Impact of the 3D morphology on the hygro-thermal transfer of hygroscopic materials: application to spruce wood

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Abstract. Spruce wood is a bio-based material that is well known in the building construction field because of its good thermal and acoustic properties. It has a heterogeneous anatomical structure and also hygroscopic nature which offers the possibility to swell or shrink—in accordance to—relative humidity solicitations. In this context, the aim of this paper is to investigate the influence of the microstructure of spruce wood on the mechanisms of heat and mass transfers. The novelty of this article is that a real 3D spruce wood structure is taken into account to model hygrothermal transfer within the material. A 3D X-ray micro-tomography was investigated for the reconstruction of the material at a resolution of 3.35 µm/pixel. Hygrothermal model was developed in order to predict the influence of the anatomical structure of wood on the material behaviour. The resulting 3D temperature and relative humidity profiles show a significant dependence on the morphological structure of the material and the mechanisms that are at the microscopic scale have an influence on the macroscopic scale.

1. Introduction
The building sector is one of the main energy consuming fields that has a destructive effect on the environment. It uses millions of tons of construction materials that contain high embodied energy content which is responsible for the contribution of climate change, global warming, landfill waste, increase in greenhouse gases mainly CO\textsubscript{2}, and raise in the percentage of pollutants in the atmosphere. Therefore, the need for implementing materials that are eco-friendly is essential. These materials should follow several measures that are concerned in improving the thermal performance and reducing the environmental impact of the building [1].

Bio-based materials have been recently the center of attention for most researchers and engineers in the civil engineering field. These materials are considered sustainable building materials which are known for their hygrothermal and acoustic performance, their resistance to fire and heat and most importantly their environmental and energy performance [2,3].
Spruce wood is a bi-phasic bio-based material which is characterized by its complex, heterogeneous and anisotropic nature and has been massively used in construction sector over the years. It is well known for its thermal properties, however its hygroscopic nature presents some disadvantages which are presented in the swelling and shrinkage it generates during the sorption and desorption cycles respectively. These caused phenomena can be clearly observed at the macroscopic scale and are caused by the microscopic morphological changes following internal mechanical stresses [4]. Most of the existing literature considered the material as a black box without taking into account its microscopic structure which leads to non-significant results. For instance, [5-8] have developed numerous macroscopic models for the prediction of the coupled Heat and Mass transfers (HAM) in porous building materials. Indeed, it is crucial to consider the morphological structure of the material because the macroscopic behavior is strongly related to the mechanism that act at the level of the microscopic scale. That is why, this paper proposes the study of heat and mass transfers of spruce wood at the microscopic scale using three-dimensional modelling approach. This study was carried out on a real 3D model volume taking into account its morphological traits and heterogeneities. To do this, X-ray tomographic scans are performed to visualize the internal structure of the spruce wood. Segmentation is then performed to distinguish between the phases that compose the structure of spruce wood, before finite element mesh is generated on the 3D reconstructed volume. Moreover, the hygrothermal model is presented and the input parameters are calculated for both solid and air phase of the material. Finally, the numerical modelling results of the transfers’ phenomena are analyzed so that a prediction of the profiles of temperature and moisture transfers, mass and heat flux can be drawn.

2. Materials and Methods
Spruce wood presents two types of morphology. Earlywood that grows in spring and latewood that grows in summer. Earlywood is characterized by its thin cell walls and large internal diameters allowing a greater passage of sap. It grows by reproducing layers where each layer represents a cycle while latewood has thick cell walls and small internal diameters with high density [9]. First, X50 micro-tomograph in the Laboratory of Mechanics and Technology (LMT) at ENS Paris-Saclay was used to scan spruce wood samples. X-ray tomography is a non-destructive technique which accesses the core of the material without causing any defect or change in its structure and morphology and reconstructs its real 3D volume. In this work, a voltage of 80 KV and a current of 50 µA were applied. At each position, 10 acquisitions were taken, with an image acquisition time of 0.5 s. In order to work on a sufficiently large volume, the resolution of the acquisition is fixed at 3.35 µm / voxel where a voxel is defined as 1x1x1 pixel³ and the scanning time was almost 2 hours. During each scan, a 360° sample rotation takes place so that several images from several angles can be taken to get a digital image. The 3D object is reproduced using sectional images. This step is carried out with <<efX>> software, in order to obtain a volume formed by several pixels in each of the 3 directions of space. The size of a pixel represents the resolution reached by the considered scan. The resolution attained allowed us to distinguish the different phases constituting the spruce wood material which are the fibrous and the porous phases. Figure 1 shows a 3D reconstruction after X ray tomographic scan of the spruce wood.

