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ORIGINAL ARTICLE

One-dimensional numerical solution of the diffusion equation to describe wood drying: comparison with two- and three-dimensional solutions

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Abstract This article describes drying of wood cut into parallelepiped shaped pieces. A one-dimensional numerical solution of the diffusion equation with boundary condition of the third kind was proposed to describe the process. The lumber was cut into the following dimensions: thickness $T = 36$ mm, height $H = 100$ mm and length $L = 745$ mm. The convective drying experiment was carried out with forced air at temperature of 40 °C, relative humidity of 40 % and velocity of 3 m s^{-1}. An optimizer was coupled with the proposed numerical solution to determine the process parameters. Comparison of the results obtained in this article (one-dimensional) with results from the literature (two- and three-dimensional) indicated good agreement between the process parameters (and also simulations). However, the optimization time for one-dimensional model is about 15 times less than the optimization time for the two-dimensional case.

Keywords Numerical simulation · Variable diffusivity · Finite volume · Optimization · Lumber

List of symbols

A, B, a, b	Coefficients of the discretized diffusion equation or fitting parameters
D	Effective mass diffusivity (m^2 s^{-1})
H	Height of the lumber (m)
L	Length of the lumber (m)
M	Local moisture content at the instant t (kg$_{\text{water}}$ kg$^{-1}_{\text{drymatter}}$)
$\overline{M}$	Average moisture content at instant t (kg$_{\text{water}}$ kg$^{-1}_{\text{drymatter}}$)
N_p	Number of experimental points (dimensionless)
N	Number of control volumes (dimensionless)
R^2	Coefficient of determination (dimensionless)
T	Thickness of the lumber (m)
t	Time (s)
Δx	Thickness of a control volume (m)
σ_i	Standard deviation of the experimental point i (dimensionless)
χ^2	Chi square or objective function (dimensionless)

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Introduction

In several industrial sectors, several production processes involve a stage in which water is transferred to or removed from the products during their manufacture. Among these production processes, it can be cited those referring to the industry of ceramic materials, pharmaceutical products, foodstuff and wood. For wood, the main operation of water removal is the drying process and, nowadays, the main technique is the use of hot air at given velocity. According to Dincer [1], drying is one of the most important stages in the processing of wood, having an important influence on the quality of the final product. Thus, understanding this process of water removal allows to obtain a dry product with superior quality. In this sense, a mathematical model is usually used to describe wood drying. The more accurate information can be extracted from the model used to describe the process, the better model could be considered. In the literature, one of models used to describe drying of products is that which describes the water migration by diffusion. Diffusion models are used to describe many types of processing such as cooling [2, 3], heating [4], osmotic dehydration [5], and drying of porous materials [6]. In particular, several works are available in the literature involving diffusion models in the description of wood drying [1, 7–15]. According to Silva et al. [14], an advantage of diffusion models when compared, for example, with empirical models, is the possibility to determine the moisture distribution within the wood at any instant during drying. This information is essential to identify regions prone to warping and cracking formation.

In the literature, several analytical solutions of the diffusion equation are used to describe drying processes of wood [1, 11, 13]. Dincer [1] used a one-dimensional analytical solution for the infinite slab to describe drying of lumber cut in the radial direction all-heartwood specimen of Douglas-fir (*Pseudotsuga menziessi* (Poir.) Britton). According to the author, a practical experimental moisture content and time data set for a slab wood dried with hot air was used, and the results were reasonable when compared with the results predicted by his model. Ricardez et al. [11] used a two-dimensional analytical solution of the diffusion equation to describe drying of red oak (*Quercus* spp.) samples at vacuum pressure. The authors concluded that their model was able to reproduce the drying kinetics of wood that occurred in two stages: constant and falling rates. Silva et al. [13] used several analytical models, including a three-dimensional model to describe drying of lumber (*Pinus elliottii* Engelm.). The authors concluded that three-dimensional model with boundary condition of the third kind reasonably described the process. However, these authors commented that analytical models normally presuppose restrictive assumptions such as constant volume and effective mass diffusivity. Thus, these authors have suggested in their conclusions that numerical solutions instead analytical solutions should be used to describe wood drying, to avoid those restrictions.

