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Modeling of moisture transport in wood below the fiber saturation point

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ABSTRACT

This paper describes a multiscale homogenization model for macroscopic diffusion properties of wood. After a short introduction the physical background of steady state diffusion processes in wood will be highlighted, resulting in a physically motivated macroscopic description of diffusion processes with only one diffusion equation and thus one diffusion tensor. This macroscopic diffusion tensor is derived by revisiting the morphological structure of wood in the framework of continuum micromechanics. Starting point is the cellular structure of wood; further homogenization steps include wood rays and the succession of annual rings. The quality of the model is assessed by a comparison of model predictions and measured values at different temperatures and moisture contents.

INTRODUCTION

Computational simulations of physical processes have gained in importance significantly in the last decades, along with the incessant advancement of computer hardware. Such simulations were of course also applied in the field of moisture transport in wood, for example by Truscott and Turner 2005 and Frandsen, Damkilde and Svensson 2007.

Beside the sample geometry, the material properties are the main input parameters for any simulation. In wood, these properties are characterized by a wide variability at the macroscale. This variability results from differences in geometry and composition observed at the macro-, micro-, and ultra-structural scale of a wood tissue. So it has been striven for long to relate the macroscopic properties to physical quantities at lower scales (see e.g. Siau 1984).

The present article describes a new model capable to predict macroscopic diffusion coefficients of wood applicable to moisture transport problems at conditions below the fiber saturation point, by including the entire hierarchical structure of clear (knot-free) wood, ending up with a multiscale analytical description. Similar models for the estimation of mechanical properties (see e.g. Hofstetter et al 2005) and thermal conductivities (Eitelberger et al 2009a) showed good agreement with measured results and motivate the application also to diffusion properties.

PHYSICAL BACKGROUND OF STEADY STATE MOISTURE TRANSPORT IN WOOD

Moisture in wood exists in three different phases: Liquid water and water vapor in the cell lumens as well as bound water in the cell wall. Liquid water is permanently present only in the living tree. Below the fiber saturation point (FSP) changes in moisture content are accompanied by changes of other material properties and by deformations. For this reason this paper deals only with such conditions.

For conditions below the fiber saturation point it further can be assumed that all interconnecting pits are aspirated. Thus, moisture can only pass from one lumen to another by diffusion through the cell wall. This is accompanied by two phase changes: on the one side of the cell wall water vapor is adsorbed, while on the other side the bound water is desorbed to water vapor again. Each phase change is accompanied by a change in enthalpy; heat is released during adsorption and consumed during desorption.

Steady state conditions denote that there is no change of moisture content in each material point in time. The two phases of water – water vapor in the lumens and bound water in the cell walls – are in equilibrium, which allows the description by only one macroscopic gradient holding for both phases.

Consequently, the amount of adsorbed and desorbed water in the cell wall is equal for steady state conditions, so that the heat generation and consumption upon the phase changes only results in a small heat flux through the cell wall parallel to the moisture flux, but no macroscopically relevant temperature gradients.

Based on this physical background, steady state moisture diffusion in wood can be described by one macroscopic gradient and therefore one Fickian process with one diffusion tensor. In one (spatial) dimension this is,

$$J = -D\frac{\partial c}{\partial x}, \qquad (1)$$

where J denotes the flux, c is the concentration, x is the position and D is the diffusion coefficient. For two or more dimensions Eq. (1) is generalized to

$$\mathbf{J} = -\mathbf{D}\cdot\nabla c, \qquad (2)$$

where ∇ is the gradient operator, and $\mathbf{D}$ is the second order diffusion tensor. Wood is in good approximation an orthotropic material, therefore the macroscopic three-dimensional diffusion tensor $\mathbf{D}$ can be written as:

$$\mathbf{D} = D_{ij} = \begin{bmatrix} D_L & 0 & 0 \\ 0 & D_R & 0 \\ 0 & 0 & D_T \end{bmatrix}, \qquad (3)$$

with D_L, D_R, and D_T denoting the longitudinal, radial, and tangential diffusion coefficients.

In order to consider the influence of the microstructure of wood on the diffusion behavior, homogenization methods are applied, which will be presented in the following chapter. A coupling to heat conduction processes is not necessary, since heat transport is negligible at the macroscale.

