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TRANSFORMATION RELATIONS AND MATRIX IMPLEMENTATION OF MULTIPHYSICS MODEL FOR TEMPERATURE AND MOISTURE FIELDS IN WOOD

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ABSTRACT

This paper deals with the numerical simulation of 3D heat and moisture transfer in wood. The appropriate mathematical model is based on a set of coupled heat and mass transfer equations.

The main contributions of this paper are: first, the transformation relations between matrixes of material coefficients (diffusion and thermal conductivity coefficients) in anatomical and geometrical directions in three-dimensional case; second, the implementation of a numerical solution for the three-dimensional problem of nonisothermal moisture transfer in the anisotropic structure of wood in convective drying with transient phenomena (Soret effect, Duffour effect).

The simulation is based on the unsteady-state nonisothermal nonlinear diffusion of moisture and heat with respect to the orthotropic nature of wood. It deals with a transport model which makes use of the gradient of moisture and temperature for motive power and respects the dependence of material coefficients on temperature and moisture.

KEYWORDS: Moisture and heat transfer, multiphysics, wood drying, transformations.

INTRODUCTION

Wood drying is still controlled by experience to a great degree. For this reason, many scholars have been trying to develop a drying model to describe wood drying processes completely, both in the theory and practice for years. There is an attempt to use the model to guide, design and optimize the wood drying process and to find out the way to increase the drying quality, decrease the energy consumption and decrease the drying time. The development of the wood drying model is based on the study of three fundamental phenomena (heat transfer, moisture transfer and strain-stress analysis).

The theory of transport phenomena in porous materials was summarised by Luikov (1975, 1980) and Whitaker (1977). Luikov (1975) developed a set of coupled partial differential equations to describe the heat and mass transport in capillary porous media by assuming that the transfer of moisture is analogical to heat transfer and that capillary transport is proportional to moisture and temperature gradient. This approach was used by Thomas et al. (1980) and Irudayaraj (1990). But the solution, even numerical, is complicated, involving complex eigenvalues (Liu and Cheng 1991). Malan and Lewis (2003) and Lewis et al. (1996) demonstrated the efficacy of the finite element method in solving highly non-linear drying systems.

A number of theoretical models have been suggested in wood drying (Chen and Pei 1989) but they are not completely applicative to simulate real drying processes as seen in industry. It is caused by a low level of generality of the proposed models that is brought about by a wide range of coupled physical fields included in the model, the specification of boundary conditions, the evaluation of experimental characteristics, etc. Koňas (2008, part I) assembled a coefficient form of a coupled stress-strain task with moisture/temperature dependency of wood with orthotropic, viscoelastic material properties suitable for current numerical solvers. The weak solution of this task and the subgrid upscaling homogenization method for the large scale hierarchical structure which is typical for wood was obtained in Koňas and Přemyslovská (2008, part II). The modified Ritz-Galerkin method was derived for a simple solution of this problem. The difficulty with the mathematical formulation of the wood drying process lies in the number of combined transfer mechanisms, the interdependencies among these mechanisms, and the different variables controlling them. Many external factors can also affect the wood drying speed, of which temperature, humidity (equilibrium moisture content) and airflow speed are the primary factors, and these three main factors determine the change of the wood moisture content. Therefore, the establishment of a phenomenological model based on the relation between the macroscopical characteristics of wood and drying conditions is another important focus of research in modelling.

