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Comparison of different models for the high-temperature heat-treatment of wood

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Abstract

The high temperature thermal treatment of wood is an environment-friendly method for wood preservation. This technique has attracted considerable attention in recent years. The GRTB (groupe de recherche sur la thermotransformation du bois) at the University of Quebec at Chicoutimi, Canada, has been working on this subject for the past number of years. In this article, the work is presented with a focus on the mathematical modelling of the process.

Three models (model based on Luikov's approach, diffusion model, and multiphase model) have been developed for the high temperature treatment of wood. The predictions of the models are compared with the experimental data. The diffusion model was found to be the most practical approach when the accuracy of the results and the computation times are both taken into account.

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Keywords: Mathematical modelling of wood thermal treatment; High temperature wood treatment; Thermotransformation of wood; Luikov's approach; Diffusion model; Multiphase model

1. Introduction

Wood preservation is mostly carried out by chemical treatment using different chemicals such as tar oil based chemicals (creosote, pentachloro-phenol) and chromated copper arsenate (CCA). These chemicals contain components that are poisonous for the environment and human health. The American and Canadian wood manufacturers started to decrease gradually the amount of chemicals used in wood treatment and are looking for alternative ways of wood preservation. The thermal treatment of wood at high temperatures seems to be a viable alternative. In this process, wood is heated to temperatures above 200 °C which changes the structure of wood. Hemicelluloses start to decompose, lignin softens, and cellulose is modified; consequently, the hydrophilic groups are modified [1,2]. As a result, wood subjected to high temperatures loses its capacity to reabsorb water contrary to the hydrophilic behavior

of the conventionally dried wood. Therefore, its hardness increases and it becomes dimensionally more stable compared to untreated wood. Hemicelluloses and cellulose are the main nutrients for fungi. Due to the lack of water and nutrients, heat-treated wood becomes more resistant to biological attacks. Its color also becomes darker and more attractive. However, this treatment might cause a decrease in wood elasticity due to the modification of long chain molecules. Therefore, optimization of the treatment parameters is necessary for a quality product [3].

The high temperature heat treatment technology for wood has recently attracted a lot of interest in North America, particularly in Saguenay–Lac–St-Jean, the principal forest region of Quebec, Canada. However, the transformation of its forest products is limited to first transformation (pulp, paper, and timber industries). To generate new products from its forest resources, this region decided to develop the second and third transformations of wood by which finished products such as floor coverings, sidings, kitchen cabinets, other furniture, windows, and doors are produced. The heat treatment of wood at

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| No | Nomenclature | | | | | |
|----------------------------|--|---------------|--|--|--|--|
| c_m | moisture capacity $kg_{(moisture)} kg_{(dry wood)}^{-1} {}^{\circ}M^{-1}$ | U | moisture potential °M | | | |
| c_q | heat capacity $J kg^{-1} K^{-1}$ | Greek | letters | | | |
| Ĉ | moisture concentration $kg_{(moisture)} kg_{(dry wood)}^{-1}$ | | $\mathbf{w} = -2\mathbf{v} - 1$ | | | |
| D | diffusion coefficient m ² s ⁻¹ | α_q | convective heat transfer coefficient W m ⁻² K ⁻¹ convective mass transfer coefficient: | | | |
| D_v | vapor diffusion coefficient | α_m | in Luikov model $kg_{(moisture)} m^{-2} s^{-1} \circ M^{-1}$ | | | |
| D_{bt} | transverse bound water diffusion | | in diffusion and multiphase models $m^2 s^{-1}$ | | | |
| | coefficient | ρ | density kg m ⁻³ | | | |
| G_m | specific gravity | ε | ratio of vapor diffusion coefficient to coefficient of | | | |
| h | enthalpy Jkg ⁻¹ | | total moisture diffusion | | | |
| J | spatial directions, x , y , z | δ | thermal gradient coefficient $kg_{(moisture)} kg^{-1} K^{-1}$ | | | |
| $oldsymbol{J} k_q$ | vector of total moisture flux $kg m^{-2} s^{-1}$ thermal conductivity $W m^{-1} K^{-1}$ | μ | dynamic viscosity $kg m^{-1} s^{-1}$ | | | |
| k_q | moisture conductivity . $kg_{(moisture)} m^{-1} s^{-1} {}^{\circ}M^{-1}$ | μ_b | chemical potential for bound water | | | |
| K_l | Permeability kg N^{-1} s^{-1} | λ | latent heat of vaporization $J kg^{-1}$ | | | |
| M | moisture content $kg_{\text{(moisture)}} kg_{\text{(dry wood)}}^{-1}$ | ν_a | porosity | | | |
| m_v | molar mass kg mole ⁻¹ | φ | relative humidity | | | |
| n | normal | Subscripts | | | | |
| Nu | Nusselt number | 0 | initial | | | |
| P | partial water vapor pressure in wood Pa | a | air (or gas) | | | |
| P_{c} | capillary pressure in wood Pa | b | bound water | | | |
| $P_{\scriptscriptstyle S}$ | saturation pressure Pa | d | dry wood | | | |
| $P_{ m sv}$ | saturation water vapor pressure in wood Pa | eff | effective | | | |
| Pr | Prandtl number | eq | equilibrium | | | |
| Re | Reynolds number | f | free water | | | |
| R | ideal gas constant J mole ⁻¹ K ⁻¹ | final | final | | | |
| Sc Sh | Schmidt number Sherwood number | fsp | fiber saturation points | | | |
| sn t | times | $_{l}^{g}$ | gas liquid | | | |
| T | time | ı m | mixture | | | |
| u | specific internal energy | v | vapor | | | |