CONTINUUM MICROMECHANICS

Continuum micromechanics is the analysis of a heterogeneous material with several material phases of known morphologies and diffusivities. This material is understood as micro-heterogeneous, but macro-homogeneous. The inhomogeneous microstructure is defined by means of a representative volume element (RVE), in which separate phases with specific properties are differentiated. To comply with the separation of scales requirement, the characteristic length d of the inhomogeneities within the RVE making up a phase, has to be much smaller than the characteristic length ℓ of the RVE, $d \ll \ell$ (see Fig. 1).

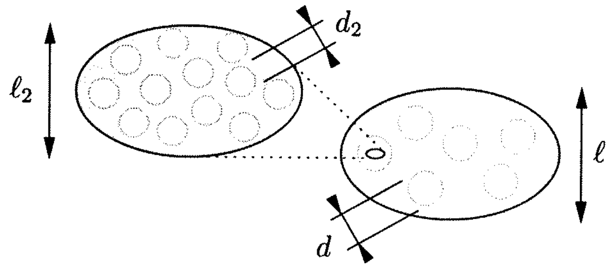

FIGURE 1: Multiscale homogenization with two RVEs

The response of the overall material, i.e. the relation between concentration gradients acting on the boundary of the RVE and the resulting diffusive fluxes, is determined using an adaption of Eshelby's solution for matrix-inclusion problems. In combination with averaging of concentration fluxes and gradients (Dormieux 2005), an estimate for the homogenized diffusion tensor $\mathbf{D}^{\text{hom}}$ of the material is obtained:

$$\mathbf{D}^{\text{hom}} = \frac{\sum_r f_r \mathbf{D}_r \cdot \left[\mathbf{I} + \mathbf{P}_r^0 \cdot \left(\mathbf{D}_r - \mathbf{D}^0\right)\right]^{-1}}{\sum_s f_s \left[\mathbf{I} + \mathbf{P}_s^0 \cdot \left(\mathbf{D}_s - \mathbf{D}^0\right)\right]^{-1}}, \qquad (4)$$

where $\mathbf{D}_r$ and f_r denote the second order diffusion tensor and the volume fraction of phase r, respectively, and $\mathbf{I}$ is the second order unity tensor. The two sums are taken over all phases of the heterogeneous material in the RVE. The second order Hill-tensor $\mathbf{P}_r^0$ contains information about the characteristic shape of phase r in a matrix phase with diffusion tensor $\mathbf{D}^0$. Choice of this diffusion tensor $\mathbf{D}^0$ allows the consideration of two different types of arrangement of the phases: the case of a continuous matrix with inclusions is represented by a Mori-Tanaka scheme and $\mathbf{D}^0 = \mathbf{D}_{matrix}$; an intimately mixed arrangement is described by a self-consistent scheme with $\mathbf{D}^0 = \mathbf{D}^{\text{hom}}$.

Formulating Eshelby's solution for an ellipsoidal inclusion with given radii a_1, a_2, and a_3, the components of the P-tensor are obtained as

$$P_{ell,ij} = \frac{1}{4\pi}\int_{-1}^{+1}\int_{0}^{2\pi} \xi_i \xi_j \left(D_{kl}^0 \xi_k \xi_l\right)^{-1} d\hat{\varphi}\, d\hat{\xi}_3, \qquad (5)$$