The use of Fick's law for the description of the moisture content has been questioned by (Babiak 1995). The process of wood drying can be interpreted as a simultaneous heat and moisture transfer with local thermodynamic equilibrium at each point within the timber (Horáček 2004). Drying of wood is in its nature an unsteady-state non-isothermal diffusion of heat and moisture, where temperature gradients may counteract with the moisture gradient. For a theoretical description of these phenomena, thermodynamic models seem to be the most suitable. Although unsteady-state non-isothermal experiments have been conducted (e.g. Avramidis et al. 1994), we are convinced that practical solutions of mathematical models that couple moisture and heat transfer with inhomogeneous material, combined with an experimental verification, are still lacking (Irudayaraj et al. 1990). A considerable volume of research has been carried out regarding the modelling of the moisture and heat transfer in materials like polymers, wood, or agricultural products (Salin 1991, Kamke and Vanek 1994). The modelling of moisture fluxes under unsteady-state non-isothermal conditions has been noticeably absent in literature (Avramidis et al. 1994), although the theory behind was proposed twenty years ago (Siau 1983). The heat and moisture transfer should be considered as coupled processes: a thermally induced mass transfer, the Soret effect (Siau 1984, Avramidis et al. 1994, Horáček 2004) and the heat flux resulting from the moisture diffusion, the Duffour effect (Siau 1992), should be all taken into account. Luikov (1966), and in much details Whitaker (1977) developed a unique approach that describes the simultaneous heat and moisture transfer in drying processes, based on irreversible thermodynamic processes.

The determination of the moisture diffusion coefficient is based on models derived by Siau (1995) and Skaar (1988), the thermal conductivity by MacLean (1941), the specific heat of wood by Skaar (1988), and the density of wood by Kollmann (1951). In contrast to the usually applied assumption by Crank (1975), the initial values of temperature and moisture do not have to be uniformly distributed within the specimen. The numerical value used for the heat and mass transfer coefficient in the simulation of wood drying has been discussed in Söderström and Salin (1993), Salin (1996a,b), Avramidis et al. (1994), Siau (1995) and Pang (1996) together with the correction coefficient introduced by Plumb et al. (1985) and Siau (1995).

The coupled and highly non-linear nature of the transport equations that govern the drying process highlights the applicability of numerical simulation in this field (Perré and Turner 1999). The mathematical model used in the present work is formed by a system of two partial differential equations and corresponding third-order boundary conditions. It is a purely mathematic treatment of wood as a continuous and homogenous medium, without explaining those physical mechanisms associated with the moisture transport that takes place simultaneously inside wood. The moisture content and the temperature gradient are set as driving forces, since all the other possible factors related to the moisture content are applicable only in the hygroscopic region. The proposed equations are inspired by Siau (1992) and Avramidis (1994), who with these equations found the best agreement between the experimental fluxes and thermodynamic model. The three-dimensional transfer of heat and moisture is generally described as follows:

$$\frac{\partial w}{\partial t} - \nabla(\mathbf{D}\nabla w + s\mathbf{D}\nabla T) = 0 \tag{1}$$

$$C\rho\frac{\partial T}{\partial t} + \frac{E_b}{1.8C}\frac{\partial w}{\partial t} - \nabla\boldsymbol{\lambda}\nabla T = 0 \tag{2}$$

where: D is the matrix of moisture diffusion coefficients of wood ($m^2.s^{-1}$), λ the matrix of thermal conductivity coefficients of wood ($Wm^{-1}K^{-1}$), s is the Soret effect (-/K), w is the moisture content (-), T is the temperature (K), C is the specific heat of heat ($Jkg^{-1}K^{-1}$), ρ is the wood density (kgm^{-3}).

The relationship

$$s = \frac{\varphi}{RT}\frac{\partial EMC}{\partial \varphi}\frac{E_b}{T} \tag{3}$$

refers to the Soret effect (thermodiffusion) based on the slope of the sorption isotherms and the activation energy for water diffusion E_b, where φ is the relative air humidity and R is the universal gas constant. In general, these isotherms are specific to wood specimens, since differential heat of sorption for different wood differs noticeably (Babiak 1990).

Boundary conditions are obtained from the heat and moisture transfer between wood surfaces and external air. The following boundary conditions were applied for the numerical solution:

$$-\mathbf{n}(\mathbf{D}\nabla w + s\mathbf{D}\nabla T) = \alpha_w(w_{\partial\Omega} - EMC) \tag{4}$$

where: α_w is the mass transfer coefficient ($m.s^{-1}$), $w_{\partial\Omega}$ is the surface moisture (-), EMC is the equilibrium moisture content of wood (-)

$$\mathbf{n}\boldsymbol{\lambda}\nabla T = \alpha_T(T_{\partial\Omega} - T_{air}) \tag{5}$$

where: α_T is the heat transfer coefficient ($Wm^{-2}.K^{-1}$), $T_{\partial\Omega}$ is the surface temperature (K), T_{air} is the air temperature (K).

