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Coupled heat and mass transfer in porous media: insight and perspective of multiscale modelling

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Abstract: This conference is devoted to multiscale approaches of coupled transfer in porous media, with particular attention to configurations leading to the failure of the assumption of local thermodynamic equilibrium.

Upscaling methods, such as homogenization or volume averaging, allowed a well-established set of macroscopic equations to be obtained. This approach is powerful but needs to be supplied by relevant effective parameters. Nowadays, thanks to the spectacular progresses in 3D imaging and computational tools, these effective parameters can be obtained by 3D calculations on real pore morphologies. Recent examples will be presented to predict properties of bio-based building materials.

The remaining part of the conference will be devoted to configurations generating the absence of local thermodynamic equilibrium. Such situations, arising more often than expected, require a comprehensive multiscale approach (concurrent coupling). In such configurations, the local history of the product must be embedded in the formulation. Three approaches will be discussed here:

- The concept of distributed microstructure models, with various assumptions regarding the coupling between scales,
- The transfer of all the information at the micro scale (downscaling),
- The transfer of all the information at the macroscopic level, in which the concept of internal variable allows the history of the microscopic field to be transferred at the macroscopic level,

Finally, the new trends will be briefly presented: thanks to the impressive development of 3D imaging tools together with High Performance Computers, direct numerical simulation of transfer in porous media will be widely used in the future.

Keywords: absence of local thermodynamic equilibrium, direct numerical simulation, lignocellulosic materials, memory effect, nanotomography.

1. The macroscopic formulation of coupled transfer in porous media

It is worthwhile to remember that the widespread formulation of transfers in the form of differential equations was launched about 200 years ago. This approach started with heat transfer by conduction, formulated and solved by Fourier in 1822^[1]. Mass transfer, in continuous media and in porous media, was formulated with similar expressions at the end of the 19th century (Fick, 1855, Darcy 1856)^[2,3].

Following these outstanding advances in the formulation of continuous media, a scientific approach of drying was initiated at the beginning of the 20th century. Lewis (1921)^[4] describes drying as the combination of two mechanisms: humidity evaporation at the exchange surface and moisture diffusion within the solid. In 1929, in a paper entitled "*The drying of solids*"^[5], Sherwood describes drying as a combination of internal and external

¹ This invited conference, to be presented in Monastir, is dedicated to Prof. Sassi Ben Nasrallah, who passed away in June 2017. Sassi was not only a colleague since more than 30 years, but above all, a friend who accompanied me throughout my career.

resistance to transfers. At this time, the nature of moisture migration within the porous medium was the object of active discussion. A diffusion equation gave nice results for some materials (clay and wood in the hygroscopic range, for example), but failed in other cases. The importance of capillary forces was definitely proved in the case of sand by Ceaglske and Hougen (1937) ^[6]. In this work, moisture content profiles during drying were analyzed as quasi-equilibrated moisture content profiles due to gravity. Nevertheless, none of these expressions, diffusion or capillary action, could be applied to all configurations. The need for a more comprehensive formulation became obvious.

In the 1950s, comprehensive sets of equations were proposed from the analysis of careful experiments by Krischer's school in Germany ^[7]. Some years later, from their works on heat and mass transfer in soils, Philips and de Vries ^[8] proposed a comprehensive set of coupled transfers in porous media. In the USSR, Luikov ^[9] produced an important work, especially in the mathematical formulation of coupled heat and mass transfer⁽²⁾. In the sets of equations resulting from these three schools, most coupled phenomena involved in heat and mass transfer were considered: moisture migration due to a gradient of moisture content, thermo-migration, capillary forces, latent heat of vaporization in the energy balance, etc.

As introduction, it is useful to summarize the different macroscopic formulations used to model coupled heat and mass transfer in porous media. The "modern" way to formulate heat and mass transfers in porous media was achieved in 1977 by Whitaker ^[10], who derived a justification of the macroscopic formulation from the microscopic level using the volume averaging technique published by Slattery some years earlier ^[11]. Coupled and simultaneous heat, mass, and momentum transfer in porous media is a complex problem, which requires the development of transport equations derived from the standard conservation laws inside each phase, as well as from fluxes at the phase interfaces. The challenge, however, is to overcome the problems associated with structural dependencies and the complex geometries evident in the internal pore network within the medium. Typically, transport phenomena are represented according to macroscopic equations that are valid at the relevant level of description.

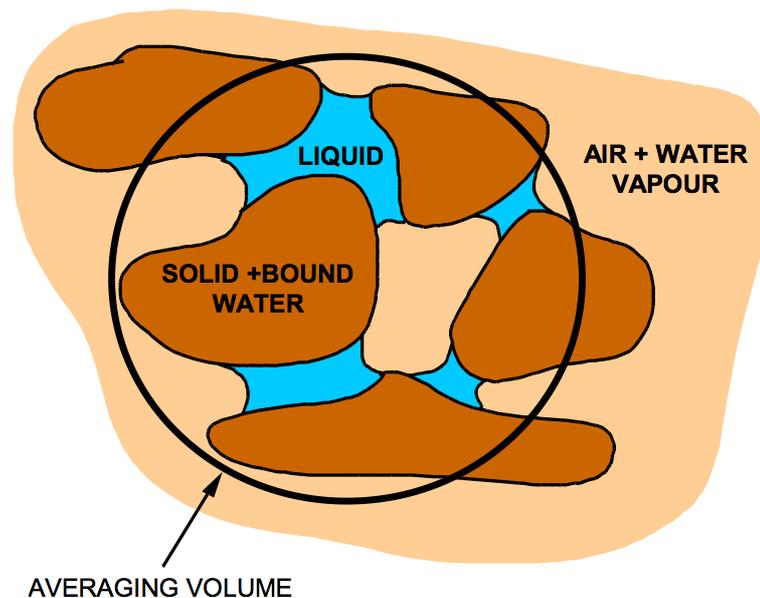


Fig. 1. Concept of Representative Elementary Volume (REV) ^[17].