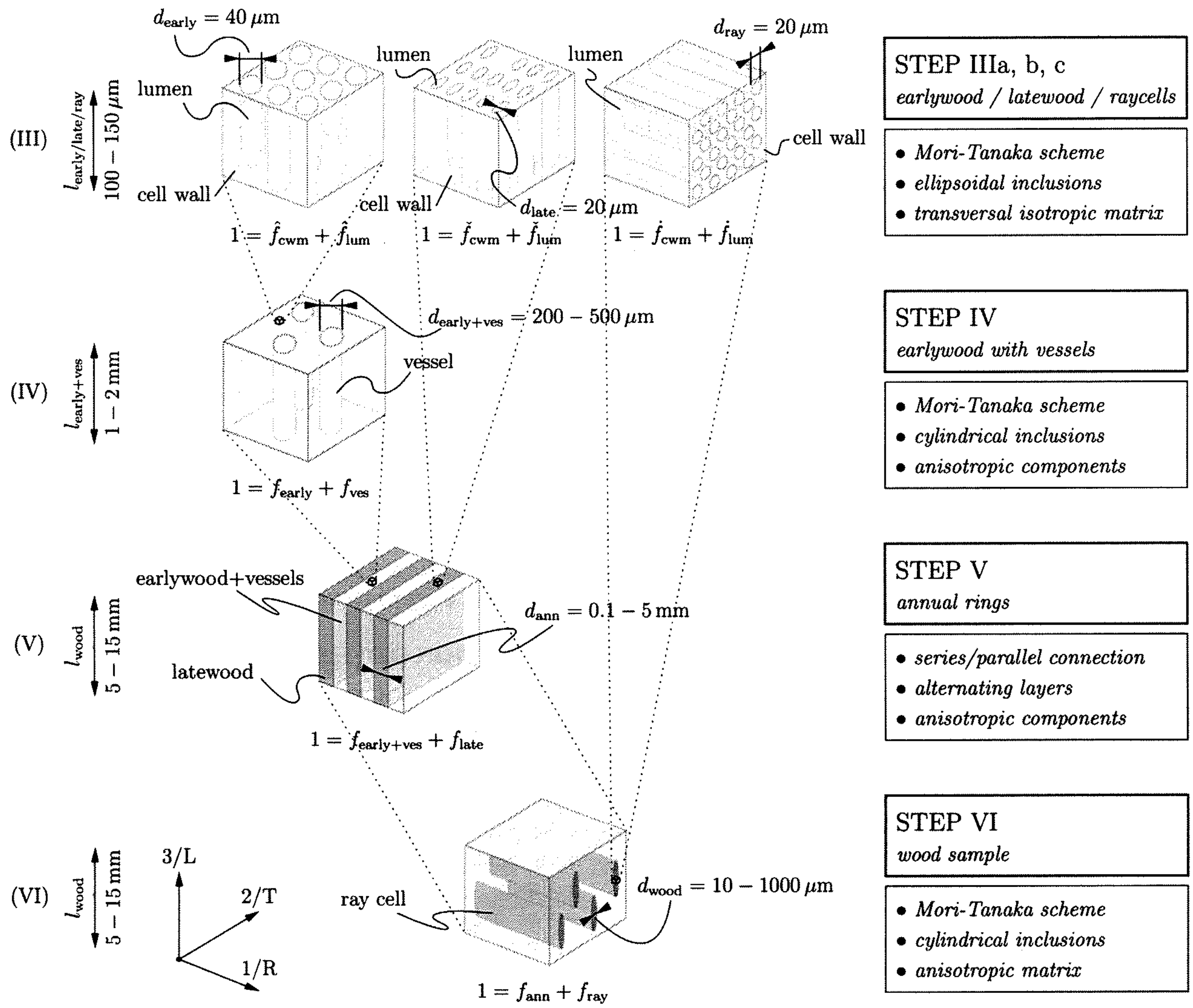

FIGURE 2: Four-level homogenization procedure for diffusion properties of wood

with

$$\xi_1 = \frac{\sqrt{1-\hat{\xi}_3^2}\cos\hat{\varphi}}{a_1},\ \xi_2 = \frac{\sqrt{1-\hat{\xi}_3^2}\sin\hat{\varphi}}{a_2},\ \xi_3 = \frac{\hat{\xi}_3}{a_3}. \quad (6)$$

This general case of ellipsoidal inclusions can be easily specialized to cylindrical inclusions (e.g. $a_3 = \infty$) and spherical inclusions ($a_1 = a_2 = a_3$).

If a single phase exhibits a heterogeneous microstructure itself, its behavior can be estimated by introduction of an additional RVE within this phase, with dimensions $\ell_2 << d$. This procedure can be repeated until a scale is reached, on which the properties of all phases are independent of the particular wood tissue, resulting in a multiscale homogenization scheme (see Fig. 1).

A material like wood suggests the use of such a multiscale approach. In the following section the material phases at the different length scales and their morphological properties are described.

HOMOGENIZATION MODEL FOR DIFFUSION PROPERTIES OF WOOD

When formulating a homogenization model for material properties, the ambition is to start at tissue-independent phases in order to enable its application to any wood species. Such phases in wood can only be found on the nanometer scale. Namely they are cellulose, hemicelluloses, lignin, water and extractives. Similar models for mechanical and thermal properties (see Hofstetter et al 2005 and Eitelberger et al 2009a) start at this scale, including up to six homogenization steps. However, moisture diffusion coefficients of these universal phases are not available.

Therefore we have chosen the cellular structure of wood on a scale of about 150 µm as starting point for the homogenization of diffusion coefficients. Fig. 2 shows the resulting four-level homogenization procedure for diffusion coefficients of wood. To be consistent with other existing models by the authors, the present model starts at step III; step I and II are only present in models that start on the molecular scale.

