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Heat and moisture diffusion in spruce and wood panels computed from 3-D morphologies using the Lattice Boltzmann method

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ABSTRACT

In this paper, the Lattice Boltzmann method is used to simulate heat and mass diffusion in bio-based building materials. The numerical method is presented and the methodology developed to reduce the calculation time is described. The 3-D morphologies of spruce and wood fibers are obtained using synchrotron X-ray micro-tomography. Equivalent macroscopic properties (heat conductivity and mass diffusivity) are therefore determined from the real micro-structure of the materials. The results reveal the anisotropy of the studied materials. The computed equivalent heat conductivity varies from $0.036\ \mathrm{W\,m^{-1}K^{-1}}$ to $0.52\ \mathrm{W\,m^{-1}K^{-1}}$ and the computed dimensionless mass diffusivity varies from 0.0088 to 0.78 depending on the materials and on the diffusion directions. Using these results, morphology families are identified and simple expressions are proposed to predict the equivalent properties as a function of phase properties and solid fraction.

1. Introduction

The use of bio-based materials in building construction is increasing because of their renewability and their insulation properties. As they are hygroscopic, understanding their hygrothermal behavior is necessary for appropriate building design. Over the last decade, it became obvious that the computational thermal codes used in buildings have to account for the coupling between heat and mass transfer [1,2]. These requirements gave rise to several experimental and theoretical works intended to deeply describe the effects of coupled heat and mass transfer in hygroscopic materials. These works are performed at the scales of wall assembly or building envelope [3–6].

These new requirement of building simulation are likely to benefit from the mature domain of drying and processing of hygroscopic materials [7,8]. With the increasing performances of the building envelops, accurate characterization of building materials in terms of heat and mass transfer is crucial. This can be done by clever characterization protocols. Lelievre et al. [9] investigated heat and moisture transfer within hemp concrete by accounting for hysteresis and phase change effects. Moisture transport in plywood under isothermal and non-isothermal conditions has been measured by Glass [10]. Effective thermal conductivity and mass diffusivity of bio-based materials are among the important properties engineers need to know to predict the energy consumption of buildings. An essential factor affecting such properties is the micro-structure of materials, which is particularly complex and difficult to characterize in the case of wood and derived materials. Therefore, a prediction approach that can compute the macroscopic properties from the medium morphology is of great interest.

Tomography allows a non-destructive description of the internal structure of a material. By its feature of non-destructive imaging and its ability to observe without the need to prepare a surface, the use of X-ray computed micro-tomography became a classical facility to observe various aspects of wood structure, for example to quantify anatomical features or determine density [11–13], to observe musical instrument [14], to observe archaeological wood [15] or to assess wood decay [16,17]. Lux et al. [18] studied the morphology of wood-based fibrous materials using X-ray tomography.

In the last decades, the possibility to obtain sub-micrometric resolutions, at first using synchrotron facilities and more recently thanks to laboratory nano-tomographs, offered brand new possibilities. Indeed, with sub-micrometric resolution, the morphology of secondary cell wall can be clearly observed and quantified [19,20].

Computed tomography with very high resolution (sub-micrometric resolution) was used by Standfest et al. [21] and Walther and Thoemen [22] to investigate an industrially produced Medium Density Fiberboard (MDF). Beyond imaging, these tools are also used for in situ experiments, either with mechanical or hydric loading [23–26].

Therefore, it appears to be a great tool for micro-structural characterization of wood-based materials, and we used high-resolution X-ray micro-tomography in this paper. Using such 3-D description at high

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resolution involves a huge amount of information and complex geometrical shapes. Suitable computational methods are therefore needed to predict the equivalent macroscopic properties.

Based on the kinetic theory of gases, the Lattice Boltzmann method (LBM) is a computational method widely used in fluid dynamics [27–29]. Unlike the traditional CFD methods, which solve the conservation equations of macroscopic properties after discretization, the LBM is an ascendant method where the macroscopic behavior of a fluid or a solid emerges from the discrete movement (consecutive propagation and collision processes) of particles [29]. The LBM has become a general numerical method to solve partial differential equations. As no connectivity is needed in the grid used for the resolution, the LBM is usually classified in the family of so-called meshless methods [30,31] with a local formulation. In the domain of heat or mass transfer, the scientific community remains very active in methodological developments able to open new configurations to LBM [32–34].

Considering those characteristics, the LBM provides several advantages: simple numerical development, suitability for parallel computing and easy processing of complex morphologies. We would just emphasize here that the choose of LBM was guided by these advantages in using simply the 3-D morphologies of the materials. Other computational strategies to solve the solution such as Finite Elements or Control Volumes would have produced similar results.

For these properties, the LBM has been used to predict effective conductivity and diffusivity of heterogeneous media. Wang and Pan [35] calculated the thermal conductivities of moist porous brick sands, in both frozen and unfrozen states. Wang et al. [36] focused on the effective thermal conductivity of carbon fiber composites. Xuan et al. [37] investigated the effective mass diffusivity in porous media. Yablecki et al. [38] determined the anisotropic and heterogeneous effective thermal conductivity of the gas diffusion layer of a polymer electrolyte membrane. Walther et al. [39] predicted the effective diffusivity of cement paste during hydration.