high temperatures is considered as an important part of these transformations. Since this technology is first developed in Europe, the processes developed for European species have to be modified for North American species.

Wood is a highly heterogeneous and anisotropic material. The properties change not only from one species to another or from one region of origin to another for the same species, but also in different directions in a given piece of wood. Therefore, an adaptation of the technology is required for each species. This is a very costly procedure at the industrial scale. The GRTB has developed a procedure for such an adaptation. This is the first North American university which has an industrial treatment furnace, a prototype treatment furnace, and a small laboratory furnace at its disposal for research purposes. The adaptation starts in the laboratory where small wood samples are treated in a thermogravimetric system under different conditions, and the properties of the treated samples are measured. Consequently, the trends are identified for a given species [4,5]. The promising treatment procedures are then tried in the prototype furnace to narrow down the options. The last step is the testing of the most favorable ones in the industrial furnace to finalize the recipe.

The mathematical modelling is an important tool for adaptation. A reliable and predictive furnace model can be used to determine the results of the subsequent treatments; and this decreases the cost of adaptation procedure substantially. Such a global model, however, requires an accurate representation of the important phenomena occurring not only in the gas surrounding the wood, but also in the wood itself. In addition, these two parts of the model have to be coupled through an appropriate interphase. For this global furnace model to be manageable in terms of memory and computation time, the models for gas and wood have to be reasonably fast and should not require a large memory. This article focuses on the modelling of the phenomena occurring in the wood and compares three hightemperature wood heat-treatment models. Their predictions are compared with the experimental data and with each other. Also, considering the accuracy of the predictions, the computation times, and the memory requirements, the most suitable model for the heat-treatment furnace modelling is identified.

2. Mathematical models

During treatment, simultaneous heat and mass transfer takes place. Wood is usually heated by a hot gas. The heat is transferred from the gas to the surface of the wood mainly by convection and to the interior by conduction. The heat transfer is very slow within the wood since wood has a very low thermal conductivity. As the heat is transferred within the wood, the moisture present in wood is heated, partially evaporated, and transferred to the surface; subsequently, it is removed by the gas. Moisture in wood can exist in different forms such as free water, bound water or water vapor during treatment. In the literature, there are various models reported for the conventional drying process, but very few are available for the thermal treatment of wood at high temperature [6-10]. Three different models have been used to represent the thermal treatment process, which predict the temperature and moisture distributions in wood as a function of time. The predictions of the models are compared with the experimental data from the laboratory experiments. The three models considered are:

- (a) Model based on Luikov's approach
- (b) Diffusion model
- (c) Multiphase model

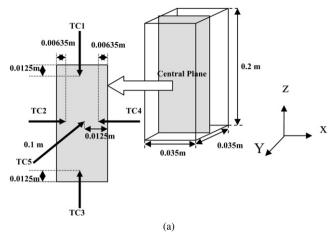
In all of these models, constant or variable properties (as a function of temperature and moisture content) can be used. However, the properties used in this study are obtained from the literature. The thermophysical properties used by all three models were taken identical, and these are shown in Table 1. The equations of the model based on Luikov's approach and the multiphase model are solved with the commercial software FEMLAB [11] which uses the finite element approach. The diffusion model equations are solved based on the finite difference approach.