In steps IIIa and IIIb, wood cells are represented by hollow tubes aligned in the stem direction. Two phases can be defined for this homogenization step: the cell wall material and air filling the lumens, with diffusion coefficients according to Eitelberger et al 2009b:

$$D_{cwm} = D_0 \cdot \exp\left(\frac{44533 - 23197 \cdot u - 1125 \cdot \ln u}{-R \cdot T}\right), \quad (7)$$

$$D_{air} = 2.31 \cdot 10^{-5} \cdot \left(\frac{p_{atm}}{p_{atm} + p_v}\right) \cdot \left(\frac{T}{273.15}\right)^{1.81} \text{ m}^2\text{/s}, \quad (8)$$

where u is the moisture content, R is the universal gas constant, T is actual temperature in [K], p_{atm} and p_v are the atmospheric and vapor pressure, respectively. The prefactor in Eq. (7) is $D_0 = 2.453 \cdot 10^{-4}$ m²/s for diffusion in the transversal direction of the cell wall, and $D_0 = 6.133 \cdot 10^{-4}$ m²/s for diffusion in the longitudinal direction.

Formulating step III for different volume fractions of cell walls and lumens and for different lumen geometries results in diffusivity estimates for earlywood and latewood (see Fig. 2).

An additional cell type are the ray cells, which form pathways in the radial direction of the stem. The behavior of these cells is calculated by step IIIc (see Fig. 2) with a Mori-Tanaka scheme.

In hardwood species, which exhibit a more specialized structure than softwood species, large vessels with a diameter of 200-500 µm support the transport of water in the living tree. They are incorporated in the model with step IV (see Fig. 2). Vessels are mainly located in earlywood so that they are only considered in this material part. The two phases of this step are the earlywood material of step IIIa and air filling the vessel pores. The morphology of the vessels as approximately ellipsoids again motivates the use of a Mori-Tanaka scheme.

Step V accounts for the succession of earlywood and latewood in the annual rings. The effective diffusivity is computed by either a series connection (R direction) or a parallel connection (L and T direction) of the diffusion coefficients of earlywood and latewood calculated in steps IIIb and IV. The typical length scale of the RVE in this step is about 5-15 mm.

In the last homogenization step wood rays are included in the material. Again a Mori-Tanaka scheme is used, with the material of step V as matrix and the ray cells of homogenization step IIIc as inclusions. The typical length scale is again about 5-15 mm as in step V. Nevertheless, this does not violate the separation of scales requirement, since the decisive dimensions of step V and VI refer to different material directions (longitudinal and tangential in step V, radial in step VI).

A more detailed description of the steps, including the calculation of volume fractions, morphological parameters and diffusion coefficients of the single phases, is available in Eitelberger et al 2009a and 2009b.

VALIDATION OF THE MODEL

The validation of the model was done by comparison of measured diffusion coefficients under steady state conditions and corresponding model estimates. Input values for the model are wood species (which is chosen as indicator of ray content, ray dimensions, and volume fractions in step V), density, moisture content, and temperature. The validation shows a good correlation between model predictions and measurements (Eitelberger et al 2009b).

To display the predictive qualities of the model, a set of measured values for a spruce tissue with an oven-dry density of ρ_{dry} = 0.404 g/cm³ (according to Kollmann 1951) is recalculated by means of the homogenization model. The input parameters differ in terms of moisture content and temperature. The results are shown in Fig. 3, where the dash-dotted lines are the model predictions for different moisture contents at a given temperature. Each cross denotes one measurement with reported temperature and moisture content.

A good agreement of measurements and model predictions is observed. Reasons for deviations could be the use of a constant approximate diffusion coefficient for the cell wall, irrespective of the chemical composition of the cell wall and the degree of pit aspiration. Another reason could be the measurement accuracy, the thus resulting broad spread of the measurement results can be seen in Fig. 3.

