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ORIGINAL ARTICLE

Effects of the method of identification of the diffusion coefficient on accuracy of modeling bound water transfer in wood

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Abstract An alternative approach to determining the bound water diffusion coefficient is proposed. It comprises a method for solving the inverse diffusion problem, an improved algorithm for the bound-constrained optimization as well as an alternative submodel for the diffusion coefficient's dependency on the bound water content. Identification of the diffusion coefficient for Scots pine wood (*Pinus sylvestris* L.) using the proposed inverse approach is presented. The accuracy of predicting the diffusion process with the use of the coefficient values determined by traditional sorption methods as well as by the inverse modeling approach is quantified. The similarity approach is used and the local and global relative errors are calculated. The results show that the inverse method provides valuable data on the bound water diffusion coefficient as well as on the boundary condition. The results of the identification can significantly improve the accuracy of mass transfer modeling as studied for drying processes in wood.

Keywords Inverse method · Computer-aided identification · Fick's law · Scots pine wood · Sorption experiments · Validation of identification

Nomenclature

a	Constant in Eqs. 13 and 14 $(-)$
b	Constant in Eq. 14 $(-)$
D	Diffusion coefficient (m^2/s)
D_0	Coefficient in Eqs. 12–14 (m^2/s)

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e_1	Local relative error (%)
e_2	Global relative error (%)
E	Reduced bound water content (−)
l	Half-thickness (m)
M	Water content ($\mathrm{kg/kg_{dry\,base}}$)
M_∞	Equilibrium water content ($\mathrm{kg/kg_{dry\,base}}$)
M_0	Initial water content ($\mathrm{kg/kg_{dry\,base}}$)
$M(t)$	Global water content in selected time instants ($\mathrm{kg/kg_{dry\,base}}$)
$M_{\mathrm{exp}}(t)$	Experimental water content ($\mathrm{kg/kg_{dry\,base}}$)
$M_{\mathrm{pred}}(t)$	Predicted water content ($\mathrm{kg/kg_{dry\,base}}$)
NT	Number of time intervals in computation
NT_{exp}	Number of time intervals in experiment
S	Objective function
t	Time (s)
t_{F}	Final time (s)
w_i	Weight function
x	Space dimension (m)

Greek symbols

Γ	Points located at the two boundary sides of the domain (two points in the one-dimensional model)
σ	Surface emission coefficient (m/s)
Ω	Geometric domain of the R^1 space
$\overline{\Omega}$	Geometric domain of the R^1 space with the boundary

1 Introduction

The modeling of wood drying as well as the description of moisture transfer in products made of wood already dried below the fiber saturation point requires credible data on the material properties. The bound water diffusion coefficient describes one of the most important properties responsible for obtaining good quality predictions of water transfer processes. The diffusion coefficient is usually determined using the sorption method. During recent decades a number of different approaches to the sorption method have been developed and applied. The simplest and the most frequently used was the initial sorption technique (e.g., Siau 1995; Stamm 1959, 1960; Wadsö 1994). Unfortunately, the assumptions that the coefficient does not depend on moisture content and the wood surface comes instantly to hygroscopic equilibrium with moist air were the most important disadvantages of the technique. It was shown early on that the second assumption is not valid in the case of wood (Skaar 1988; Shmulsky et al. 2002). Therefore, methods were developed, which took into consideration the gradual approach of the wood surface to equilibrium. The methods were able to separate the surface resistance from the internal resistance by identifying both the surface emission coefficient and the bound water diffusion coefficient in wood (Choong and Skaar 1969, 1972). Unfortunately, the methods were based on the analytical solution of the diffusion problem, which required the assumption of a constant value of the coefficient. This may cause significant errors in the identification of the coefficients and lead to false values. The problem of false values was extensively reported by Söderström and Salin (1993).

The inaccuracy in the diffusion coefficient's determination may be significantly reduced by applying the inverse approach for solving mass transport problems. The authors of the present paper have already shown the effectiveness of the inverse problem concept for analyzing the heat and mass transport in forest products (Weres et al. 2000; Olek et al. 2005; Weres and Olek 2005). However, the improvement in the accuracy of the diffusion coefficient's identification obtained by the application of the inverse approach was never quantified. Therefore, the objective of the present paper was to analyze the accuracy of predicting the diffusion process with the use of the coefficient values determined by traditional sorption methods as well as the inverse modeling approach.

2 Methods

2.1 Experimental data

Experimental material was obtained from freshly cut Scots pinewood (*Pinus silvestris* L.) with clearly oriented growth rings and uniform density of 490 ± 10 kg/m^3. The material was carefully dried to a moisture content lower than the fiber saturation point and then equilibrated to an initial moisture content of ca. 0.08 kg/kg$_{\text{dry base}}$. Two types of samples, i.e., radial and tangential ones, in the shape of rectangular prisms, were cut from the equilibrated material. The dimensions of the samples were 70, 35 and 8 mm. The last dimension always corresponded to the thickness ($2l$) of a sample. The sides of the samples were sealed by covering with a few layers of chlorinated rubber enamel (Fig. 1).