2.1. Model based on Luikov's approach

In this model, wood is represented as a capillary porous medium based on Luikov's approach [6–8]. The wood was assumed to be homogeneous and isotropic with initially uniform temperature and moisture distribution. The effect of gravity and all the mechanical deformations of wood and chemical reactions are neglected. The model solves the simultaneous, 3D,

Table 1 Thermophysical parameters used in models

| Parameter | Unit | Value |
|---------------------|--------------------------------|----------------------|
| ρ | ${\rm kg}{\rm m}^{-3}$ | 660 |
| c_q | $\rm Jkg^{-1}K$ | 1884 |
| $k_z = 2k_x = 2k_y$ | ${ m W}{ m m}^{-1}{ m K}^{-1}$ | 0.18 |
| α_q | ${ m W}{ m m}^{-2}{ m K}^{-1}$ | 15 |
| α_m | ${ m Ms^{-1}}$ | 1.6×10^{-5} |
| M_0 | $\% (kg kg^{-1})$ | 7–25 |
| T_0 | K | 298 |
| λ | $\rm Jkg^{-1}$ | 2.5×10^{6} |



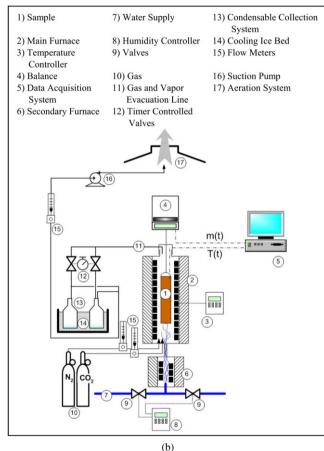


Fig. 1. Schematic view of thermogravimetric analyzer: (a) Sample; (b) Experimental system.

unsteady-state heat and mass transfer equations together with the initial and boundary conditions given below:

Equations

Heat transfer:

$$\rho c_q \frac{\partial T}{\partial t} = \vec{\nabla} \cdot \left[\left(k_q + \frac{\varepsilon \lambda k_m \delta}{c_m} \right) \vec{\nabla} T + \varepsilon \lambda k_m \vec{\nabla} U \right] \tag{1}$$

Mass transfer:

$$\rho c_m \frac{\partial U}{\partial t} = \vec{\nabla} \cdot \left[\left(\frac{k_m \delta}{c_m} \right) \vec{\nabla} T + k_m \vec{\nabla} U \right]$$
 (2)

Boundary conditions

Heat transfer:

$$-k_q \frac{\partial T}{\partial j} = \alpha_q (T - T_g) + (1 - \varepsilon) \lambda \alpha_m (U - U_g)$$
 (3)

at the surfaces

Mass transfer:

$$-k_m \frac{\partial U}{\partial j} = \left(\frac{k_m \delta}{c_m}\right) \frac{\partial T}{\partial n} + \alpha_m (U - U_g) \tag{4}$$

at the surfaces

Initial conditions

Heat transfer:

$$T = T_0 \quad \text{at } t = 0 \tag{5}$$

Mass transfer:

$$U = U_0 \quad \text{at } t = 0 \tag{6}$$

In the above equations, U is the moisture potential of wood in $^{\circ}$ M defined by Luikov and given by the following equation:

$$C = c_m U \tag{7}$$

The thermophysical properties are obtained from the literature [12]. The thermal conductivity in the axial direction is taken as twice the radial and tangential thermal conductivities [13]. The heat transfer and mass transfer coefficients are calculated using the empirical relations reported in the literature [14,15]:

$$Sh = \frac{h_m L}{D} = 0.664 Re^{0.5} Sc^{0.33}$$

$$Nu = \frac{hL}{k_q} = 0.664 Re^{0.5} Pr^{0.33}$$
(8)

The equations are solved using the FEMLAB software based on the finite element technique. A grid independent solution is ensured by comparing the result of different grid meshes (see Fig. 2(a)). Simulations were carried out using three grids with 3182, 6580 and 8394 elements. The predictions did not vary significantly. The rest of the simulations were carried out with a grid of 1466 nodes and 6580 elements. The time step was 360 s. In the simulations, the computation time for a typical run was 16 minutes. The details of the model are given elsewhere [16,17]. The thermophysical properties and parameters of the model used in the simulations are shown in Tables 1 and 2.

2.2. Diffusion model

In the diffusion model, it is assumed that the mass transfer in wood takes place only by diffusion, and the coupled heat and

Table 2
Parameters of the model based on Luikov's approach

| Unit | Value |
|---|---|
| kg _{moisture} kg ^{−1} K ^{−1} | 0.025 |
| _ | 0.3 |
| $kg_{moisture} m^{-1} s^{-1} M^{-1}$ | 1.8×10^{-8} |
| $kg_{moisture} kg^{-1} M^{-1}$ | 0.01 |
| | kg _{moisture} kg ⁻¹ K ⁻¹ |

mass transfer equations are solved. The equations describing the 3D heat and moisture transfer in wood during heat treatment are given as follows [18,19]:

Equations

Heat transfer:

$$\rho_m \frac{\partial h_m}{\partial t} = \vec{\nabla} \cdot [k_q \vec{\nabla} T] \tag{9}$$

Mass transfer:

$$\frac{\partial M}{\partial t} = \vec{\nabla} \cdot [D\vec{\nabla}M] \tag{10}$$

Boundary conditions

Heat transfer:

$$-k_q \frac{\partial T}{\partial j} = \alpha_q (T - T_g) + \alpha_m \lambda (M - M_g)$$
 (11)

at the surfaces

Mass transfer:

$$-D\frac{\partial M}{\partial j} = \alpha_m (M - M_g) \tag{12}$$

at the surfaces where j is the spatial direction (x, y, z).