This assumes the variables to be defined at the level of many pores, and the porous material to be represented as a fictitious continuum ^[12]. In this framework, it is possible to rigorously derive the macroscopic equations from microscopic balance equations by means of volume averaging ^[10,11,13-15]. The underlying idea of volume averaging ^[11,16] is to average the dependent variable (for example, the liquid or gas phase water vapour density) over some representative localized volume, as depicted in figure 1. The averaging volume, V (REV), comprises the individual phase volumes, each of which can vary with space, as well as time, for the liquid and gas phases. Averages are then defined in terms of these volumes, which are said to be associated with the centroid of the averaging volume V , which assumes the existence of a representative volume that is large enough for the

²Unfortunately, Luikov's formulation involves the so-called phase conversion factor of liquid into vapour, which is not an intrinsic parameter and drove several scientists to pursue a misleading track of inquiry.

averaged quantities to be defined and small enough to avoid variations due to macroscopic gradients and non-equilibrium configurations at the microscopic level

The development of the volume-averaged transport equations requires the introduction of what are called superficial and intrinsic averages. For example, the superficial average of the density of the liquid phase is given by

$$\bar{\rho}_w = \frac{1}{V} \int_{V_w} \rho_w dV \quad (1)$$

And its intrinsic average by

$$\bar{\rho}_w^w = \frac{1}{V_w} \int_{V_w} \rho_w dV \quad (2)$$

Where V_w is the volume of the liquid phase contained in V . One also notes the relationship $\bar{\rho}_w = \varepsilon_w \bar{\rho}_w^w$ in which $\varepsilon_w = V_w / V$ is the volume fraction of the liquid phase. The latter average is claimed to be the best representation in the sense that if ρ_w were a constant given by ρ_w^0 , then the intrinsic average gives $\bar{\rho}_w^w = \rho_w^0$, whereas the superficial average gives $\bar{\rho}_w = \varepsilon_w \rho_w^0$.

The comprehensive set of macroscopic equations that result from this volume averaging procedure and that are adapted to the case of hygroscopic products is as follows ^[14,17,18].

1.1.1. Water conservation

$$\begin{aligned} \rho_s \frac{\partial X}{\partial t} + \nabla \cdot (\rho_w \bar{\mathbf{v}}_w + \rho_v \bar{\mathbf{v}}_g) \\ = \nabla \cdot (\rho_g \mathbf{f} \mathbf{D}_v \nabla \omega_v + \mathbf{D}_{b,\rho_v} \nabla \rho_v) \end{aligned} \quad (3)$$

1.1.2. Energy conservation

$$\begin{aligned} \frac{\partial}{\partial t} (\varepsilon_w \rho_w h_w + \varepsilon_g (\rho_v h_v + \rho_a h_a) + \bar{\rho}_b \bar{h}_b + \varepsilon_s \rho_s h_s) + \nabla \cdot (\rho_w h_w \bar{\mathbf{v}}_w + (\rho_v h_v + \rho_a h_a) \bar{\mathbf{v}}_g) \\ = \nabla \cdot (\lambda_{eff} \nabla T + \rho_g \mathbf{f} \mathbf{D}_v (h_v \nabla \omega_v + h_a \nabla \omega_a) + h_b \mathbf{D}_{b,\rho_v} \nabla \rho_v) \end{aligned} \quad (4)$$

1.1.3. Air conservation

$$\frac{\partial (\varepsilon_g \rho_a)}{\partial t} + \nabla \cdot (\rho_a \bar{\mathbf{v}}_g) = \nabla \cdot (\rho_g \mathbf{f} \mathbf{D}_v \nabla \omega_a) \quad (5)$$

These equations are able to compute the coupling between heat and mass transfer occurring in a porous medium. It allows three independent variables to be computed (for example, temperature or enthalpy, moisture content, air density, or gaseous pressure). This is required, for example, if an important part of mass transfer occurs as convective flow (Darcy's regime). This comprehensive set of equations will be named the **three-variable model** in this paper. Because this formulation accounts for the internal pressure through the air balance (equation 5), this formulation has proven its ability to tackle numerous configurations involving intense transfers: high temperature convective drying, vacuum drying, and microwave drying ^[17, 21-23]. By intense transfers, we mean all drying processes able to give rise to a significant overpressure inside the porous medium. This includes all configurations of "high temperature" drying, for which the product temperature can be higher than the boiling point of water. These configurations are sometimes called "drying with internal vaporization" in opposition with processes with evaporation.

This comprehensive set of macroscopic equation can be simplified using successive simplifications. In particular, the 3-variable model can be reduced to a 2-variable model and even a 1-variable model ^[24].

If the total gaseous pressure is assumed to be equal to the external pressure, the mass balance of the air part of the gaseous phase (5) can be discarded to obtain a set of two independent equations that are able to compute two

independent variables (typically temperature and moisture content). In this case, the effect of gravity on the gas flow is often neglected and the gaseous velocity is set to zero. Consistently, the enthalpy of the air phase may also be neglected, as it is negligible with respect to the sensible heat of the solid phase (this assumption is not valid when the air velocity may be large). This simplified set defines the **two-variable model**. Using the **two-variable model**, the porous medium is described with only two independent variables (temperature or equivalent, and moisture content or equivalent). This model can be analysed as a simplification of the comprehensive model. This set is obviously not suitable to drying configurations with internal vaporization (high temperature configurations). However, through the enthalpy difference between vapour and liquid, it accounts for the latent heat of vaporization. In this way, it takes into account **the most important feature of drying**: the coupling between heat and mass transfer (this two-way coupling is due to the latent heat of vaporization and the relationship between temperature and saturated vapour pressure).