The sorption experiments were performed in a setup with controlled air parameters, i.e., temperature of 23.4°C, relative humidity corresponding to the equilibrium moisture content of ca. 0.14 kg/kg$_{\text{dry base}}$ and forced air flow of 0.8 m/s. The individual samples were placed on a balance of accuracy of 0.001 g and weighed at time instants. The results were collected by a data acquisition system. The final moisture content of each sample was determined by the gravimetric method after the sorption experiment. The results of sorption experiments were stored in an empirical database as the moisture content values of the samples depending on the time instants.

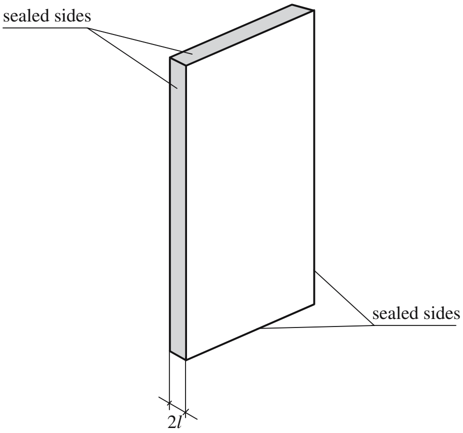

Fig. 1 Schematic representation of a sample with four sealed sides

2.2 Mathematical model

The mathematical model of the unsteady state bound water diffusion is traditionally given by the transient form of Fick's second law:

$$\frac{\partial M}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial M}{\partial x}\right), \quad (x,t) \in \Omega \times [0, t_{\mathrm{F}}] \tag{1}$$

with the initial condition

$$M(x,0) = M_0, \quad x \in \overline{\Omega} \tag{2}$$

and the third kind boundary condition:

$$\left(-D\frac{\partial M}{\partial x}\right) = \sigma \cdot [M(x,t) - M_\infty], \quad (x,t) \in \Gamma \times [0, t_{\mathrm{F}}], \tag{3}$$

$$\left(-D\frac{\partial M}{\partial x}\right) = \sigma \cdot [M(x,t) - M_\infty] \quad (x,t) \in \Gamma \times [0, t_{\mathrm{F}}], \tag{4}$$

or the first kind boundary condition:

$$M(x,t) = M_\infty, \quad (x,t) \in \Gamma \times [0, t_{\mathrm{F}}], \tag{5}$$

$$M(x,t) = M_\infty, \quad (x,t) \in \Gamma \times [0, t_{\mathrm{F}}]. \tag{6}$$

2.3 Methods used for diffusion coefficient estimation

The diffusion coefficient was estimated with the use of the two traditional sorption methods as well as the inverse approach. The basic assumptions of all methods applied in the present analysis are given below.

2.3.1 Initial sorption

The diffusion problem given by (1), (2), (5), and (6) has an analytical solution for the initial stage of sorption with the assumption of a constant value of the diffusion coefficient. The solution can be written for the total bound water content and reduced to the following relation (Crank 1975):

$$E = 2\left(\frac{D\,t}{\pi\,l^2}\right)^{1/2}, \tag{7}$$

where for adsorption, reduced bound water content (E) is defined as

$$E\,(t) = \frac{M(t) - M_0}{M_\infty - M_0}. \tag{8}$$

The diffusion coefficient was calculated from results of the sorption experiments presented in the form of plots of E versus $\sqrt{t}$ (linear part of the relation) and the following equation derived from (7):

$$D = \frac{\pi}{4/l^2}\left(\frac{\Delta E}{\Delta\sqrt{t}}\right)^2. \tag{9}$$

2.3.2 *Separation of diffusion and surface emission coefficients*

Liu (1989) proposed a method for the simultaneous determination of the diffusion coefficient as well as surface emission coefficient. It was based on the analytical solution of the diffusion problem given by (1)–(4) and originally obtained by Newman (1931). The earlier methods of coefficient separation (Choong and Skaar 1969, 1972) required the results of sorption experiments done on samples of different thickness. Liu (1989) proposed an analytical procedure that required results to be obtained for one thickness only. The diffusion coefficient was determined from the relation:

$$D = l^2 \left. \frac{-0.1654}{0.7010 \cdot dt/dE + 2.05 \cdot t} \right|_{E=0.5} \tag{10}$$

and the surface emission coefficient (σ) was calculated as:

$$\sigma = \left. \frac{0.7010 \cdot D}{D \cdot t/l - 0.1963 \cdot l} \right|_{E=0.5}. \tag{11}$$