Initial conditions

Heat transfer:

$$T = T_0 \quad \text{at } t = 0 \tag{13}$$

Mass transfer:

$$M = M_0 \quad \text{at } t = 0 \tag{14}$$

There are two type of diffusion occurring in wood [15]. The diffusion of water vapor through air in the cell lumens (inter gas diffusion) and the diffusion of water within the cell wall of wood (bound water diffusion). In this study, both types of diffusion are taken into account.

The diffusion coefficient D depends on the temperature and moisture content. As suggested by Baronas et al. [18], this coefficient is expressed as a function of instantaneous wood moisture content below the fiber saturation point. When the wood moisture content is higher than its value at the fiber saturation point $(M_{\rm fsp})$, the diffusivity is only a function of this value as shown below and given in Table 3:

$$D = \begin{cases} f(M, T) & \text{if } M < M_{\text{fsp}} \\ f(M_{\text{fsp}}, T) & \text{if } M \geqslant M_{\text{fsp}} \end{cases}$$
 (15)

The diffusion coefficient D can be expressed by, the transverse bound water diffusion coefficient $D_{\rm bt}$ of wood, the vapour diffusion coefficient D_v in the lumens and the porosity of wood v_a (Table 3) [18].

A computer program was written using FORTRAN to solve the finite difference equations. The solution of the matrix at each step is obtained using the Gauss–Seidel iterative method. A mesh consisting of $20 \times 20 \times 30$ elements with a time step of 360 s were used for all the subsequent computations considering both accuracy and computation time (see Fig. 2(b)). The time necessary for a typical run is 4 minutes. Table 3 gives the parameters of the model used in the simulations.

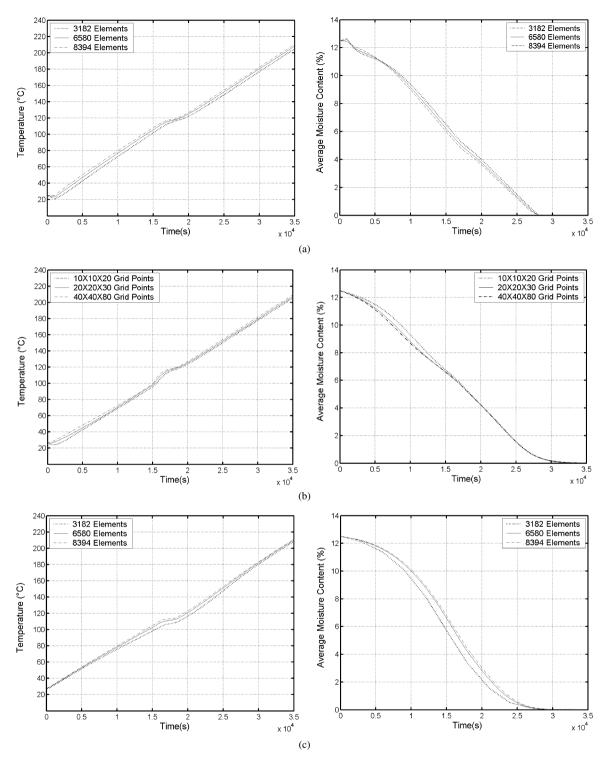


Fig. 2. Grid independence test: Temperature and average moisture content evolutions for different grid size $(T_{g,\text{final}} = 220 \,^{\circ}\text{C})$, heating rate $20 \,^{\circ}\text{C} \,^{-1}$, $M_0 = 12.50\%$): (a) Diffusion model; (b) Luikov's approach; (c) Multiphase model.

2.3. Multiphase model

This model is based on the approaches proposed by Whitaker [8], Bear [9], Hassanizadeh and Gray [10]. All the phases present (free water, bound water, water vapor, wood) and their possible transfer mechanisms are represented in the solution of simultaneous heat and mass transfer equations. It was as-

sumed that the wood is porous, the enthalpies of all phases are linear functions of temperature, Darcy's law represents the transport of free water in wood and the bound water transfer takes place due to chemical potential gradient. The mechanical deformations of wood, gravity effects, and chemical reactions are neglected. A mesh consisting of 1466 nodes and 6580 elements were used in the simulations for a grid-independent