The Representative Elementary Volume (REV) should be determined in the next step. It is important as it gives all the needed data that can express the whole volume. The size of the volume that should be carried in this study has to be equal or greater than the selected REV which will be used in the study of hygrothermal transfers in the real heterogeneous geometry of spruce wood. It is selected when the porosity does not show any more significant variations. The studied sample was exposed for dry and wet humidity conditions. The volume was initially at its dry state (0% RH) where a tomographic scan was taken. Then, it was exposed to a high relative humidity at 72% and79 % respectively. The sample is placed in a closed transparent plexiglas to maintain a constant humidity during the scanning test. Once the specimen reached its mass equilibrium, another tomographic scan was taken. During these steps, several Regions of Interests (ROI) were chosen to compare the variation
of the porosities. When the porosities of the ROIs show no more significant variation, a REV was selected. The porosity measurements were carried out using the ImageJ plugins from [10].

The interest of exposing the sample to high relative humidity is to evaluate the swelling of the material in order to predict its performance while implementing it in building envelopes. Figure 2 expresses the porosity as a function of the volume size of the considered spruce wood. This graph can be divided into three main zones. The first zone expresses a strong variation which represents the microscopic heterogeneous medium then the transition that appears next shows an approximate stable zone expressing the porous medium domain which the REV can be selected from. Finally, the third zone displays the heterogeneous medium at the macroscopic scale.

![X-ray tomography reconstruction](image)

**Figure 1.** X-ray tomography reconstruction of a resolution of 3.35 µm/pixel.

![Porosity evolution curve](image)

**Figure 2.** Porosity evolution curve as a function of the volume.

After 3D reconstruction << AVIZO.9>> comes as a preliminary step to remove all the noise obtained in the image [11]. This is because the captured 2D images obtained from micro CT contain a lot of parasitic information that can be defined by “noise” or “artefacts” which affect the quality of the image and disturb the analysis and interpretation of it. The appearance of artefacts is due to several factors such as the X-ray flux and scatter, finite resolution and discrete sampling. Thus, the need to remove these artefacts comes as a prior step in order to obtain a clearer image that can be analyzed properly [12,13].

Moreover, the segmentation/thresholding tool is used to separate and distinguish the two phases that identify the components of spruce wood microstructure [14,15].

3. Numerical Modelling

Modelling heat and mass transfers is very important to consider because it has a direct and indirect impact on affecting the indoor air quality, the energy saving and the performance of the building. However, it is very critical to identify an exact model describing heat and mass transfers because of
the complex and porous structure of the material which can be defined as the orientation, size and shape of the voids.

3.1. Implemented model

In our study, a coupled heat and mass transfer model is used for simulation of hygroscopic porous building materials [5]. It is based on Fick’s and Fourier laws with consideration of temperature and moisture content as driving potential, as indicated in in equations (1) and (2):

\[
\frac{\partial \omega}{\partial t} = \text{div}[D_m (\nabla \omega + \delta \nabla T)] \\
\rho C_p \frac{\partial T}{\partial t} = \text{div}[\lambda \nabla T] + h_{tv} \cdot \rho \chi \frac{\partial \omega}{\partial t}
\]

Where: \(\omega\) [Kg/Kg] is the water content, \(D_m = (D_v + D_f)\) [m²/s] is the moisture diffusion coefficient, \(\delta\) [Kg/Kg. K] is the thermo-gradient coefficient, \(\rho\) [Kg/ m³] is the density, \(C_p\) [J/Kg. K] is the specific heat, \(\chi\) [-] is the phase constant ratio, \(\lambda\) [W/m.K] is the thermal conductivity and \(h_{tv}\) [J/Kg] is the mass enthalpy.