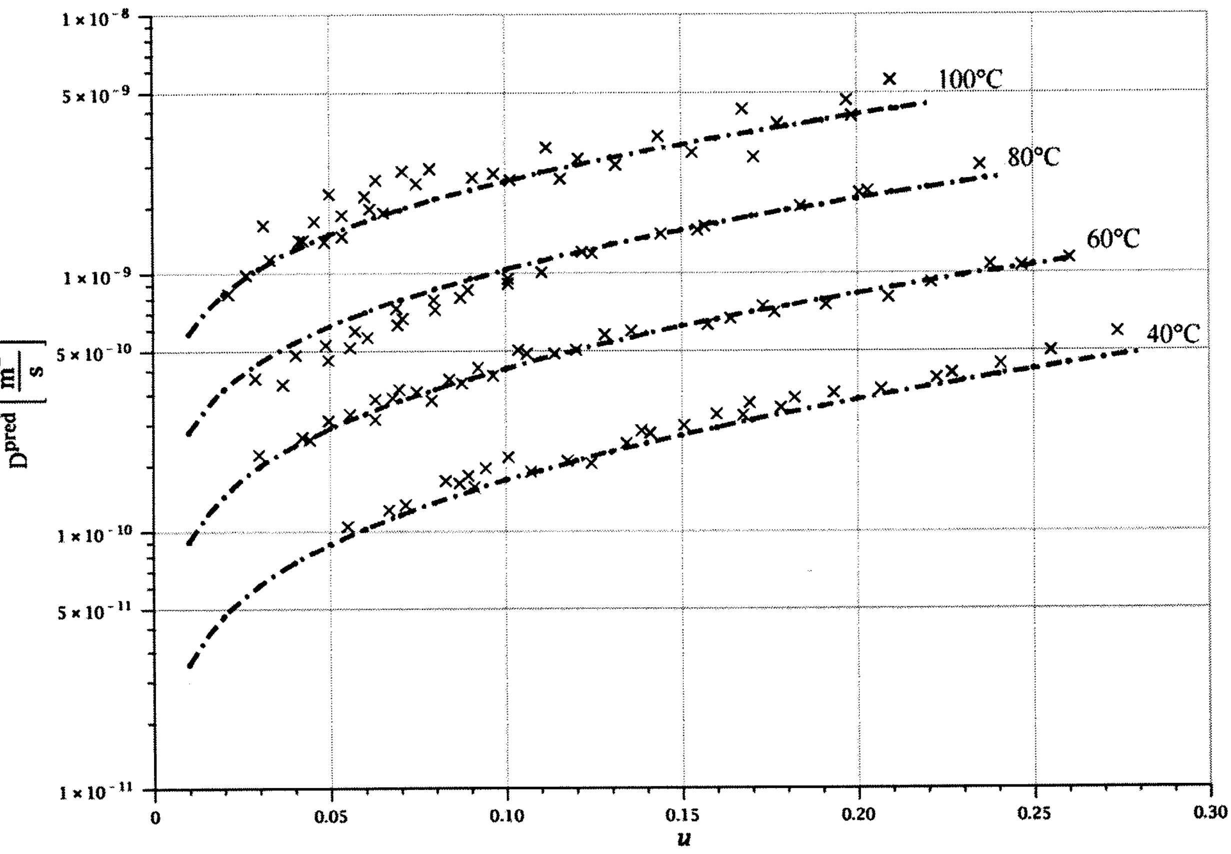

FIGURE 3: Model predictions (dash-dotted lines) compared with measured diffusion coefficients for a sample of spruce (ρ_{dry} = 0.404 g/cm³) according to Kollmann 1951. The tests were conducted at four different temperatures (40, 60, 80, 100°C) Each marker indicates one measured value at moisture content u.

SUMMARY AND OUTLOOK

A multiscale model for moisture diffusion in wood below the FSP is presented. Due to the lack of input values below the cell wall scale, it starts at a length scale of about 150 μm, where wood cells form a honeycomb-like structure. Within six homogenization steps at four length scales the morphology of wood is remodeled more accurately than in existing models, which are limited to the wood cell structure. The obtained results demonstrate the good predictive capabilities of multiscale homogenization models and continuum micromechanics as homogenization method.

With the presented approach, only diffusion coefficients for steady state moisture diffusion can be calculated. The simulation of transient diffusion processes is more complicated, since the two water phases that are present below the fiber saturation point are not in equilibrium anymore. Thus, they have to be accounted for by two separate phases also on the macroscale. Further a macroscopically relevant generation and consumption of heat due to phase changes requires the coupled simulation of heat transport. The present steady state model will serve as practical tool for determination of input parameters, together with a similar multiscale model for heat transfer properties (see Eitelberger et al 2009a).

We are positive, that the presented model will contribute to future research of moisture transport simulations in wood.

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