Table 3
Parameters of the diffusion model

| Property | Reference | Expression |
|---|-----------|---|
| M_{fsp} | (15) | $M_{\rm fsp} = 0.57315 - 0.001T$ |
| Gm | (12) | 0.66 |
| v_a | (15) | $v_a = 1 - G_m(0.667 + M)$ |
| $D [\mathrm{m}^2 \mathrm{s}^{-1}]$ | (15) | $D = \frac{\sqrt{\nu_a} D_{bt} D_v}{(1 - \nu_a)(\sqrt{\nu_a} D_{bt} + (1 - \sqrt{\nu_a}) D_v)}$ |
| $D_v [{\rm m}^2 {\rm s}^{-1}]$ | (15) | $D_v = \frac{1.29.10^{-13}(1.0+1.54M)p_sT_K^{1.5}}{(T_K+245.18)} \cdot \frac{d\varphi}{dM}$ |
| $D_{\rm bt} [{\rm m}^2 {\rm s}^{-1}]$ | (15) | $D_{\rm bt} = \exp(-9.9 + 9.8M - 4300/T_K)$ |
| p_s [Pa] | (15) | $p_s = 3390 \cdot \exp(-1.74 + 0.0759T_C)$ |
| | | $-0.000424T_C^2 + 2.44 \times 10^{-6}T_C^3$ |
| h_l [J kg ⁻¹] | | 419 000 |
| h_g [J kg ⁻¹] | | 2 676 000 |
| $c_{\rm ql}$ [J kg ⁻¹ K] | | 4185 |
| $c_{\rm qg}$ [J kg ⁻¹ K] | | 2000 |

solution (see Fig. 2(c)). The time step was taken as 500 s. The computation time for a typical run is 25 minutes. The equations are solved with FEMLAB software. Details of the model are given elsewhere [20].

Equations

Heat transfer:

$$\frac{\partial}{\partial t}(\rho_a u_a + \rho_v u_v + \rho_b u_b + \rho_f u_f + \rho_d u_d) + \nabla \cdot (\mathbf{J}_a h_a + \mathbf{J}_v h_v + \mathbf{J}_b h_b + \mathbf{J}_f h_f) = \nabla (k_a \nabla T)$$
(16)

Mass transfer:

$$-\rho \frac{\partial M}{\partial t} = \nabla \cdot \mathbf{J} = \frac{\partial J_x}{\partial x} + \frac{\partial J_y}{\partial y} + \frac{\partial J_z}{\partial z}$$
 (17)

In the above equations, ρ , u, h, k are the density, specific internal energy, specific enthalpy, and thermal conductivity, respectively. The subscripts "a", "v", "b", "f", "d" represent air (or gas), water vapor, bound water, free water, and dry wood, respectively. **J** is the total mass flux vector, ρ is the dry wood density, M is the water moisture content per unit mass of dry wood

If \mathbf{J}_v , \mathbf{J}_b , and \mathbf{J}_f are the fluxes of moisture of water vapor, bound water, and free water, respectively, the total mass flux is given by:

$$\mathbf{J} = \mathbf{J}_v + \mathbf{J}_b + \mathbf{J}_f \tag{18}$$

The vapor flux can be determined as follows using Fick's law:

$$\mathbf{J}_{v} = -\frac{m_{v} \cdot D_{\text{eff}}}{R \cdot T} \cdot \nabla P_{v} \tag{19}$$

Equation suggested by Stanish et al. [21] is used to determine the bound water flux as follows:

$$\mathbf{J}_{b} = -\frac{D_{b}}{m_{v}} \cdot \left\{ -\left[187 + 35.1 \ln\left(\frac{T}{298.15}\right) - 8.314 \ln\left(\frac{P_{v}}{101325}\right)\right] \nabla T + 8.314 \frac{T}{P_{v}} \nabla P_{v} \right\}$$
(20)

Liquid water flux is given by Darcy's law at moisture contents higher than the Fiber Saturation Point (FSP) as shown below:

$$\mathbf{J}_f = -\frac{K_l \rho_l}{\mu_l} \nabla P_l = -\frac{K_l \rho_l}{\mu_l} \nabla P_c \tag{21}$$

 m_v is the molar mass of vapor, R the ideal gas constant, P_v is the partial vapor pressure of water which is calculated using the correlation given by Moyne [22], D_b is the diffusion coefficient of bound water is given by Siau [14], P_c is the capillary pressure given by Spolek and Plumb [23], ρ_l and μ_l are the density and viscosity of the liquid water, and K_l is the permeability.

Boundary conditions

Heat transfer:

$$[k_{\text{eff}} \nabla T] \cdot \vec{n} = \alpha_a (T - T_e) + \lambda J_n \tag{22}$$

Mass transfer:

$$J_n = \alpha_m \rho_v (M - M_{\rm eq}) \tag{23}$$

Initial conditions

Heat transfer:

$$T = T_0 \tag{24}$$

Mass transfer:

$$M = M_0 \tag{25}$$

 $k_{\rm eff}$ is the effective thermal conductivity, λ is the latent heat of vaporization, α_q is the heat transfer coefficient. The values of convective mass and heat transfer coefficients (α_m and α_q) at each point on the surfaces are calculated using the expressions given in literature [14]. ρ_v is the water vapour density, and $M_{\rm eq}$ is the equilibrium moisture content obtained from the Hailwood–Horrobin equation adopted for wood by Simpson and Tenwold [12]. The values of convective mass and heat transfer coefficients (α_m and α_q) at each point on the surfaces are found from Eq. (8).