The transformation from a dimensional equation to a dimensionless formulation simplifies the problem and gives an idea of the relative dimensions of the different phases for the different parameters of the material and consequently a physical quantization phenomenon can be reached.

To make the problem dimensionless, it is necessary to introduce physical quantities without dimensions. Each parameter must be divided by a reference value. The dimensionless variables proposed are:

\[
\tilde{\rho} = \frac{\rho_{\text{phase}}}{\rho_{\text{air}}}, \quad \tilde{\lambda} = \frac{\lambda_{\text{phase}}}{\lambda_{\text{air}}}, \quad \tilde{C}_p = \frac{C_{p_{\text{phase}}}}{C_{p_{\text{air}}}}, \quad \tilde{D}_m = \frac{D_{m_{\text{phase}}}}{D_{m_{\text{air}}}}, \quad \tilde{\delta} = \frac{\delta_{\text{phase}}}{\delta_{\text{air}}}, \quad \tilde{T} = \frac{T - T^-}{T^+ - T^-}, \quad \tilde{m} = \frac{w - w^-}{w^+ - w^-}, \quad \tilde{F}_0 = \frac{D_{m_{\text{air}}} \cdot t}{1 (m^2)}, \quad \tilde{\vartheta} = 1(m), \tilde{\varphi}
\]

The reference variables are the properties of the porous phase (air), assumed to be known. The sign “~” designates dimensionless quantities. Let M be a point belonging to the wood sample. If M ∈ to the air phase: \(\tilde{\rho} = \tilde{\lambda} = \tilde{C}_p = \tilde{D}_m = \tilde{\delta} = 1\). Using these dimensionless variables, the heat and mass transfer equations can be written in dimensionless form as following:

\[
\tilde{\rho} \cdot \tilde{C}_p \cdot \frac{\partial \tilde{T}}{\partial \tilde{F}_0} = \tilde{\lambda} \cdot \tilde{L} \cdot \tilde{T}^{-1}, \quad \tilde{\varphi}^2 \theta + \tilde{K}_o \cdot \tilde{\vartheta} \cdot \frac{\partial \tilde{m}}{\partial \tilde{F}_0}
\]

(3)

\[
\frac{\partial \tilde{m}}{\partial \tilde{F}_0} = \text{div}[	ilde{D}_m \cdot (\tilde{\vartheta} \tilde{m} + Pn. \tilde{\varphi} \theta)]
\]

(4)

The considered problem depends on four dimensionless numbers: Luikov \(Lu = \frac{D_{m_{\text{air}}}}{\rho_{\text{air}} C_{p_{\text{air}}} \cdot \vartheta}\), Kossovitch \(Ko = \frac{h_{tv}}{C_{p_{\text{air}}} \cdot \vartheta}\) and Fourier \(F_o = \frac{D_{m_{\text{air}}} \cdot \vartheta}{1 (m^2)}\).

3.2. Boundary conditions

The boundary conditions chosen in this work are Dirichlet Type, where the dimensionless relative humidity and temperature parameters are directly applied to the exterior surfaces of the spruce wood sample: \(\theta(x=0) = 0, \theta(x=L) = 1, m(x=0) = 0\) and \(m(x=L) = 1\).

The study was conducted at the stationary state and the initial conditions at \(t = 0\) are considered constant in the spruce wood material and are expressed as the following: \(\theta_{(t=0)} = 0 \text{ et } m_{(t=0)} = 0\).

Continuity conditions of mass and heat transfer are considered on the wood air interface, respectively:

\[
\frac{\partial m_w}{\partial x} n_{wa} = \frac{\partial m_a}{\partial x} n_{wa} \quad \text{and} \quad \frac{\partial \theta_a}{\partial x} n_{wa} = \frac{\partial \theta_w}{\partial x} n_{wa}.
\]

Where, the indices “w” and “a” designates wood and air phases, respectively.