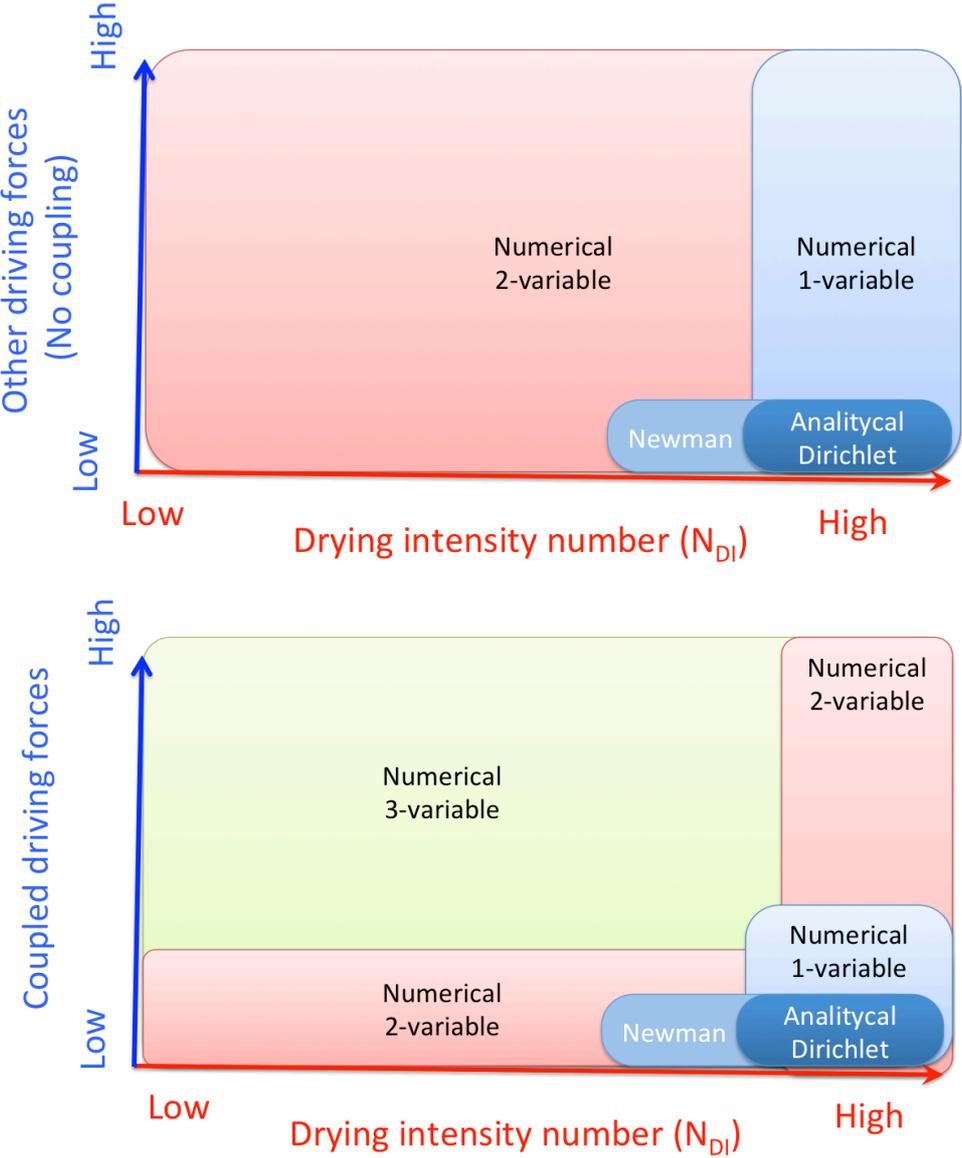


Fig. 2. How to choose the right modelling level as a function of the drying configuration. Top) When the other driving forces are known, bottom) When the other driving forces have to be computed by the model [24].

From this two-variable model, it is still possible to imagine something simpler: just forget about temperature. By doing so, one assumes, in fact, that the product temperature immediately follows the airflow temperature, despite the energy required to evaporate liquid water. Therefore, it is no longer necessary to differentiate liquid and vapour flows even though they have different enthalpies. A very simple **one-variable model** is then obtained. In this case, the coupling between heat and mass transfer is not taken into account, which is a severe simplification. The reader is invited to refer to paper [24] for further detail regarding the formulation and limitations of the 2-

variable and 1-variable models. Figure 2, reproduced from paper [24], summarises the possibilities and limitations of these different models. In these figure, the drying intensity number (N_{DI}), is defined as a ratio of two time constants. The time constant tied to internal mass transfer is simply the time constant of a diffusion process:

$$\tau_{int} = \frac{\ell^2}{D} \quad (6)$$

The time constant tied to the external transfer conditions is evaluated as the time required to remove the total moisture, assuming the drying flux to be that of the CDR (constant drying rate) period:

$$\tau_{ext} = \frac{m_{water}}{q_v^0} = \ell \rho_s \Delta X \times \frac{L_v}{h \Delta T} \quad (7)$$

Where ΔX is the moisture content change ($X_{ini} - X_{eq}$) and ΔT is the difference between the dry bulb temperature and the wet bulb temperature.

The Drying Intensity Number is then simply defined as the ratio of these two time constants:

$$N_{ID} = \frac{\tau_{int}}{\tau_{ext}} = \frac{\ell h \Delta T}{D \rho_s \Delta X L_v} \quad (8)$$

Accordingly, a high value of N_{DI} means that the resistance to internal mass transfer governs the drying process. Three main conclusions should be emphasised:

- A one-variable model is very poor in the physical description of coupled transfer in porous media. It can be justified only when the resistance to internal transfer dominates. Even in this case, analytical solutions impose further simplifications, namely constant mass diffusivity, which is never the case in reality,
- The tow-way coupling between heat and mass transfer requires at least a **two-variable model** to be chosen.
- When a gradient of internal pressure develops during the process, a **three-variable model** is needed. It includes a balance over the inert gas components, which allows the pressure field to be computed. This includes high temperature configurations, vacuum drying, reactive transfer (production of volatiles), large deformation of the solid matrix...