However, in most studies, the effective properties of heterogeneous materials are calculated on model media or reconstructed morphologies and not on real morphologies (stochastic generation growth method [40], uniformly distributed inclusions and randomly generated fibrous medium [41], stochastic fibers placement algorithm [38] and correlated random field [39]). Wulf et al. proposed a full 3D approach applied to metallic foams [42]. Perré et al. [43] studied both thermal and mass diffusivities in real morphologies of wood but only in two dimensions (2-D) whereas it is necessary to know the material properties in all directions because of their anisotropy.

In this paper, we investigate both heat and mass transfers in bio-based materials using the LBM to predict the effective thermal conductivity and mass diffusivity. The calculations are done on real 3-D morphologies obtained by micro-tomography, in each direction. The next section of this paper describes the materials studied, the imaging technique used, synchrotron X-ray micro-tomography and image processing. Then, we present the Lattice Boltzmann method in the case of diffusion and describe the computation of equivalent (or effective) properties. The methodology to reduce calculation time (choice of numerical parameters, determination of a convergence criterion and parallel computing) is explained in Section 4. Finally, the results for both heat and mass transfers are presented in Section 5.

2. Material morphologies

Several bio-based building materials are studied in this paper: spruce (*Picea abies*) earlywood (EW) and latewood (LW), Low-Density Fiberboard (LDF) and Medium-Density Fiberboard (MDF). These products are all wood-based materials but present a wide range of properties as a result of their internal structure (porosity, pore connectivity, directional orientation). Therefore, depending on their properties, these materials have different roles in building, such as mechanical structure, furniture, partition and insulation. These materials were chosen because they have the same solid phase, which will allow us to concentrate on the effect of morphology on macroscopic properties in the present work.

2.1. Sample preparation

To obtain 3-D images at high resolution, we had to prepare small cylindrical samples of our materials. Depending on the toughness of the product, we used two different methods. For spruce, we used a wood-turning machine to make cylinders and carefully reduce their diameter down to a few millimeters. This method does not work for LDF and MDF due to their low cohesion. Instead, we used a laser cutting device to prepare, without any mechanical stress, cylinders of 10 mm and 5 mm, respectively. However, we had to face another problem: for LDF, the density is so low, hence the air circulation so easy, that the samples burnt during laser cutting. To avoid this, we pre-cut larger samples with a hole saw and placed them in an open-top aluminum container free of oxygen thanks to an intense nitrogen flux during laser cutting.

2.2. Microtomography

X-Ray micro-tomography is a non-destructive and non-invasive 3-D imaging technique. It is used to characterize material micro-structure at a micron level spatial resolution. It has become a relatively common tool in materials science and is suitable for bio-based materials [44].

Classical X-ray tomography is based on the attenuation of an X-ray beam by matter. A sample is scanned at different rotation angles by X-ray beams and the attenuation of the X-ray beam intensity is measured by a 2-D detector, which acquires a collection of projections. Then an algorithm reconstructs the 3-D object from the 2-D radio-density images.

Our samples have been scanned at ESRF (European Synchrotron Radiation Facility, line ID19) by Novitom, a company specializing in advanced analytical imaging powered by synchrotron technology. The tomography analysis mode used is phase contrast. In contrast to classical tomography, it is not the attenuation of the X-rays that is measured but the beam phase shift (transformed into variations in intensity) that is recorded by the detector. The energy of the X-ray beam was 19 keV for the highest resolution and ca. 80 keV for the other resolutions. The exposure time was about 0.1 s per projection. With a total of 6000 projections, the time required per reconstructed volume is ca. 10 s. For wood samples, 2 or 3 volumes were needed to scan the whole sample in the longitudinal direction. All scan were done with samples equilibrated with the surrounding air, i.e. at a moisture content of about 10%. We scanned at different resolutions: 3.05 μm for LDF, 0.97 μm for MDF and 0.62 μm for spruce. The dimensions of the scanned volume are $12 \times 12 \times 13\ \mathrm{mm}^3$ for LDF, $4.4 \times 4.4 \times 2.1\ \mathrm{mm}^3$ for MDF and $1.4 \times 1.4 \times 2.6\ \mathrm{mm}^3$ for spruce. The scanned spruce volume contains both early- and latewood.

2.3. Image processing and 3-D morphologies

Image processing of the reconstructed datasets is needed to define the 3-D morphologies of materials in a form suitable for the LBM code. The image processing is performed with *Fiji*, which is an open source image processing package based on *ImageJ*. For spruce (late- and earlywood), the sample is rotated to align the material directions of wood (longitudinal, radial and transverse) along the x-, y- and z-axes. The reconstructed datasets are cropped to have $200 \times 200 \times 200$ voxels for fibers and around $100 \times 150 \times 400$ voxels for spruce. To have enough tracheids with only $100 \times 150 \times 400$ voxels, we used a $2 \times 2 \times 2$ binning factor on earlywood. We apply a global threshold-based segmentation on each sample, the threshold level is determined by the moment method. Finally, the morphology is defined as a file with the coordinates and the corresponding grey level (0 for the solid phase or 1 for the gaseous phase). The four bio-based materials that have been