The initial conditions can be defined as functions of the position in the body of wood. In this work the initial conditions are taken as constants:

$$w = f_w(x,y,z) = w_0 \tag{6}$$

$$T = f_T(x,y,z) = T_0$$

MATERIAL AND METHODS

During physical analysis and mathematical modelling it is necessary to consider the anisotropic wood structure. Often the values of the diffusion and heat conductivity coefficients in geometrical directions are not known. These coefficients are established (measured, analytically determined) only in anatomical directions and it is necessary to transform them into geometrical directions before solving the system of partial differential equations (PDEs) describing the simultaneous, nonisothermal, nonlinear, nonstationary moisture and heat transfer in a generally orthotropic wood body. The transformation relations and the matrix form of the mentioned system of PDEs are described below.

The numerical simulations are performed for pinewood 0.045 m thick, 0.2 m wide and 5 m long with initial moisture of 0.25 and an initial temperature of 20°C. The air temperature is kept at a constant value of 80°C and the relative humidity (φ) and the corresponding equilibrium moisture content (EMC) depend on time as featured in Tab. 1. The air flow is constant - 2 ms^{-1}.

Tab. 1: Time drying schedule.

t (hours)	T_{air} (°C)	φ (-)	EMC (-)
4.5	80	0.77	0.108
9	80	0.67	0.087
17	80	0.59	0.073
29	80	0.46	0.056
45.5	80	0.34	0.042
54.5	80	0.3	0.039

Transformation relations and implementation into COMSOL Multiphysics

Let L: V→V be a linear operator on a vector space V. Let $\mathbf{L}_\alpha$ be the matrix of *L* relative to a basis α for V. Let $\mathbf{L}_\beta$ be the matrix of L relative to another basis $\mathbf{P}_\beta$ for V. Let $\mathbf{L}_{\beta\alpha}$ be the transition matrix from the basis α to β. Then

$$\mathbf{L}_\beta = \mathbf{P}_{\beta\alpha}\mathbf{L}_\alpha\mathbf{P}_{\beta\alpha}^{-1} \tag{7}$$

Thus, if the matrix of diffusion coefficients is known relative to a basis α, it can be expressed relative to any other basis β.

Then the matrix $\mathbf{L}_\alpha$ has a diagonal form:

$$\mathbf{L}_\alpha = \begin{pmatrix} D_R & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_L \end{pmatrix} \tag{8}$$

For generally orthotropic material as wood is this matrix $\mathbf{L}_\alpha$ must be transformed to a matrix of diffusion and heat-conductive coefficients $\mathbf{L}_\beta$ in general axes of the model at the deviation of anatomic directions from these axes

$$\mathbf{L}_\beta = \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{pmatrix} = \mathbf{P}_{\beta\alpha}\begin{pmatrix} D_R & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_L \end{pmatrix}\mathbf{P}_{\alpha\beta} \tag{9}$$

The transition matrixes are assembled from the following relations: $\mathbf{P}_{\alpha\beta} = \mathbf{P}_{\beta\alpha}{}^{-1}$, $\mathbf{P}_{\beta\alpha} = \boldsymbol{\beta}^{-1}\boldsymbol{\alpha}$, where α, β are matrixes with columns formed by vectors of bases α, β. In this work β is assumed to be the standard basis (thus it is formed by unit vectors and then β is the identity matrix) and consequently $\mathbf{P}_{\beta\alpha} = \boldsymbol{\alpha}$.

The previous information is important, because it enables us to gain transition matrixes $\mathbf{P}_{\alpha\beta}$ and $\mathbf{P}_{\beta\alpha}$ easily. Consequently, by using relation (9) the matrix of diffusion (or thermal conductivity coefficients) can be obtained and be used at Fick´s (or Fourier´s) laws for the mathematical description of moisture (or heat) transfer inside generally orthotropic material. This theory is valid for an arbitrary basis *α* and therefore the above mentioned relations are applicable for an arbitrary fibre lean.