2. Prediction of effective parameters from real morphologies using upscaling techniques

The former set of macroscopic equations involves many effective parameters. Traditionally, these parameters are just determined experimentally (for example the thermal conductivity of an heterogeneous medium, such as composites panels). However, these effective properties result from a deterministic effect of i) the local properties of each phase and ii) the spatial morphology of these phase in the heterogeneous medium. Computational approaches, which take advantage of advances made in applied mathematics and mechanics regarding scaling approaches [25,26], together with relevant computational methods, allows these effective properties to be predicted. Upscaling, such as the homogenisation of periodic structures, is a deterministic approach that includes several steps (Fig. 3):

- 1) Representation: choice of the representative elementary volume (REV), also called the Unit Cell. This REV should be defined in a suitable way for subsequent calculation (Finite Element mesh, collection of material points...),
- 2) Characterisation of the properties for each phase of the unit cell.
- 3) Solution: the theoretical formulation (i.e., the homogenisation of periodic media) has to be solved using a suitable computational method,
- 4) Validation: the predicted macroscopic properties should be tested against experimental data,
- 5) Localisation: this step is not mandatory, but it allows the local (microscopic) fields (shrinkage, strain, stress, temperature, etc.) to be computed inside the REV under the macroscopic conditions applied to the product.

Figure 3 indicates that a macroscopic property depends on both the local properties of the different phases of the REV (Representative Elementary Volume) (2) and their spatial organisation (morphology) (1). This can be summarized in the well-known formula resulting from homogenisation in periodic media regarding the elastic

properties (equ. 9) ^[25]. This equation confirms that the macroscopic properties are the sum of i) the weighted averaged of the local properties of the different phases and ii) a correction term whose calculation requires the solution ξ^{lm} of elementary problems over the REV. The last term of the right side represents the effect of the phase morphology.

$$\begin{aligned}
 A_{ijkh} &= \langle a_{ijkh} \rangle + \langle a_{ij/lm} e_{y/lm}(\xi^{kh}) \rangle \\
 \text{Homogenised} &= \text{Average of the} + \text{Corrective} \\
 \text{values} &= \text{microscopic values} + \text{term}
 \end{aligned}
 \tag{9}$$

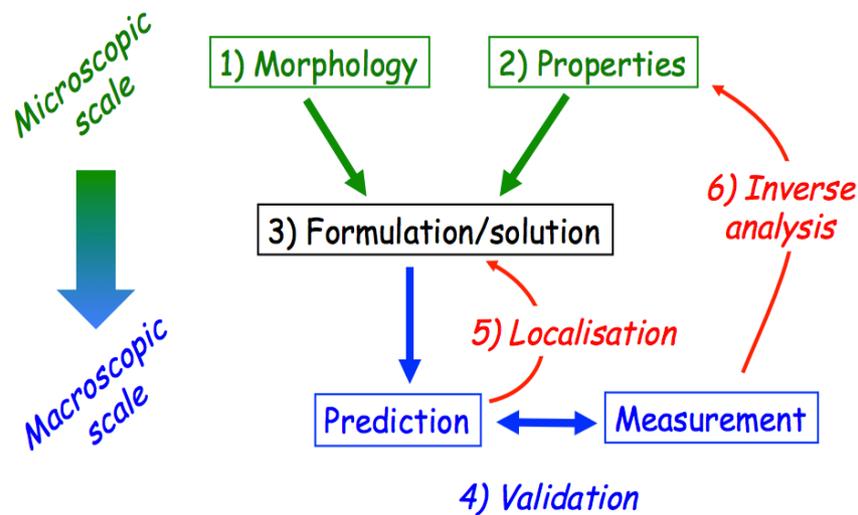


Fig. 3. Upscaling in material sciences: principle ^[27].

Nowadays, thanks to the development of 2D and 3D imaging techniques, together with the power of High Performance Computers and the development of meshless computational methods ^[28,29], it is possible to apply the upscaling techniques on real morphologies of porous medium, at a volume large enough to be representative of the macroscopic medium.

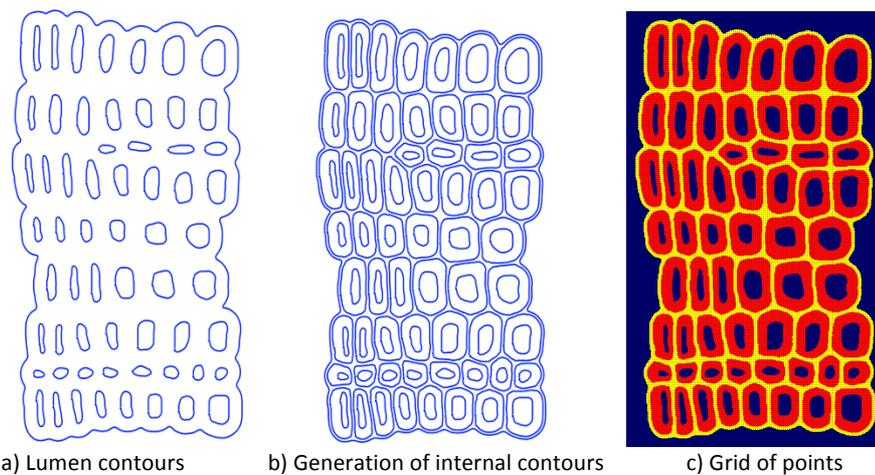


Fig. 4. Generation of internal contours and allocation of two solid phase types (blue = lumens, red = secondary wall and yellow = middle lamella) ^[27].