Olek and Weres [12] used the finite element method to solve the one-dimensional diffusion equation in Cartesian coordinates. The authors proposed a variable effective mass diffusivity as a function of the moisture content to use their numerical solution for describing drying of Scots pinewood (*Pinus sylvestris* L.). The authors concluded that the best results were obtained for the effective mass diffusivity given by an exponential expression in which the exponent is a quadratic function of the moisture content. On the other hand, Silva et al. [14] described convective drying of lumber (*Pinus elliottii* Engelm.) at low air temperature. Silva et al. [14] described the drying process using a three-dimensional numerical solution of the diffusion equation, in which was supposed variable effective mass diffusivity. The model permitted a rigorous description of the drying process, and it can predict the moisture content in any position within the parallelepiped that represents the lumber, at any time. However, Silva et al. [15] observed that the determination of the process parameters through optimization technique, using three-dimensional model, takes a long time to perform. Because of that, these last authors used a two-dimensional numerical solution of the diffusion equation to describe same drying studied by Silva et al. [14]. In this two-dimensional study, Silva et al. [15] reported good results, and the optimization time for their model was about 20 times less than the optimization time with the typical three-dimensional solution. Naturally, in this context, a question should be answered: is the one-dimensional model a good option to describe same drying? In this sense, the aim of this article is defined in the following.

The objective of this article was to describe drying of wood cut into parallelepiped shaped pieces, considering the effective mass diffusivity as a variable property. For this purpose, a numerical solution of the one-dimensional diffusion equation was proposed and coupled with an optimizer to determine the process parameters. In addition, a second objective was to compare the results obtained herein with other found in the literature supposing the lumber with two- and three-dimensional geometry.

Materials and methods

The one-dimensional diffusion equation in Cartesian coordinates, used to describe water migration during drying of lumber can be written as [16]:

$$\frac{\partial M}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial M}{\partial x}\right), \tag{1}$$

where M is the local moisture content ($\mathrm{kg_{water}\ kg_{drymatter}^{-1}}$); t is the time (s); x is the position (m) within the infinite slab with origin in the center; and D is the effective mass diffusivity ($\mathrm{m^2\ s^{-1}}$). The following assumptions were assumed to numerically solve Eq. (1): (a) liquid diffusion was considered as the main mass transport mechanism inside the product; (b) the boundary condition is of the third kind; (c) the product was considered homogeneous and isotropic; (d) the diffusion process presents symmetry with respect to the midpoint of the slab.

Numerical solution

Equation (1) was numerically solved using the finite volume method [16], with a fully implicit formulation. To discretize Eq. (1), an infinite slab with thickness T (m) is presented in Fig. 1a. Figure 1b shows a uniform grid with

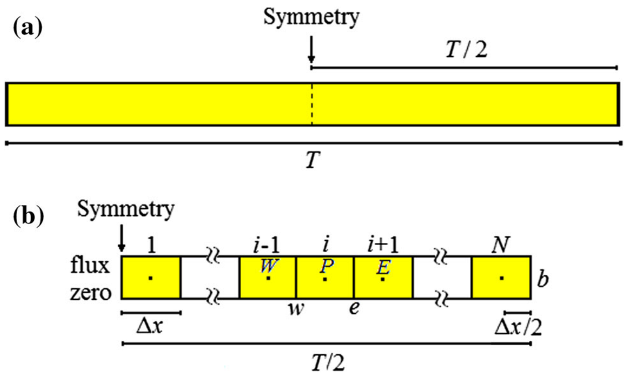

Fig. 1 **a** Infinite slab; **b** uniform grid with N control volumes in a symmetrical piece of the infinite slab

N control volumes in a symmetrical piece of the infinite slab, and each control volume has a thickness given by Δx (m). Figure 1b also shows an internal control volume "i" with nodal point "P", and its neighbors to west "W" and east "E". The lowercases "w" and "e" refer to the interfaces of the control volume "P" to west and east, respectively.

The integration of Eq. (1) with respect to space (Δx) and time (from t up to $t + \Delta t$), for a control volume P, gives the following result:

$$\frac{M_P - M_P^0}{\Delta t}\Delta x = \Gamma_e \frac{\partial M}{\partial x}\bigg|_e - \Gamma_w \frac{\partial M}{\partial x}\bigg|_w \quad (2)$$

in which the superscript "0" means "former time t" and its absence means "current time $t + \Delta t$".