The simulations of wood drying were provided for wood with a fibre lean as illustrated in Fig. 1. The angle u denotes the transverse fibre lean and v denotes the longitudinal fibre lean.

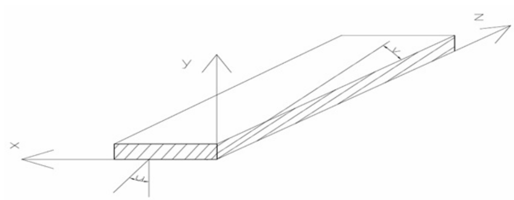

Fig. 1: Deviation of anatomic directions (R, T, L) from geometric axes (x, y, z) of the model (u=35°, v=10°).

For the fibre lean as illustrated in Fig. 1 the transition matrix $\mathbf{P}_{\beta\alpha}$ is following:

$$\mathbf{P}_{\beta\alpha} = \begin{pmatrix} \cos(u) & -\sin(u) & 0 \\ \sin(u) & \cos(u) & \sin(v) \\ 0 & 0 & \cos(v) \end{pmatrix} \tag{10}$$

and the searched matrix :

$$\mathbf{L}_{\beta} = \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{pmatrix} = \begin{pmatrix} \cos(u) & -\sin(u) & 0 \\ \sin(u) & \cos(u) & \sin(v) \\ 0 & 0 & \cos(v) \end{pmatrix} \begin{pmatrix} D_R & 0 & 0 \\ 0 & D_T & 0 \\ 0 & 0 & D_L \end{pmatrix} \begin{pmatrix} \cos(u) & -\sin(u) & 0 \\ \sin(u) & \cos(u) & \sin(v) \\ 0 & 0 & \cos(v) \end{pmatrix}^{-1}$$

$$\mathbf{L}_{\beta} = \begin{pmatrix} D_R\cos^2(u) + D_T\sin^2(u) & \sin(u)\cos(u)(D_R - D_T) & \sin(u)\cos(u)(D_R - D_T)\tan(v) \\ \sin(u)\cos(u)(D_R - D_T) & D_T\cos^2(u) + D_R\sin^2(u) & -(D_T\cos^2(u) + D_R\sin^2(u) - D_L)\tan(v) \\ 0 & 0 & D_L \end{pmatrix} \tag{11}$$

Regarding the notations in the previous theory section, the matrix $\mathbf{L}_{\beta}$ is written as D ($\mathbf{L}_{\beta}$ = D) so that it is obvious that this is the matrix of diffusion coefficients.

The system of PDEs (1, 2) can be written into the FEM environment of COMSOL Multiphysics 3.4 as follows:

$$\mathbf{u} = \begin{pmatrix} w \\ T \end{pmatrix}, \quad \mathbf{c} = \begin{pmatrix} \mathbf{D} & s\mathbf{D} \\ \mathbf{0} & \boldsymbol{\lambda} \end{pmatrix}, \quad \mathbf{d}_{\mathbf{a}} = \begin{pmatrix} 1 & 0 \\ \dfrac{E_b}{1.8C} & C\rho \end{pmatrix} \tag{12}$$

where:

$$\mathbf{D}=\begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{pmatrix},\ s\mathbf{D}=\begin{pmatrix} sD_{xx} & sD_{xy} & sD_{xz} \\ sD_{yx} & sD_{yy} & sD_{yz} \\ sD_{zx} & sD_{zy} & sD_{zz} \end{pmatrix},\ \boldsymbol{\lambda}=\begin{pmatrix} \lambda_{xx} & \lambda_{xy} & \lambda_{xz} \\ \lambda_{yx} & \lambda_{yy} & \lambda_{yz} \\ \lambda_{zx} & \lambda_{zy} & \lambda_{zz} \end{pmatrix}$$

and others input parameters are zero matrixes 0.
Thus:

$$\mathbf{c}\nabla\mathbf{u}=\begin{pmatrix} \mathbf{D} & s\mathbf{D} \\ \mathbf{0} & \boldsymbol{\lambda} \end{pmatrix}\begin{pmatrix} \nabla w \\ \nabla T \end{pmatrix} \tag{13}$$