Figure 4 and 5 depicts an example of simulation of the mechanical behaviour of the cellular structure of spruce submitted to a radial loading. This includes two important steps:

- **Image-based representation** (Fig. 4): in this example focused on the cellular structure of wood, the lumen contours were extracted from ESEM images. Then, in order to mimic the development of the secondary cell wall in tress, the contours of the middle lamella are generated. The final representation consists in the generation of a collection of points, either within the secondary cell wall (in red) or within the middle lamella (yellow). Each point had its own local directions of the anisotropic cell wall.
- **Solution of the problem** (Fig. 5): meshless methods (i.e. Lattice Boltzmann Method, Material Point Method, Peridynamic) are excellent computational techniques to deal with complex morphologies ^[27,29]. MPM (Material Point Method) were used here to solve this solid mechanics formulation ^[27].

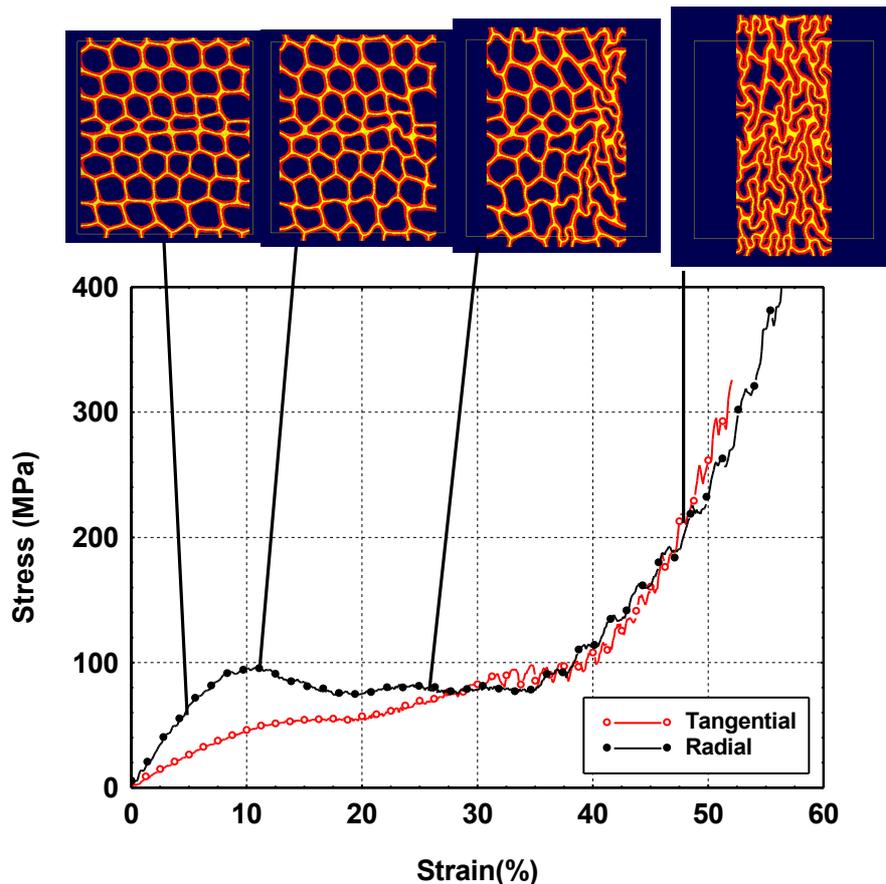


Fig. 5. Stress-strain curves obtained for spruce earlywood in the radial and tangential directions. Computational images of the cellular deformation for the radial test were selected at strain levels of 5, 12, 25 and 48 % ^[27].

The 3D prediction of mass diffusivity is proposed as second example. Figure 6 depicts the REV chosen for different materials (low and medium density fibreboard, earlywood and late wood parts of spruce) as obtained using nanotomography. The scans were performed at the ID19 line of the ERSF synchrotron (0.7 μm of spatial resolution). For all REV, the mass diffusivity values were computed in the 3 material directions using LBM, Lattice Boltzmann Method (Fig. 7) ^[30].