Internal control volumes

For an internal control volume, the following algebraic equation was obtained from the discretization of Eq. (1):

$$A_w M_W + A_p M_P + A_e M_E = B \quad (3)$$

and the coefficients A_w, A_p, A_e and B are given in Silva et al. [5], where the diffusion equation was discretized for the boundary condition of the first kind. Naturally, for an internal control volume, Eq. (3) is independent of the boundary condition.

Control volume 1

For the control volume 1, the boundary condition was supposed to be of the second kind, with flux zero at west side due to the symmetry. Thus, the following algebraic equation was obtained:

$$A_p M_P + A_e M_E = B. \quad (4)$$

Again, the coefficients A_p, A_e and B are given in Silva et al. [5] and, for that, they were omitted herein.

Control volume N

For the control volume N, the derivatives of Eq. (2) were approximated by:

$$\frac{\partial M}{\partial x}\bigg|_w \cong \frac{M_P - M_W}{\Delta x} \quad (5)$$

and

$$\frac{\partial M}{\partial x}\bigg|_e \cong \frac{M_b - M_P}{\Delta x / 2} \quad (6)$$

where M_b is the value of M at the east boundary. Thus, for the control volume N, the subscript "e" (east) is equivalent to "b" (boundary). The boundary condition of the third kind to east side is expressed by

$$-D\frac{\partial M}{\partial x}\bigg|_e = h_b(M_b - M_{eq}), \quad (7)$$

in which h_b is the convective mass transfer coefficient at east boundary, and M_{eq} is the equilibrium moisture content. Combining Eqs. (6) and (7) to express M_b, and substituting M_b into Eq. (6), this new equation and also Eq. (5) can be used to rewrite Eq. (2). The following algebraic equation is obtained:

$$A_w M_W + A_p M_P = B, \quad (8)$$

where

$$A_w = -\frac{1}{\Delta x} D_w, \quad (9a)$$

$$A_P = \frac{\Delta x}{\Delta t} + \frac{D_w}{\Delta x} + \frac{D_b}{\frac{D_b}{h_b} + \frac{\Delta x}{2}}, \quad (9b)$$

$$B = \frac{\Delta x}{\Delta t} M_P^0 + \frac{D_b}{\frac{D_b}{h_b} + \frac{\Delta x}{2}} M_{eq}. \quad (9c)$$

In Eq. (9c), M_P^0 is the moisture content in the control volume P at the beginning of the time step.

Equations (3), (4) and (8) constitute a system of equations in each time step, and such system was solved by the method "tri-diagonal matrix algorithm" [17], also called TDMA. The average value of M at any instant, denoted by $\overline{M}$, was calculated by a arithmetic average of the moisture contents obtained for the control volumes, once the established grid is uniform.

Effective mass diffusivity

The expression used in this article for the effective mass diffusivity as a function of local moisture content during drying of wood at low temperature was proposed by Silva et al. [14, 15], and is given by:

$$D = b\ \exp(a/M), \quad (10)$$

where "a" and "b" are parameters that fit the numerical solution to an experimental data set. For a uniform grid, on the interfaces of the internal control volumes, for example, "e" (see Fig. 1), D is determined through harmonic mean [16]:

$$D_e = \frac{2D_E D_P}{D_E + D_P}, \quad (11)$$

where D_P and D_E at the nodal points "P" and "E" are calculated through Eq. (10).

As the effective mass diffusivity D is variable, the coefficients A in Eqs. (3), (4) and (8), as well as the coefficients B, are calculated in each time step, due to the nonlinearities caused by the variation of such parameter. If the time refinement is adequate, the errors due to the nonlinearities can be discarded.

Optimization

Establishing the function given by Eq. (10) to express the effective mass diffusivity D at the nodal points, the parameters a and b, as well as the convective mass transfer coefficient h, can be determined by optimization. The expression of the Chi square [18, 19] was chosen as objective function:

$$\chi^2 = \sum_{i=1}^{N_p} \left[\overline{M}_i^{\exp} - \overline{M}_i^{\text{sim}}\right]^2 \frac{1}{\sigma_i^2}, \quad (12)$$

in which $\overline{M}_i^{\exp}$ is the average moisture content measured in the experimental point i, $\overline{M}_i^{\text{sim}}$ is the correspondent simulated moisture content, N_p is the number of experimental points, $1/\sigma_i^2$ is the statistical weight referring to the point i. According to Silva et al. [20], if the statistical weights are unknown, they can be made equal to a common value, for instance 1. In Eq. (12), it is interesting to observe that the χ^2 depends on $\overline{M}_i^{\text{sim}}$, which depends on D and h. Thus, if the convective mass transfer coefficient can be considered constant and the effective mass diffusivity is given by Eq. (10), the parameters "h", "a" and "b" can be determined through the minimization of the objective function, which is accomplished in cycles involving the steps given in the following [3, 20].