3. Experimental system

In order to compare with the model predictions, experiments were carried out in a thermogravimetric analyzer using white birch as shown in Fig. 1. Wood samples with dimensions of $0.035~\text{m}\times0.035~\text{m}\times0.2~\text{m}$ were heat-treated. The samples were suspended from a balance (Mettler Toledo AG285) with an accuracy of $\pm0.001g$ into the tube furnace. The data were collected using an automatic data acquisition system (Keithley 2700). The experiments were carried out under an inert gas atmosphere. The experimental parameters studied were the maximum treatment temperature and the heating rate. The initial moisture content of the wood samples was measured before each experiment using a wood moisture meter (Delmhorst RDM-2S) which has an accuracy of 0.1% moisture content.

The samples are first heated to about 120 °C and kept there for half an hour in order to reduce the moisture content. Then they are heated at a desired heating rate until the maximum treatment temperature is reached. The weight change of the

samples and the temperatures at predetermined positions are followed during two series of experiments. From the weight change data, the average moisture loss of the sample as a function of time is obtained. The models give the moisture and temperature distribution within the sample. An average overall moisture content of the sample is calculated from the moisture distribution in order to compare with the experimental data. During this study, the emission of organic volatiles and byproducts produced by the exothermic reactions taking place at high temperatures are neglected. Although five T-type thermocouples (Copper-Constantan) which were connected to the data acquisition system are placed in the sample (see Fig. 1(a)). The accuracy of the thermocouples is ± 1 °C (Omega Engineering, 2003). The comparison between the measured temperatures by thermocouple 2 (TC2) and the temperatures predicted by the model at the same position is presented to simplify the figures.

4. Results and discussion

The temperatures as a function of time at thermocouple position 2 (TC2) and the evolution of the average moisture content of the white birch sample were compared with the predictions of the three models, namely model based on Luikov's approach, diffusion model and multiphase model. Then, a parametric study was carried out. The average moisture contents and the temperatures predicted by the models using different heating rates and different initial wood moisture contents were compared. The moisture content and temperature profiles within the wood predicted at different times by the three models are also presented.

4.1. Comparison of model predictions with experimental data

Figs. 3 and 4 compare the model predictions with the experimental data for heating rates of $20\,^{\circ}\text{C}\,h^{-1}$ and $30\,^{\circ}\text{C}\,h^{-1}$, respectively. As it can be seen from the figures, the initial moisture contents of the samples are slightly different (12.5% at $20\,^{\circ}\text{C}\,h^{-1}$ heating rate and 11% at $30\,^{\circ}\text{C}\,h^{-1}$ heating rate). These are the measured moisture contents of the wood samples used.

For the average moisture content, the model predictions cross over the data at both heating rates (see Figs. 3(a) and 4(a)). At $20\,^{\circ}\text{C}\,\text{h}^{-1}$ heating rate, the predictions of the model based on Luikov's approach are closest to the experimental data at the earlier times whereas the diffusion model underpredicts and the multiphase model overpredicts the data in this range. At later times, the multiphase model predictions are the closest to the data and the other two models overpredict the data. This trend continues until two thirds of the experiment duration. Then, the difference increases. Towards the end of the experiment, the diffusion model's predictions are the most accurate. At $30\,^{\circ}\text{C}\,\text{h}^{-1}$ heating rate, the multiphase model predictions follow the experimental data closely at all times. The other two models underpredict the data at earlier times and overpredict at later times.

The comparison of the temperatures predicted by the three models with the experimentally measured temperatures at the thermocouple position 2 (see Figs. 3(b) and 4(b)) shows that the

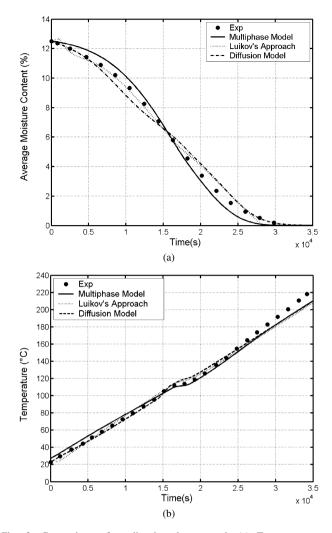


Fig. 3. Comparison of predicted and measured: (a) Temperature evolution, (b) Average moisture content evolution during heat treatment $(T_{g, \text{final}} = 220 \,^{\circ}\text{C}$, heating rate $20 \,^{\circ}\text{C} \, \text{h}^{-1}$, $M_0 = 12.50\%$).

multiphase model overpredicts the data at earlier times whereas it underpredicts at later times. The diffusion model results follow the data very closely until the very late stages of the experiment. At intermediate times the multiphase model predictions are closest to the data. The predictions of the model based on Luikov's approach and the diffusion models are almost identical at $20\,^{\circ}\text{C}\,h^{-1}$ heating rate; but, at the higher heating rate, the model based on the Luikov's approach gives higher values compared to those of the two other model. However, the predictions of all three models are very close.