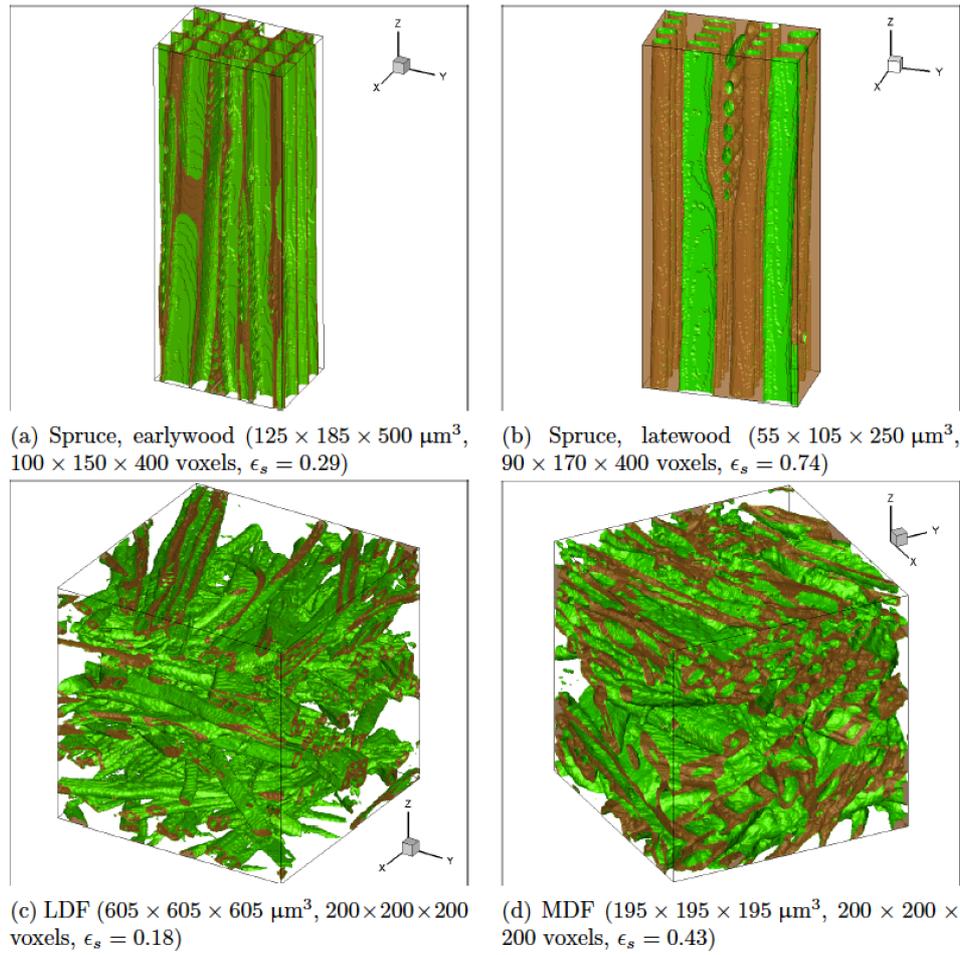


Fig. 6. 3D reconstruction of selected regions of the bio-based materials scanned by X-ray nano-tomography. The size, the voxel number and the solid fraction are given for each 3D structure^[30].

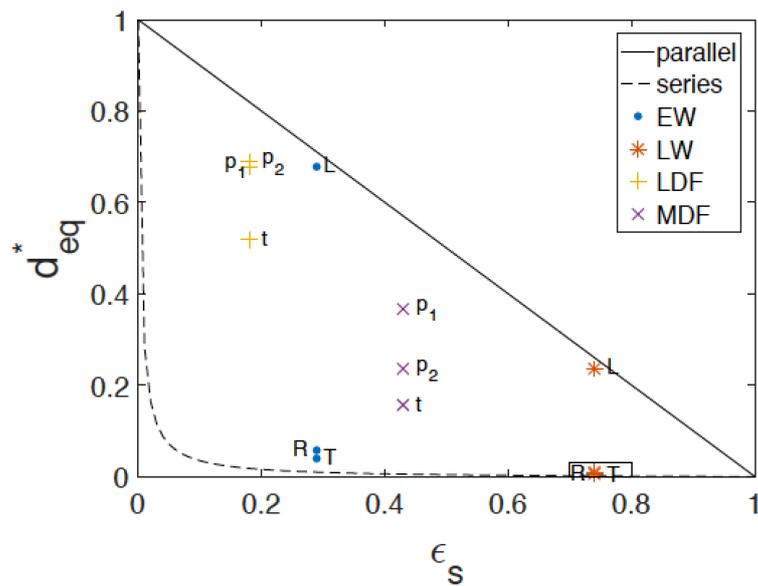


Fig. 7. Dimensionless equivalent mass diffusivity d_{eq}^* versus solid fraction for ϵ_s in the three directions of spruce earlywood and latewood, LDF and MDF. Series (dashed line) and parallel (solid line) theoretical models are represented^[30].

3. The failure of local equilibrium as the most common demand for multiscale approaches

In upscaling approaches such as homogenization, the time variable disappears when computing the effective macroscopic properties. As a consequence, the macroscopic property has to be calculated only once and subsequently used in the homogenized problem. This is a typical **sequential coupling**.

Although consistent and comprehensive, this approach is not relevant for certain configurations, namely in the case of local thermodynamical non-equilibrium. Indeed, configurations of coupled transfer whereby the scaling approach fails are well documented in the literature (see, e.g.,^[31-35]). Such configurations require a **concurrent coupling**.

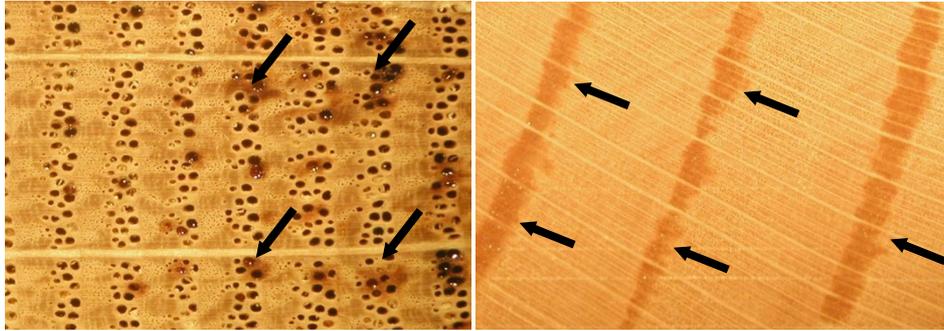


Fig. 8 – Absence of local thermodynamical equilibrium during imbibition with water of wood, oak (left) and beech (right). Views of the outlet face of 40-mm long samples, where the localised water field is manifest^[35].