1. Provide the initial values for the parameters "a", "b" and "h". Solve the diffusion equation and determine the χ^2;
2. Provide the value for the correction of "h";
3. Correct the parameter "h", maintaining the parameters "a" and "b" with constant values. Solve the diffusion equation and calculate the χ^2;
4. Compare the latest calculated value of the χ^2 with the previous one. If the latest value is smaller, return to the step 2; otherwise, decrease the last correction of the value of "h" and proceed to step 5;
5. Provide the value for the correction of "a";
6. Correct the parameter "a", maintaining the parameters "b" and "h" with constant values. Solve the diffusion equation and calculate the χ^2;
7. Compare the latest calculated value of the χ^2 with the previous one. If the latest value is smaller, return to the step 5; otherwise, decrease the last correction of the value of "a" and proceed to step 8;
8. Provide the value for the correction of "b";
9. Correct the parameter "b", maintaining the parameters "a" and "h" with constant values. Solve the diffusion equation and calculate the χ^2;
10. Compare the latest calculated value of the χ^2 with the previous one. If the latest value is smaller, return to the step 8; otherwise, decrease the last correction of the value of "b" and proceed to step 11;
11. Begin a new cycle coming back to the step 2 until the stipulated convergence for the parameters "a", "b" and "h" is reached.

According to Silva et al. [20], in each cycle, the value of the correction of each parameter can be initially modest, compatible with the tolerance of convergence imposed to the problem. For a given cycle, in each return to the step 2, 5 or 8, the value of the new correction can be multiplied by the factor 2. If the modest correction initially informed does not minimize the objective function, in the next cycle, its value can be multiplied by the factor −1.

A simplified flowchart for the optimization algorithm is shown in Fig. 2, highlighting the parameter h, referring to steps 1–4.

Da Silva et al. [3], studying the cooling kinetics of cucumbers, have used this optimization algorithm, and they estimated the uncertainty of the process parameters as follows. The experimental measurements were disrupted with 50 different Gaussian error distributions with zero mean value and standard deviation given by $\sigma = 2\sigma_\Phi{*}$ (95 %) in which $\sigma_\Phi{*}$ is the standard deviation of the original simulation. These authors found that the optimization algorithm has determined the process parameters with an uncertainty less than 1 % of the average value of the correspondent parameter.

Experimental data

To compare one-, two- and three-dimensional models, drying studied by Silva et al. [14] (three-dimensional) and Silva et al. [15] (two-dimensional) was analyzed again using the one-dimensional numerical solution proposed herein to describe the process. The experimental data set is referring to drying of lumber (*Pinus elliottii* Engelm.), in which wood with 20 years of age was used. Four lumber pieces were

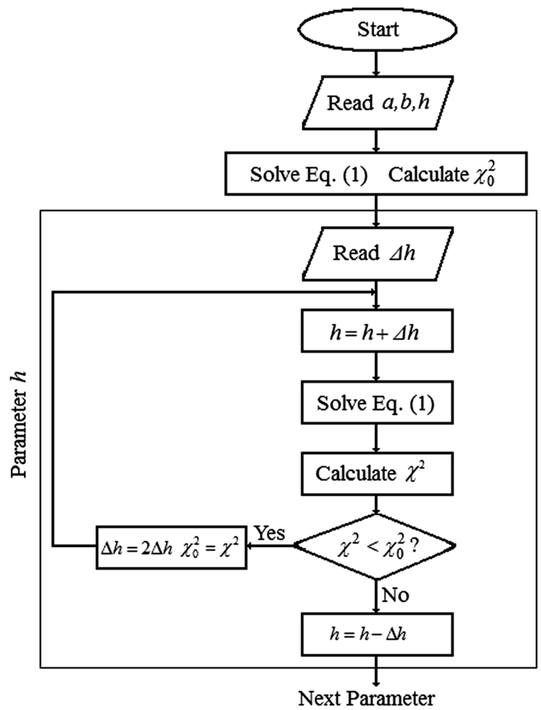

Fig. 2 Simplified flowchart for the optimization algorithm highlighting the parameter *h*