The study is conducted for the steady state on Equation (3) and (4) in COMSOL Multiphysics. The studied wood sample has a dimension of 231μm x 231μm x 231μm, in the radial direction.
3.3. Input parameters

The thermal and moisture equivalent properties of spruce wood differ with direction due to the anisotropic structure of this material. In addition, these parameters vary with the variation of relative humidity, hence the need to take this variation into consideration during the simulation. The hygrothermal properties of the spruce wood used in this work were identified in the ANR Hygrobat project [16]. A relationship giving the variation of thermal conductivity as a function of water content \( X \) proposed by [16] was used: \( \lambda_{\text{eff}} = 0.14 + 0.3 * X \). To determine the value of \( X \) as a function of relative humidity, the sorption-desorption isotherm of spruce wood was used.

Several models can be found in the literature to predict the thermal conductivity of heterogeneous media. These models predict the effective thermal conductivity \( \lambda \) and water diffusion \( D_m \) of the material as a function of the volume fraction of each phase and their local thermal and water properties.

In our case, the model of [17] was considered to determine the thermal conductivity of the solid fibers. These authors assume that the material has orthotropic thermal properties and the thermal conductivity can be determined by the following expression:

\[
\lambda_{\text{eff}}^l = \lambda_l (1 - a^2) + \lambda_{\text{air}} * a^2
\]

For the diffusion coefficient \( D_{m} \), [18] provided values for the equivalent diffusion coefficient of spruce wood for different relative humidity. To calculate the diffusion coefficient of the solid phase, we use the generalized auto-coherent model:

\[
D_{\text{eff}} = D_{s} + (1 - \Phi_{s}) \left[ (D_{a} - D_{s})^{-1} + \frac{\Phi_{s}}{3 * D_{s}} \right]^{-1}
\]

Where \( \Phi_{s} \) is the volume fraction of the solid phase.

Concerning the air properties, and according to [19], these latter are not highly dependent on the temperature. At \( T=23°C \), the density, thermal conductivity and specific heat of the air are equal to 1.2 Kg/m\(^3\), 0.025 W/ (m.K) and 1004 J/(Kg.K) respectively whatever the relative humidity. The air diffusion coefficient proposed by De vries [20] follows the equation of:

\[
D_{v\text{air}} = \frac{2.306 \times 10^{-5} P_{0} \left( \frac{T}{273} \right)^{1.81}}{p}
\]

In this work, temperature and water content gradients are applied to create heat and water transfers in the radial direction (\( \Delta T=0.5 \) K and \( \Delta w=0.01 \) Kg/Kg).

Table 1 summarizes the dimensional input parameters that were inserted for the hygrothermal modelling of the considered material.

| RH  | \( \lambda_s \)/[\( \text{Kg}\cdot\text{m}^{-1}\cdot\text{K}^{-1} \)] | \( c_{p_s} \)/[\( \text{Kg}^{-1} \cdot\text{K}^{-1} \)] | \( \rho_s \)/[\( \text{Kg}^{-1} \)] | \( B_{m_s} \)/[\( \text{Kg}^{-1} \cdot\text{K}^{-1} \)] | \( K_0 \) | \( P_n \) | \( L_u \) | \( \chi \) |
|-----|---------------------------------|-----------------|----------------|-----------------|------|------|------|------|
| 0%  | 0.53/0.025                      | 1.49            | 666.67         | 0.0027          | 49.80| 0.05 | 1.29 | 0.3  |
| 72% | 0.631/0.025                     | 1.49            | 666.67         | 0.0058          | 49.80| 0.05 | 1.26 | 0.3  |
| 79% | 0.6554/0.025                    | 1.49            | 666.67         | 0.0073          | 49.80| 0.05 | 1.25 | 0.3  |