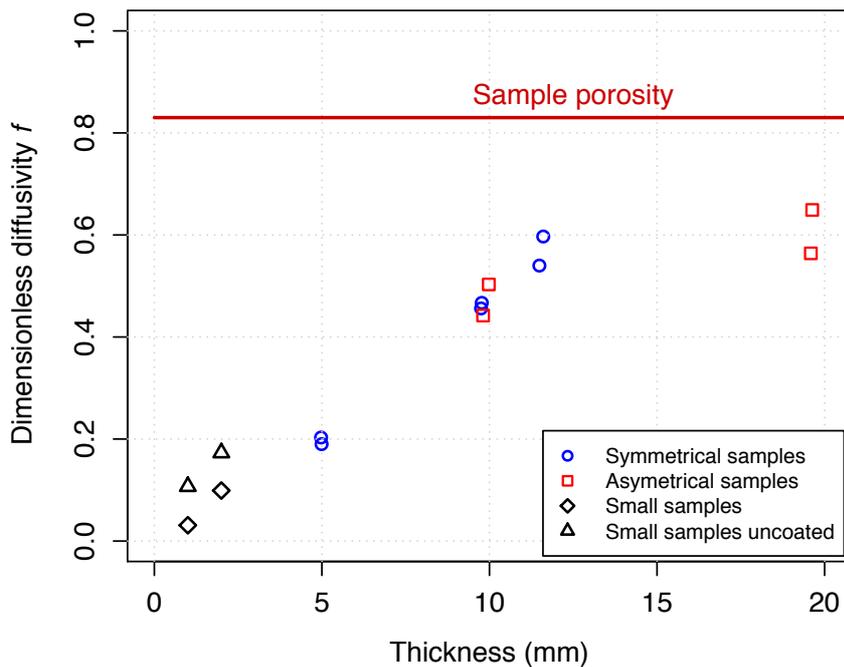


Fig. 9 – Dimensionless mass diffusivity identified by inverse analysis for Low Density Fibreboards samples of different thickness values. For a pure Fickian behaviour, the macroscopic parameter should not depend on the sample thickness^[36].

Imbibition of hardwood samples with water is a typical configuration for which the previous approach fails (Fig. 8). In these examples, migration occurs mostly in the longitudinal direction, after water has been supplied to one transverse face. The opposite face is just observed at different soaking times. In such a process, a typical dual scale mechanism occurs: the water flows very rapidly in those vessels that are open and connected. In the case of oak, this easy transfer happens in the vessels having a low amount of tyloses, whereas the early part of each annual growth ring is very active in the case of beech. Then, moisture needs more time to invade the remaining

part of the structure, by liquid transfer in low permeable tissues or by bound water and water diffusion. Such a local thermodynamical non-equilibrium occurs as soon as the macroscopic and the microscopic time scales have similar orders of magnitude. As a result, the microscopic field not only depends on the macroscopic field, but also on the history of this macroscopic field.

Similar dual-scale effects are also observed when storage inclusions are placed in a conductive matrix (fissured blocks, hygroscopic inclusions in a gaseous phase...). For example, low-density fibreboards made used for thermal insulation of building consists mostly of air (up to 90% of the volume), with a small amount of wood fibres. The connected gaseous phase allows an easy diffusion of water vapour, whereas most of the water is stored as bound water in the solid phase, with low diffusivity. Due to this contrast of diffusivity between the connected and storage phase, the moisture content field is not at equilibrium inside the inclusions in the case of transient configurations. As a consequence, the identified macroscopic diffusivity depends on the sample thickness (Fig. 9), which should not be the case for a classical Fickian law.

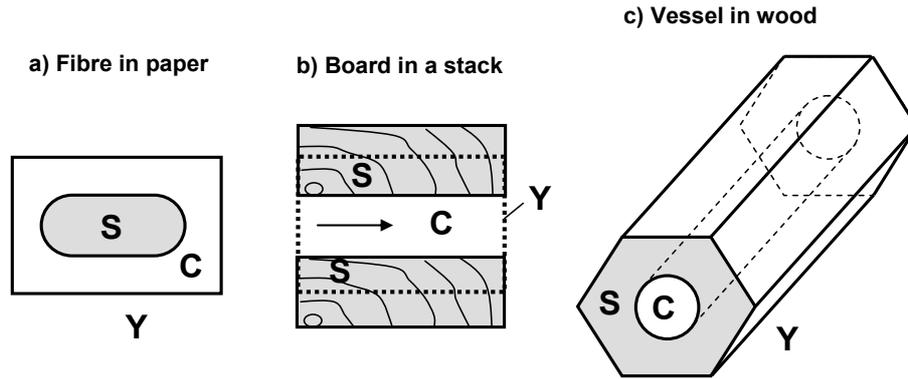


Fig. 10 – Some unit cells suitable for different configurations of dual-scale modeling: S = storage phase, C = conductive phase ^[33].

Such **concurrent coupling** between scales can be formulated by different strategies, such as parallel flow models or mesoscopic models, or distributed microstructure models ^[33,35]. Due to its excellent potential in accounting for various situations, the concept of distributed microstructure models will be presented briefly hereafter.

Distributed microstructure models are among the multiscale models with concurrent coupling ^[33,37]. In this section, a bounded macroscopic domain Ω is considered. This domain is supposed to be periodic and defined by a unit cell Y . This unit cell consists of a conductive phase, denoted C and a storage phase, denoted S (Fig. 10). Here, the conductive phase is supposed to be connected at the macroscale. By scaling the transfer property by ε^2 in the storage phase, homogenization gives rise to a model in which non-equilibrium can exist within the unit cell ^[33,37]. This results in a macroscopic equation with a delay due to the storage capacity at the microscopic level:

$$\begin{aligned} |C| \frac{\partial u}{\partial t} - \nabla \cdot (A^C \nabla u(t, x)) + Q(x, t) &= 0 \quad x \in \Omega \\ b \frac{\partial U}{\partial t} - \nabla_y \cdot (A^S \nabla_y U(t, x, y)) &= 0 \quad y \in S_x, x \in \Omega \end{aligned} \quad (10)$$

b is the accumulative coefficient for the storage phase and $|C|$ is the accumulative coefficient of the conductive phase weighted by its volume fraction in the unit cell Y . u is the macroscopic variable and U the microscopic variable in the storage phase S . These variables are connected by boundary conditions at the interface ∂S_x between phases S and C : potential continuity, in this simple example, and mass conservation

$$\begin{aligned} U(t, x, y) &= u(t, x) \quad y \in \partial S_x, x \in \Omega \\ Q(t, x) &= \frac{1}{|Y|} \int_{\partial S} A^S \nabla_y U \cdot \vec{n} \, dS \quad x \in \Omega \end{aligned} \quad (11)$$

\vec{n} is the unit normal towards the conductive phase.