obtained through tangential cut, with a density of the dry matter of 405 kg m^{-3}. To dry the product, the lumber initially 23 °C was placed into a chamber with forced air at temperature of 40 °C, relative humidity of 40 % and velocity of 3 m s^{-1}. The parallelepiped that represents the lumber is shown in Fig. 3 and the dimensions of the product were: thickness $T = 36$ mm; height $H = 100$ mm and length $L = 745$ mm. Moisture content was determined by gravimetric method, in which the four lumber pieces were weighted together. The initial and equilibrium moisture content were, respectively, 1.213 and 0.070, in dry basis, $kg_{water}\ kg^{-1}_{drymatter}$. The experimental data set obtained during the drying process of the lumber is shown through Fig. 4.

Results and discussion

An unreported study about the refinement of grid and time indicated that a grid with 48 control volumes and 2000 time steps are adequate to solve the diffusion equation using the numerical solution proposed in this article. Thus, the results in the following were obtained.

Results

The process parameters "*a*", "*b*" and "*h*" were determined by optimization, using the experimental data set presented in Fig. 4, and the obtained results are presented in Table 1.

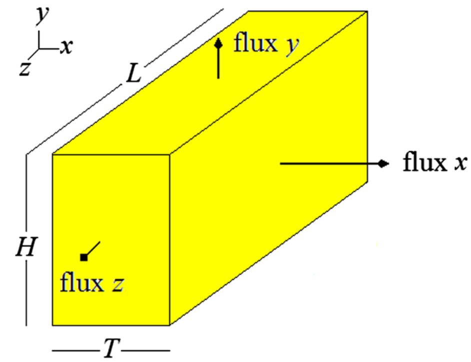

Fig. 3 Parallelepiped representing a lumber with thickness *T*, height *H* and length *L*, highlighting the three moisture fluxes at the three visible surfaces during drying

This table also presents the results available in the literature for two- and three-dimensional models (2D and 3D). The symbols χ^2 and R^2 represents the statistical indicators χ^2 and determination coefficient, respectively.

Since the process parameters have been determined, the simulation of the drying kinetics for the one-dimensional case (1D) can be presented together with the experimental data set, as is shown in Fig. 5.

Figure 6 presents the effective mass diffusivities as a function of the local moisture content for the cases one- (present work), two- [15] and three-dimensional [14].

Figure 7 presents the moisture distributions for the one-dimensional case at instants $t = 19.8$ h and $t = 31.2$ h.

Discussion

According to several authors, such as Silva et al. [13], due to some heterogeneity and anisotropy, the diffusion process in a given direction can be little different from the diffusion in other directions. Thus, the values of the parameters

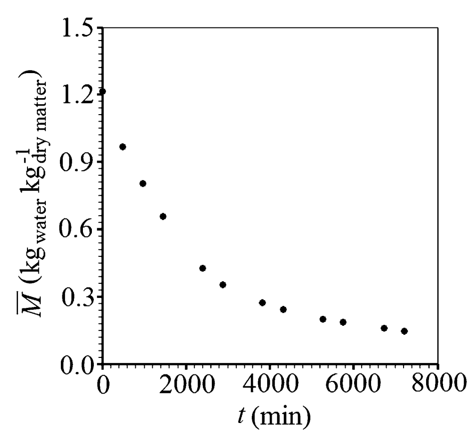

Fig. 4 Experimental data set referring to drying of lumber

Table 1 Results of the optimization using models

Model	References	D (m^2 s^{-1})	h (m s^{-1})	R^2	χ^2
1D	Present work	$1.87 \times 10^{-8}\exp(-0.477/M)$	1.56×10^{-7}	0.9992	1.127×10^{-3}
2D	Silva et al. [15]	$1.61 \times 10^{-8}\exp(-0.442/M)$	1.16×10^{-7}	0.9993	1.071×10^{-3}
3D	Silva et al. [14]	$1.57 \times 10^{-8}\exp(-0.435/M)$	1.13×10^{-7}	0.9994	1.023×10^{-3}