As it can be seen from this comparison, it is difficult to choose a model which gives the closest predictions when compared with the experimental data. It is clear that the multiphase model is the most fundamentally complete model which takes into account all the phenomena taking place and all the different phases of water present during the wood heat treatment. However, this model requires more parameters which are difficult to determine as input to the model, and it takes longer computation times when compared to the other two models. On the other hand, the diffusion model needs the least number of model parameters and the minimum computation time (16 min

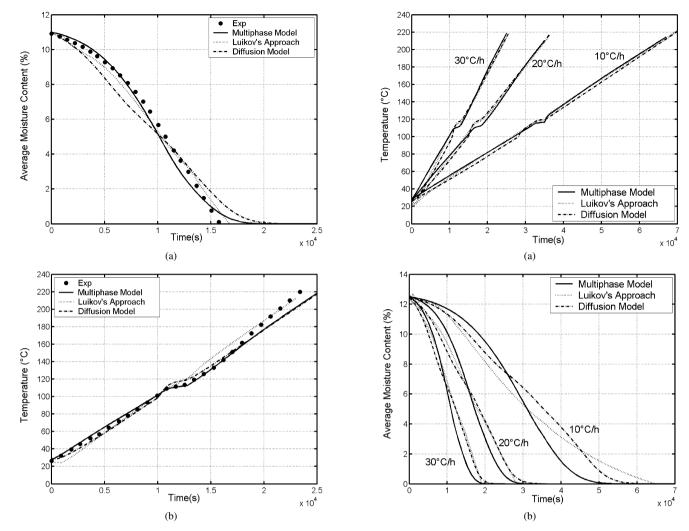


Fig. 4. Comparison of predicted and measured: (a) Temperature evolution; (b) Average moisture content evolution during heat treatment $(T_{e, \text{final}} = 220 \,^{\circ}\text{C}$, heating rate $30 \,^{\circ}\text{C} \, \text{h}^{-1}$, $M_0 = 11\%$).

Fig. 5. Predicted (a) temperature and (b) average moisture content evolutions during heat treatment at different heating rates ($M_0=12.5\%$, $T_{g,\rm final}=220\,^{\circ}{\rm C}$).

for Luikov's approach, 4 min for diffusion model and 25 min for multiphase model for a typical run) and its predictions are reasonably close to the data. As discussed previously, this aspect is very important when a model which represents the heat and mass transfer taking place in wood has to be incorporated into a global furnace model to simulate the entire heat-treatment process. In addition to wood, the global model has to account for the heat and mass transfer taking place in the gas as well as the interphase between the gas and the wood. Furthermore, it has to represent the furnace geometry reasonably well which may result in high number of nodes for the numerical solution. Therefore, a wood model which does not require a high computation time but still can predict the temperature and moisture profiles reasonably well will reduce the computation time of the global furnace model substantially.

4.2. Parametric study

A parametric study was carried out to investigate the effects of the heating rate and the initial moisture content on the temperature and overall moisture content of wood with all three models. In addition, the evolution of temperature and moisture content profiles within wood samples predicted by all three models are presented and compared.

(a) Effect of heating rate

Fig. 5(a) shows the temperatures (at thermocouple position 2) predicted by the models at three different heating rates and Fig. 5(b) presents the overall moisture contents predicted by these models under the same conditions. Very similar trends are observed when the predicted temperatures by the three models at other thermocouple positions are compared. The slight discrepancies between these results and the results shown in Fig. 4 are due to the difference in the initial moisture content of the wood samples.