Two main features have to be emphasized:

- The macroscopic property A^C is computed from a homogenization procedure applied to part C of the unit cell,
- The memory effect is not obtained thanks to an identified parameter, but from the computation of the variable field over part S of the unit cell.

Such a distributed microstructure models have been extended in the case of coupled heat and mass transfer in porous media ^[35]: both macroscopic and microscopic formulations of this model are based on a 3-variable such as the one presented in section 1 of this paper. The interested reader is invited to refer to this reference for further detail.

4. Conclusion and perspectives

This paper proposed a brief review of the state-of-the-art of coupled transfer in porous media. It includes the comprehensive macroscopic formulation, the determination of effective properties with upscaling techniques (sequential coupling between scales) and multiscale modelling (concurrent coupling between scales).

The team at CentraleSupélec, in collaboration with the laboratory LESTE at ENIM, Monastir, Tunisia and the School of Mathematical Sciences, QUT, Australia, is currently working into three complementary directions:

- **Downscaling**: we revisit the concept of distributed microstructure model to transfer the maximum information at the microscale (Fig. 11). As ultimate goal, the objective is to avoid any formulation at the macroscopic scale ^[38,39]. Such an approach is well-adapted to heterogeneous media whose morphology changes in space and/or in time,
- **Revisited macroscopic formulation**: the idea is to transfer all the concurrent coupling between scales at the macroscopic level. This formulation introduces the material history as convolution products with kernel functions. The challenge is to extend this quite well-known concept to coupled heat and mass transfer configurations and to account also for the delay due to molecular relaxation ^[40].
- **Direct numerical simulations**: as previously stated, thanks to the rapid development of High Performance Computers and 3D imaging devices, it is now possible to dream at direct numerical modelling of coupled heat and mass transfer in porous media. This is an orthogonal approach in which the basis conservation laws are solved within each phase of the heterogeneous medium, without any reference to effective parameters. Since some months, the LGPM owns a nanotomograph, which proposes a spatial resolution up to 400 nm, similar to what can be obtained in synchrotron facilities (Fig. 12). This is a perfect tool to gain the morphological information to be supplied to direct numerical simulation. A PhD project in cotutelle with ENIM started this year in this domain.

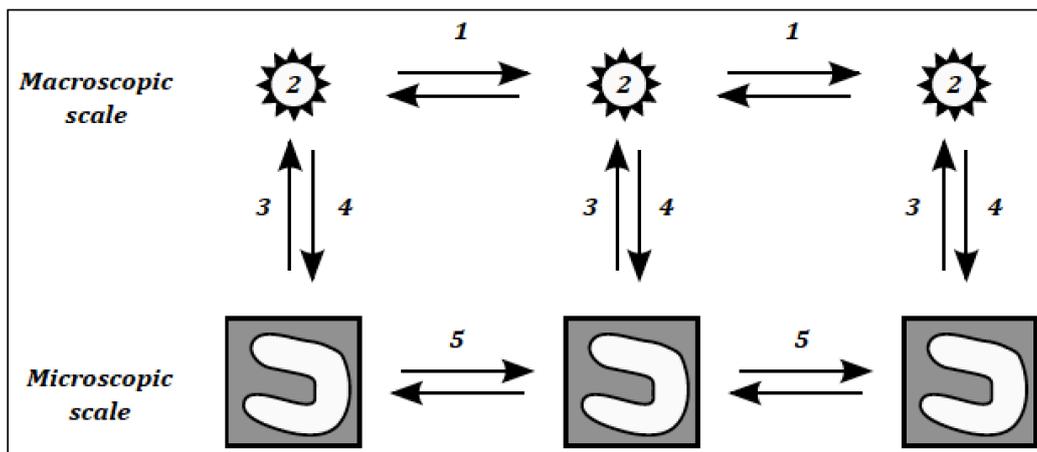


Fig. 11 – Possible interactions within and between the macroscopic and microscopic scales for the balance equations ^[38].

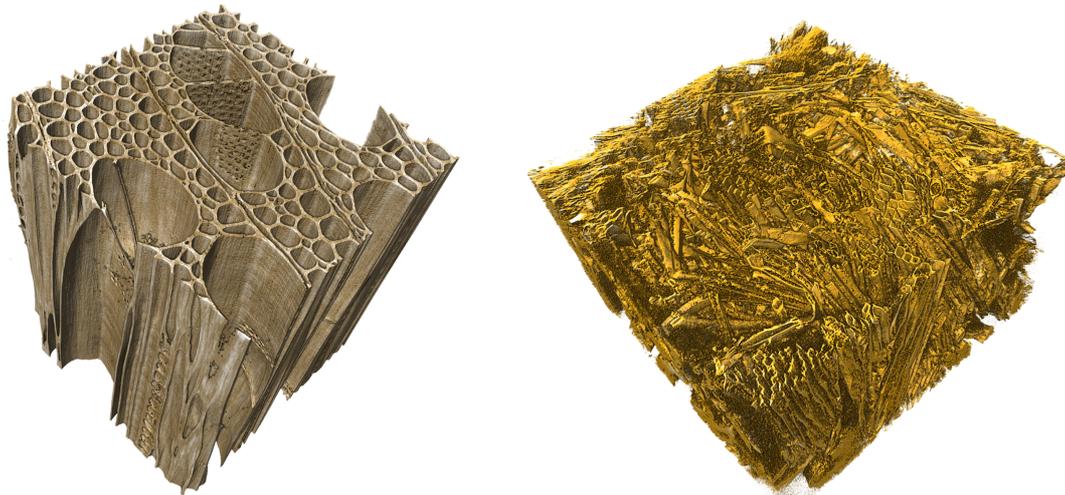


Fig. 12 – Examples of high resolution nanotomograph scans performed at LGPM : poplar and LDF (C. Breton, P Lu and P. Perré).

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