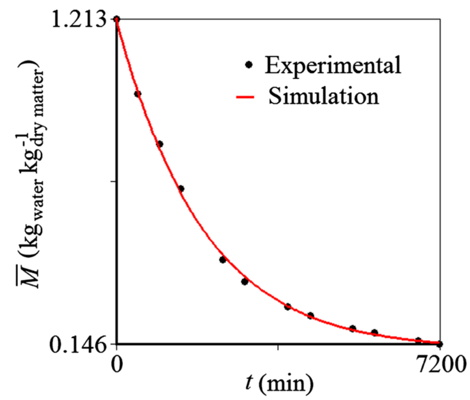

Fig. 5 Drying kinetics of lumber using one-dimensional numerical simulation

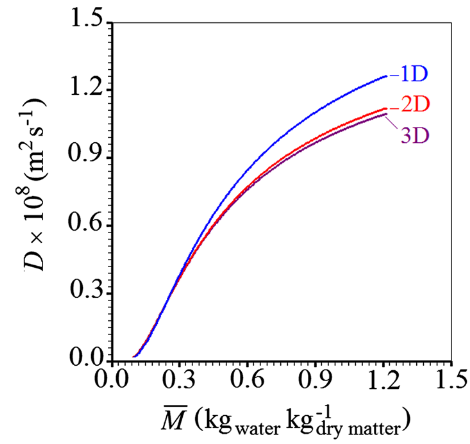

Fig. 6 Effective mass diffusivity as a function of the local moisture content for the following cases: one-, two- and three-dimensional simulations

determined by optimization should be interpreted as effective values referring to the proposed model. In addition, Silva et al. [14] observe that the consideration of the liquid diffusion as the only mechanism of water transport inside the lumber is a simplification of the proposed model, justified by the low value of the initial moisture content and drying temperature. Thus, the analyses in the following are performed in this context, i.e., considering the assumptions assumed for models 3D, 2D and 1D.

An inspection on the statistical indicators of Table 1 enables to conclude that the drying kinetics of lumber was well described by three models used to represent the process. However, as Silva et al. [13] observed, the results of Table 1 indicates that the more the considered geometry is close to the real geometry, the better the results. On the other hand, an idea on the goodness-of-fit for the one-dimensional case is given by inspection of Fig. 5, in which the experimental points and the one-dimensional simulation are in good agreement. Similar result was obtained by Dincer [1], which used with success an analytical solution of the diffusion equation to describe drying of lumber with the following dimensions: $T = 40$ mm, $H = 100$ mm and $L = 200$ mm. Note that, in this case, H and L are 2.5 and 5 times the value of T, respectively. In the present study, H and L are 2.8 and 20.7 times the value of T, and such dimensions are more favorable to consider the lumber as an infinite slab. In addition, Dincer [1] considered the effective mass diffusivity with a constant value and in the present work, this property was considered variable. This consideration is so significant that the statistical indicators obtained by Silva et al. [13] describing this same drying with an analytical three-dimensional solution (constant effective mass diffusivity) are worse than the statistical indicators obtained herein with a numerical one-dimensional solution (variable effective mass diffusivity).

As can be realized in Fig. 6, the effective water diffusivity increases with increasing of the local moisture content, and this result was also obtained by other researchers such as Silva et al. [5] studying osmotic dehydration of guava, and Olek and Weres [12] describing lumber drying. In addition, Fig. 6 indicates that the effective mass diffusivity for model 2D is moderately greater than this property obtained with 3D model. On the other hand, the effective mass diffusivity for model 1D is significantly greater than this property for model 2D and, consequently, for model 3D. The interpretation of this result can be given with basis in Fig. 3, which shows the dimensions of the lumber and the moisture fluxes at the three visible surfaces of the parallelepiped during drying. For the 3D case, the moisture flux occurs in three pairs of surfaces, involving the total area of 209840 mm^2. For the 2D case, the pair of moisture fluxes at direction z was disregarded. Thus, the area involved in the moisture flux was 202640 mm^2, representing about 97 % of the total area for the 3D case. For the 1D case, the pair of moisture fluxes at direction y was also disregarded. Consequently, with these considerations, the

