,)$, $Pe_w = O(\varepsilon^q)(q = 0, 1, 2)$.

3 MACROSCOPIC BEHAVIOURS

3.1 *Mechanical problem*

The derived macroscopic mechanical description is written as a steady-state behaviour with coupled Darcy's laws:

$$\vec{\nabla} \cdot \vec{V}_w = 0; \quad \vec{\nabla} \cdot (\rho_a \vec{V}_a) = 0; \quad p_c = p_a - p_w;$$
$$\vec{V}_w = -\tilde{K}_{ww} \vec{\nabla} p_w - \tilde{K}_{wa} \vec{\nabla} p_a;$$
$$\vec{V}_a = -\tilde{K}_{aa} \vec{\nabla} p_a - \tilde{K}_{aw} \vec{\nabla} p_w.$$

where $\tilde{K}_{\alpha\beta}$ represents the permeability of the porous medium considering both phases α and β.

3.2 *Thermal problem*

3.2.1 $CL_{wa_4} = O(1)$

This situation can occur physically but is not homogenizable. This means that there is no equivalent macroscopic description.

3.2.2 $CL_{wa_4} = O(\varepsilon^2)$, $Pe_w = O(\varepsilon^2)$

The macroscopic behaviour is purely diffusive and is given by:

$$\vec{\nabla} \cdot (\lambda^{eff} \vec{\nabla}_x T) = 0. \tag{36}$$

3.2.3 $CL_{wa_4} = O(\varepsilon^2)$, $Pe_w = O(\varepsilon)$

In this case a convective term due to the wetting phase does appear:

$$\vec{V}_w \cdot \vec{\nabla}(C_{p_w} \rho_w T) = -\vec{\nabla} \cdot (\lambda^{eff} \vec{\nabla} T) \tag{37}$$

3.2.4 $CL_{wa_4} = O(\varepsilon^2)$, $Pe_w = O(1)$

In this case we obtain a phase change term, a diffusive term and a convective term. The non-wetting phase does appear in the convective term.

$$\vec{V}_w \cdot \vec{\nabla}(C_{p_w} \rho_w T) + \varepsilon \vec{V}_a \cdot \vec{\nabla}(C_{p_a} \rho_a T) = -\varepsilon \vec{\nabla} \cdot (\lambda^{**} \vec{\nabla} T) + \varepsilon C_{p_w} T_{\Gamma_{wa}} \frac{\Gamma_{wa}}{|\Omega|} \dot{m}_w \tag{38}$$

$$\lambda^{**} = \frac{1}{|\Omega|} \int_{\Omega_w} \left[\lambda_{w_{jk}} \left(\delta_{jk} + \frac{\partial \chi'_{wj}}{\partial y_k} \right) - \chi'_i \vec{v}(0)_{wj} \right] \tag{39}$$

χ'_w is the particular solution of a boundary-value problem defined over the period. $\vec{v}(0)$ represents the first order of the development of the velocity.

3.2.5 $CL_{wa_4} = O(\varepsilon^1)$, $Pe_w = O(\varepsilon^2)$

The macroscopic behaviour is purely diffusive and is given by equation (36).

3.2.6 $CL_{wa_4} = O(\varepsilon)$, $Pe_w = O(\varepsilon)$

We get diffusive, convective and phase change terms:

$$\vec{V}_w \cdot \vec{\nabla}(C_{p_w} \rho_w T) = -\vec{\nabla} \cdot (\lambda^{eff} \vec{\nabla} T) + \frac{|\Gamma_{wa}|}{|\Omega|} \dot{m}_w C_{p_w} T_{\Gamma_{wa}} \tag{40}$$

Note that in this case all terms are of the same order of magnitude.

3.2.7 $CL_{wa_4} = O(\varepsilon)$, $Pe_w = O(1)$

The influence of the non-wetting phase now appears in the phase-change term, but is negligible at the first order.

$$\vec{V}_w \cdot \vec{\nabla}(C_{p_w} \rho_w T) + \varepsilon \vec{V}_a \cdot \vec{\nabla}(C_{p_a} \rho_a T) = -\varepsilon \vec{\nabla} \cdot (\lambda^{**} \vec{\nabla} T) + \frac{|\Gamma_{wa}|}{|\Omega|} \dot{m}_w (C_{p_w} - \varepsilon C_{pa}) T_{\Gamma_{wa}} \tag{41}$$

3.2.8 $CL_{wa_4} = O(\varepsilon^3)$

The macroscopic behaviour is purely diffusive and described by equation (36), without any phase change effect.

4 CONCLUSIONS

We have presented the results obtained by an homogenization technique for water-gas flow in porous media with phase change of water into vapor. The macroscopic behaviors are obtained from the description at the pore level. For the thermal problem, different

macroscopic behaviors were obtained depending on the order of magnitude of two dimensionless numbers. Thus, for a given practical situation, the knowledge of the order of magnitude of these two dimensionless numbers will indicate which mathematical model should be chosen for describing the evolution of the physical processes. As an example of application, we considered hot pressing of paper on an industrial point of view in which a phase change may appear in the paper web due to the high tempertaure of the rolls. Consequently, the use of such models had improved to build and optimize this new technology. The presented results may also be used so as to model any other technical process that involves porous media, corresponding to the hypotheses presented in this study.

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