4. Results and Discussions

We considered the real 3D real geometry of spruce wood obtained from the tomographic scans and we imported the meshed volume performed by AVIZO into COMSOL MULTIPHYSICS where heat and mass transfers were modelled for the spruce wood sample scanned at the three relative humidity levels: 0%, 72% and 79%. Figure 3 and 4 show the three-dimensional temperature and moisture content profiles, respectively, for the three mentioned relative humidity states.
We can notice from the obtained results inhomogeneous fields. In fact, the thermal and the hygric results profiles attained at the dry and at the wet states indicate clearly the dependence of the hygrothermal transfer on the microscopic arrangement of cell walls, that behave completely different from a relative humidity state to another. This inhomogeneous distribution is due to the heterogeneity of the spruce wood material which is of biphasic nature, variability of the hygrothermal behavior of the constituents of the material and the topology of the interfaces between solid and air in spruce wood.

Moreover, a qualitative study to determine the heat and mass flux of each phase and the total flux of coupled heat and moisture transfer was done to study the effect of dimensional variations on spruce wood.
Figure 5 shows the evolution of heat and mass flux as a function of relative humidity. For heat transfer, the heat flux in the solid phase is much larger than in the air phase. This is due to the difference in the order of magnitude of the dimensionless thermal conductivity ($\bar{\lambda}_s \gg \bar{\lambda}_a$). Therefore, the solid phase controls the heat transfer. Furthermore, the heat flux in the total volume increases with increasing relative humidity. This change is to the increase in the thermal conductivity of the solid phase when the medium becomes more humid.

For water transfer, a great difference between the mass flow in the two phases solid and air. The flux in the pores is much higher than in the solid phase. This is due to the diffusion coefficient which differs between the two phases phases ($\bar{D}_s \ll \bar{D}_a$). Therefore, the air phase indicates the transfer in spruce wood. When the relative humidity increases from 0% to 72%, the wood has not swollen too much and the total diffusion coefficient has increased, which explains the high value of mass flux. Above this value, the mass flux starts to decrease due to the swelling of the solid phase and consequently the pores are blocked, which prevents the water transfer. By increasing the relative humidity, the material continues to swell and the pores are not the same, which explains the decrease of the flux (high swelling).

5. Conclusions

In this paper, the hygrothermal behavior of spruce wood was investigated through modelling these transfers with a new approach applied on real 3D structures. First, we obtained the microstructure of spruce wood through X-ray micro-tomography then a 3D reconstruction of the material took place allowing to observe the different phases of the sample: solid and air. The processing and the numerical operations done on the real 3D volume led to a fine meshing which allowed the thermo-hygric simulations to be performed.

The thermal and hygric input parameters were calculated using scaling techniques based on equivalent parameters from the literature.

The three-dimensional fields of temperature and moisture content in the spruce wood were presented at the dry and the wet state displaying the strong heterogeneity of the thermo-hygric transfers through the real geometry of the material. A remarkable difference was observed in the surfaces between the dry and the wet states. These results show the importance of considering the morphological structure which is more significant in understanding the behavior of the material at the microscopic scale and how is this phenomenon reflected at the macroscopic level.

However, shrinkage or swelling lead in both cases to variation in the fibrous dimensions of the material, due to the presence of bound water. In addition, the deformation of the fibers inside the wet sample is due to the adsorption of water causing the expansion of the isothermal surfaces, which is evidence of the swelling that occurred in the cell wall when subjected to high relative humidity, which causes an increase in the size of the fibers while shrinking is the drying process where water cell releases water content.

As perspective of this study, it is essential to consider the dimensional variation under hygric adsorption when modelling the 3D hygrothermal transfer. Moreover, it is essential to consider the influence of the sorption hysteresis phenomena because it characterizes the behavior of the porous material that tends to have different water contents at equilibrium at both states: the adsorption or desorption state along with determining the swelling coefficient. However, applying the hysteresis phenomena and identifying the swelling coefficient need a lot of time and careful study which will be investigated in a further paper where simulations will be done also on the transient state and development of statistical and fine imaging (3D image correlation) will take place.

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