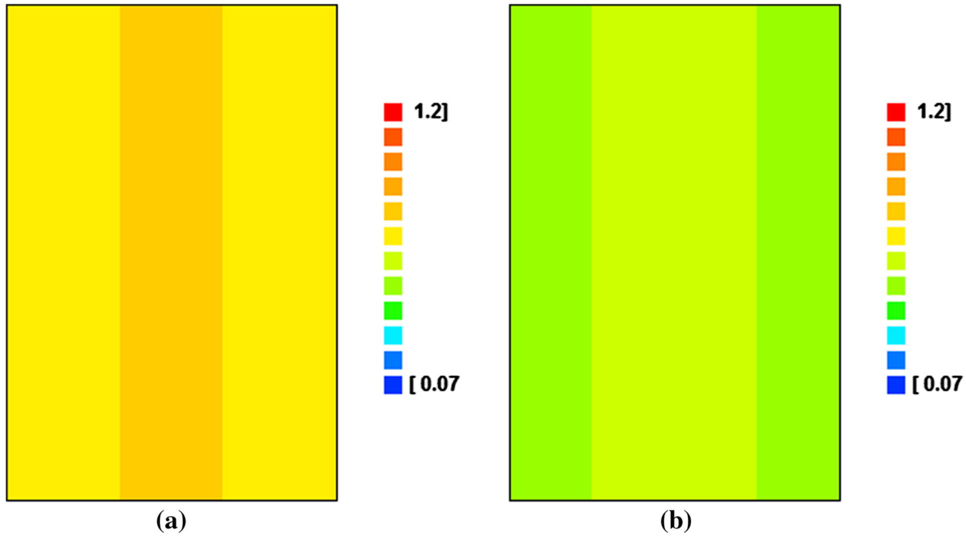

Fig. 7 Moisture distributions at: **a** $t = 19.8$ h; **b** $t = 31.2$ h

moisture flux occurs in an area equal to 149000 mm^2, which represents only about 71 % of the area for the 3D case. As it is observed, the great reduction in area when models 3D or 2D are substituted by model 1D explains the significant increasing in its effective mass diffusivity, as it can be seen in Fig. 6. On the other hand, the small reduction in area when model 3D is substituted by model 2D explains the little difference in their effective mass diffusivities. An inspection of Table 1 enables to conclude that similar results are also obtained for the convective mass transfer coefficients for the cases one-, two- and three-dimensional.

To determine the average value for the effective mass diffusivity, the following expression was used:

$$\overline{D} = \frac{\int_{M_{eq}}^{M_0} D(M)\mathrm{d}M}{\int_{M_{eq}}^{M_0} dM} \tag{13}$$

in which M_0 and M_{eq} are, respectively, the initial and equilibrium moisture content. For the one-dimensional case, the average effective mass diffusivity was 8.7×10^{-9} m^2 s^{-1}. This average value is compatible with the constant value obtained by several authors that use diffusion models in wood drying considering some resistance on the boundary, such as Dincer [1] ($h = 2.26 \times 10^{-7}$ m s^{-1} and $D = 3.24 \times 10^{-9}$ m^2 s^{-1}).

An observation of Fig. 7 indicates that the information on moisture distribution within the lumber is poor because the moisture distribution at direction z and, mainly, at direction y are not considered. Even so, if the main focus of the study is the drying kinetics, model 1D presents good results for lumber with the dimensions involved in this work. As Silva et al. [21] observed, even whether the proposed model is not completely acceptable in a given study, the one-dimensional numerical solution presented in this article is useful because, through this solution, the obtained results serve as initial values for other optimization processes involving a model 3D (or 2D).

Finally, as observed by Silva et al. [15], the drying kinetics of wood at low temperature was well described by models with an effective water diffusivity expressed by an exponential function, in which the exponent is proportional to the inverse of the local moisture content. However, this function was obtained for the specific dataset studied in this article, and more tests should be performed to know whether good results are also obtained.

Conclusion

One-dimensional model considering variable effective mass diffusivity well describes the drying kinetics of the studied lumber. The obtained statistical indicators are comparable with those obtained for two- and three-dimensional models.

The strong reduction in area of moisture flux of model 1D significantly overestimates the effective mass diffusivity and the convective mass transfer coefficient when compared with these properties obtained with model 3D (and also 2D). In addition, the moisture distribution is simplified to the one-dimensional case and, for that, such distribution is not appropriate to provide information for a subsequent study on stress and crack formation. However, the process parameters obtained in this study by optimization serve, at least, as initial values for other optimization processes involving a model 3D.

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