Fig. 5(b) shows that the difference between the overall moisture contents predicted by different models increases with the decreasing heating rate. The multiphase model predictions are higher at earlier times and lower at later times than those of the other two models. At high and intermediate heating rates, the

model based on the Luikov's approach and the diffusion model give similar results although the predictions of the models cross each other. At the lowest heating rate, the diffusion model predictions are higher compared to those of the model based on the

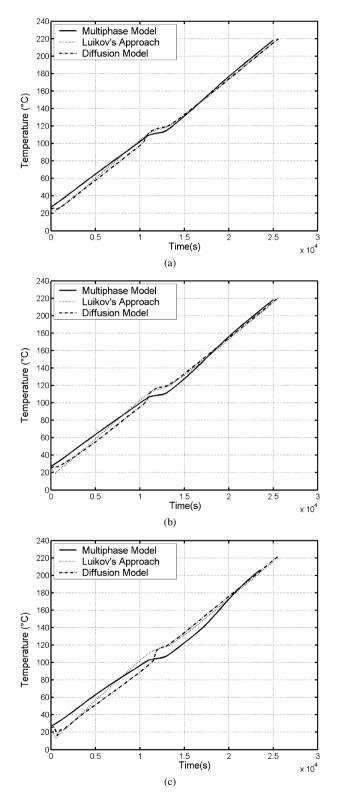


Fig. 6. Predicted temperature evolution during heat treatment with different initial moisture contents: (a) $M_0=10\%$; (b) $M_0=15\%$; (c) $M_0=25\%$ ($T_{e,\mathrm{final}}=230\,^{\circ}\mathrm{C}$, heating rate $30\,^{\circ}\mathrm{C}\,\mathrm{h}^{-1}$).

Luikov's approach except for a short period towards the end of the treatment.

(b) Effect of initial moisture content of wood

The temperatures with respect to time for three initial wood moisture contents (10%, 15%, 25%) predicted by three models are presented in Fig. 6. Although the predicted temperatures are very close, the difference between them increases with increasing initial wood moisture content.

Similarly, Fig. 7 shows the predicted average moisture content of the wood sample with respect to time predicted by the three models for different initial wood moisture contents. Again the differences between the predictions of the models become more significant with increasing initial moisture content.

(c) Moisture content and temperature profiles within the sample

The temperature and moisture content profiles predicted at different times by the three models in the midsection of central plane are shown in Fig. 8. The initial temperature and moisture content distributions are assumed to be uniform in the simulations.

The predicted temperature profiles are similar (see Fig. 8(b)). The temperature difference between the center and the surface of the sample is more pronounced in the predictions of the multiphase model at the intermediate times. At initial and final stages of the treatment, the temperatures predicted by the multiphase model are slightly higher than the other two models. At very early times, the diffusion model predicts slightly higher temperatures than the model based on Luikov's approach. At intermediate and later times, this trend is reversed.

The model based on Luikov's approach gives a flat profile in the center of the sample at earlier times (see Fig. 8(b)). This model predicts the highest difference between the center and

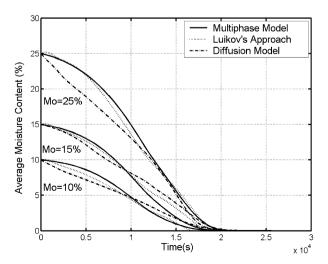
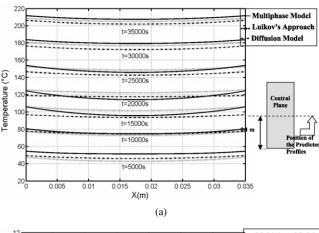


Fig. 7. Predicted average moisture content evolution during heat treatment with different initial moisture contents: (a) $M_0=10\%$; (b) $M_0=15\%$; (c) $M_0=25\%$ ($T_{g,\mathrm{final}}=230\,^{\circ}\mathrm{C}$, heating rate $30\,^{\circ}\mathrm{C}\,\mathrm{h}^{-1}$).



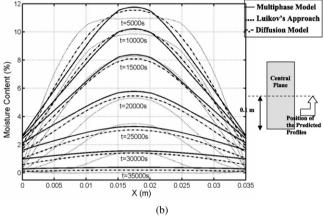


Fig. 8. Spatial profiles of (a) temperature and (b) moisture content during heat treatment ($T_{g,\text{final}} = 220 \,^{\circ}\text{C}$, heating rate $20 \,^{\circ}\text{C} \, \text{h}^{-1}$, $M_0 = 12.5\%$).

the surface resulting in a sharp moisture content gradient at all times. Predictions of the multiphase and the diffusion models are found very similar at all times.

5. Conclusions

Difficulty for all models is essentially to find the right wood properties, coefficients describing the heat and mass transfer as well as their dependence on temperature and moisture content and direction in space since wood is anisotropic. The diffusion model requires the less number of constants and shortest computation time when compared to other two models. The predictions of diffusion model seem to be reasonably similar to that of the multiphase model which is the most fundamentally sound model. Therefore, this model is very suitable to be used with treatment furnace modelling which is already costly in terms of time and computer memory. Utilization of a simple model which still represents the behavior of wood during treatment accurately is very important for treatment furnace modelling. In addition, the predictions of the diffusion model can be further improved if a better diffusivity data as a function of temperature and wood moisture content is available for the species found in North America.

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