$$\mathbf{d_a}\frac{\partial \mathbf{u}}{\partial t}=\begin{pmatrix} 1 & 0 \\ \dfrac{E_b}{1.8C} & C\rho \end{pmatrix}\begin{pmatrix} \dfrac{\partial w}{\partial t} \\ \dfrac{\partial T}{\partial t} \end{pmatrix} \tag{14}$$

$$-\mathbf{n}\begin{pmatrix} \mathbf{D} & s\mathbf{D} \\ \mathbf{0} & \boldsymbol{\lambda} \end{pmatrix}\begin{pmatrix} \nabla w \\ \nabla T \end{pmatrix}=\begin{pmatrix} \alpha_w(w_{\partial\Omega}-EMC) \\ \alpha_T(T_{\partial\Omega}-T_{air}) \end{pmatrix} \tag{15}$$

RESULTS AND DISCUSSION

Mathematical relations for the transformation of the diffusion and thermal conductivity matrixes for generally orthotropic material were developed. The above mentioned diffusion model of the coupled moisture and heat transfer was solved numerically in program COMSOL Multiphysics 3.4 (the solver is based on the finite element method) with the moisture initial condition below the fibre saturation point (w_0=0.25) and temperature initial condition (T_0=293.15 K). During numerical calculations the dependencies of material coefficients on moisture and temperature were taken into account. The simulations were performed for wood species with an absolutely dry wood density ρ_0=0.4 g.cm^{-3} (corresponding to pinewood).

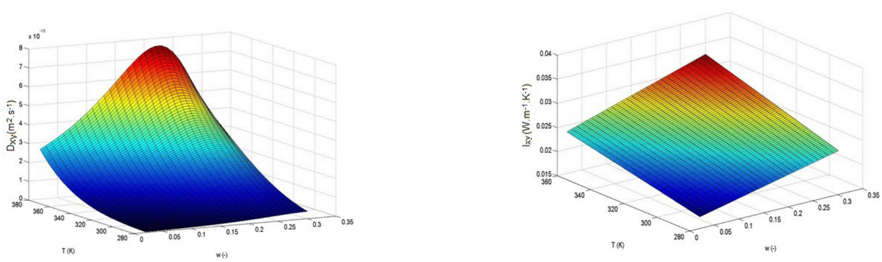

Fig. 2: Influence of temperature T and moisture w on a) diffusion coefficient D_{xy} and b) thermal conductivity coefficient l_{xy} (=λ_{xy}) with fibre lean as in Fig. 1.

Fig. 2a depicts the dependence of the diffusion coefficient D_{xy} on moisture and temperature. The coefficient and the other eight diffusion coefficients are the results of the above mentioned transformation of diffusion coefficients from anatomical to geometric directions. The pictured dependence is conditioned by the dependence of diffusion coefficients in anatomical directions on moisture and temperature according to Siau (1995).

Fig. 2b shows the dependence of the thermal conductivity coefficient l_{xy} on moisture and temperature. This coefficient is, as the diffusion coefficient, a result of the above mentioned transformation. The pictured dependence is conditioned by the dependence of thermal conductivity coefficients in anatomical directions on moisture and temperature according to MacLean (1941) and Siau (1995).

As for wood density, its dependence on moisture is considered according to Kollmann (1951) and the analytical formula for calculating of the specific heat was taken from Skaar (1972, 1988).

The numerical values used for the heat and mass transfer coefficient in the simulation of wood drying were discussed in Söderström and Salin (1993), Avramidis et al. (1994), Siau (1995) and Pang (1996) together with the correction coefficient introduced by Plumb et al. (1985) and Siau (1995). This work assumes the dependence of the mass transfer coefficient on moisture and temperature according to Avramidis et al. (1994).

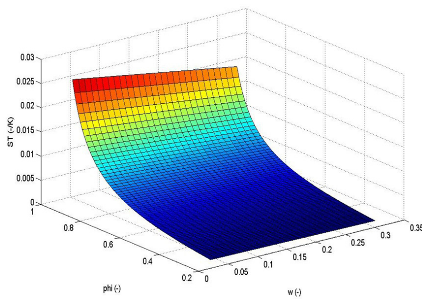

Fig. 3: Influence of wood moisture w and relative air humidity p_{hi} (=φ) on the Soret effect coefficient ST (=s).Y

The heat and moisture transfer should be considered as coupled processes: the thermally induced mass transfer, the Soret effect (Siau 1984, Avramidis et al. 1994) and the heat flux resulting from the moisture diffusion, the Duffour effect (Siau 1992), should all be taken into account. The Soret effect is displayed in Fig. 3 and we can see that both the temperature and moisture influence it. The Soret effect decreases with the increase in moisture and increases with the increase in temperature. There is a noticeable high dependence of the effect on the relative air humidity within the range of the relative air humidity from 0.6 to 1. The dependence of the Soret effect on the moisture of wood is smaller and linear. Luikov (1966), and in much details Whitaker (1977), developed a unique approach that describes the simultaneous heat and moisture transfer in drying processes, based on irreversible thermodynamic processes.

Fig. 4a shows that influence of the fibre lean (Fig. 1) on the drying speed is almost insignificant.

When comparing the simulated progess of moisture content at the beginning of drying, Fig. 4b shows that the Soret effect causes an increase in moisture content in the middle of the timber; Fig. 4c shows that it causes a faster drying of timber surface, which corresponds to the theory according to Siau (1984), Avramidis et al. (1994)

Fig. 5 displays the influence of the Soret effect on the moisture distribution within the body at the beginning of drying. We can see that from the very beginning of the drying process up to the time between 20000 s and 50000 s (about 10 hours) the effect of the temperature gradient on the moisture diffusion decreases and even vanishes.

Numerical solution of the model

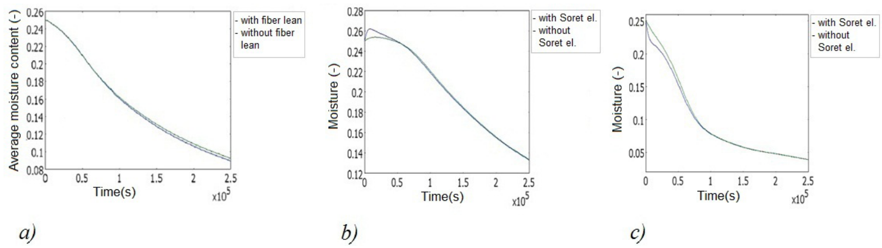

Fig. 4: a) The effect of fibre deviation on the progress of average moisture content; b) the Soret effect on the progress of moisture content in the medium part of timber; c) the Soret effect on the progress of moisture content in the surface of timber.

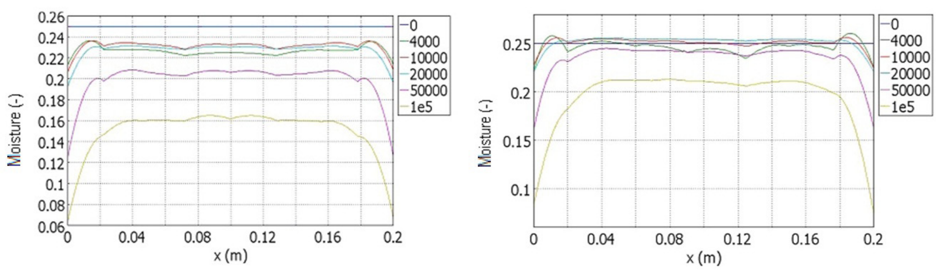

Fig. 5: Simulated moisture content profiles in the middle of the thickness (y=0.0225 m) and along the timber (along the x axis) in a) the surface plane (z=0) and b) the medium plane (z=2.5).

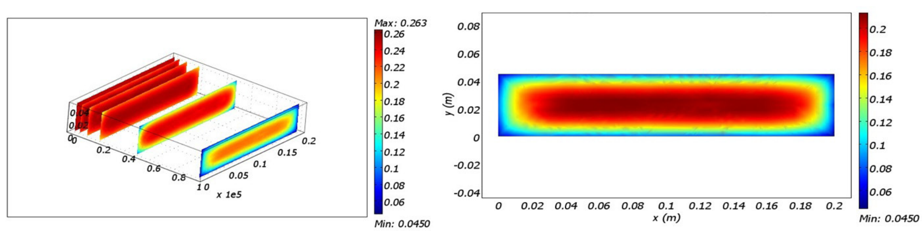

Fig. 6: Moisture distribution of cross section z=2.5 (in the middle of the length) a) for selected times in the range 0 to 100000 seconds (0 to 27.8 hours); b) in time 100000 seconds (27.8 hours).

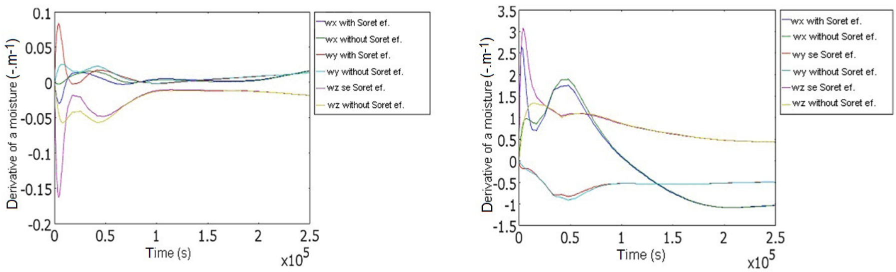

Fig. 7: Differentiations of moisture with respect to spatial variables in the middle of the wood body (0.1,0.0225,2.5) a) and at surface point (0.1,0.0225,0); b) with the Soret effect and without the Soret effect.

The graphs (Fig. 6) of moisture distribution during the drying process show that the wooden board is actually subjected to relatively high differences between the surface moisture and the inner moisture after vanishes the Soret effect.

The numerical results for the moisture gradient curves are displayed in Fig. 7. The largest gradients are at surface points at the beginning of the drying process. Thus the largest stresses (depending on the moisture gradients) are assumed at these points and times.

The predicted values by the assembled theoretical model are compared with norm data taken under actual drying conditions to show the difference between the predictive model and time drying schedules values.

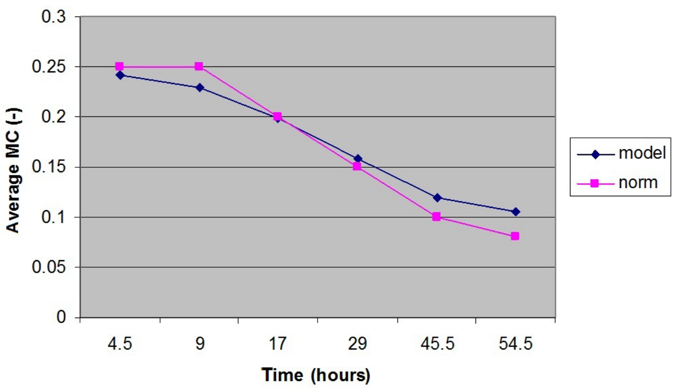

Fig. 8: The differences between simulated values of average moisture content (w) and the values stipulated by the norm (w_n).

Fig. 8 shows the prediction of the average moisture content simulated by the model together with norm values according to the drying schedule depicted in Tab. 1. The maximum difference between the values does not exceed 2.5 % of moisture content. At the beginning of the drying process the model predicts a higher drying speed than the norm features. Next, the trend reverts and the model drying speed is smaller and after about 17 hour of drying process the curves intersect. At the end of drying the model predicts average MC of 10.5 % and the norm features desired 8 % of average MC.

CONCLUSION

A mathematical model describing the coupled heat and moisture transfer in a wood body during the drying process was assembled and solved. The transformation relations between matrixes of material coefficients (diffusion and thermal conductivity coefficients) in anatomical and geometrical directions in three-dimensional case were developed. There were respected the dependencies of material coefficients on temperature and moisture. The numerical solution of the model was performed because an analytical solution to the mentioned coupled unsteady-state nonisothermal diffusion phenomena is difficult to find. This model can be used to predict the distribution of both moisture and temperature fields in the hygroscopic moisture content and below 100°C temperature ranges for single boards as well as stacked lumber.

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