2.3.3 *Inverse method*

The inverse finite element analysis approach to identifying the diffusion coefficient was based on the inverse problem concept, optimization techniques, and the finite element method for solving direct problems. A detailed description of the approach was given by Olek et al. (2005) and Weres and Olek (2005). The operational form of the mathematical model of the analyzed diffusion process was developed by applying the finite element approximation (isoparametric elements in space and an absolutely stable, threepoint recurrence scheme in time), the iteration procedure resulting from the quasi-linearity of the analyzed diffusion model, and the empirical submodels for the diffusion coefficient. The empirical submodels analyzed in the present study were parameterized by the following functions:

$$D = D_0, \tag{12}$$

$$D = D_0 \cdot \exp[-a \cdot M(t)], \tag{13}$$

$$D = D_0 \cdot \exp\Big[-\Big(a \cdot M(t) + b \cdot M^2(t)\Big)\Big], \tag{14}$$

where D_0, a, and b are the estimated coefficients. The bound water content at the hygroscopic equilibrium (M_∞) was taken as an additional parameter, estimated in all options of the inverse analysis.

The algorithm for solving the direct diffusion problem was supplemented with the module for averaging all predicted nodal values of the bound water content in the geometric domain. This allowed us to obtain the global values of the water content $M_{\text{pred}}(t)$ for each time instant. The predicted global values were used in the procedure of coefficient estimation.

The optimization algorithm was developed on the basis of the trust regions and the variable metric approach, in which gradients and Jacobians were approximated automatically, and Hessians were approximated by the quasi-Newtonian technique. The objective function was defined as the sum of the squares of the residuals of the measured and predicted global values of the bound water content (Eq. 15). We assumed $w_i = 1$, as a result of our previous analyses of differentiating values of the weight function. The invented inverse problem approach was implemented and the software package was coded in Lahey/Fujitsu Fortran 95.

$$S = \sum_{i=1}^{NT_{\mathrm{exp}}} w_i \left[M_{\mathrm{exp}}(t_i) - M_{\mathrm{pred}}(t_i) \right]^2. \tag{15}$$

3 Results

The diffusion coefficient was identified for Scots pine wood in the radial as well as tangential directions. The input data consisted of the averaged results of adsorption experiments (at least results of four processes were subjected to averaging). The values of the diffusion coefficient as well as the surface emission coefficient determined with the initial sorption method and the Liu method are presented in Table 1, and the values of the coefficients determined with the inverse method are shown in Table 2. The latter values of the coefficients were used in modeling the diffusion process. The numerically obtained bound water content changes in time were compared to the empirical data of experiments that were not used for the identification (Figs. 2, 3). In order to quantify the quality of the coefficient estimated by the three analyzed methods, two errors were defined and calculated (Olek et al. 2003, 2005), i.e., the local relative error (e_1)

$$e_1(t_i) = 100 \frac{\left| M_{\mathrm{exp}}(t_i) - M_{\mathrm{pred}}(t_i) \right|}{M_{\mathrm{exp}}(t_i)}, \quad i = 1, \ldots, NT_{\mathrm{exp}} \tag{16}$$

Table 1 Values of the coefficients estimated by the analytical sorption methods

	Applied method	σ (m/s)	D(m^2/s)
Radial direction	Initial sorption	–	$1.105 \cdot 10^{-10}$
	Liu method	$2.343 \cdot 10^{-7}$	$1.471 \cdot 10^{-10}$
Tangential direction	Initial sorption	–	$0.6794 \cdot 10^{-10}$
	Liu method	$1.218 \cdot 10^{-7}$	$0.9592 \cdot 10^{-10}$

Table 2 Values of the coefficients estimated by the inverse method

	Inverse method option	σ (m/s)	D_0 (m^2/s)	$a(-)$	$b(-)$	M_∞ (kg/kg$_{\mathrm{drybase}}$)	S
	Eq. 12	$6.751 \cdot 10^{-7}$	$1.707 \cdot 10^{-10}$	–	–	0.1376	0.09242
Radial	Eq. 13	$5.515 \cdot 10^{-7}$	$2.714 \cdot 10^{-10}$	2.400	–	0.1377	0.08928
direction	Eq. 14	$6.752 \cdot 10^{-7}$	$0.006262 \cdot 10^{-10}$	−78.80	288.0	0.1378	0.08460
	Eq. 12	$2.081 \cdot 10^{-7}$	$1.042 \cdot 10^{-10}$	–	–	0.1436	0.05195
Tangential	Eq. 13	$3.031 \cdot 10^{-7}$	$0.3041 \cdot 10^{-10}$	−6.782	–	0.1433	0.02541
direction	Eq. 14	$3.416 \cdot 10^{-7}$	$0.005259 \cdot 10^{-10}$	−60.54	185.0	0.1433	0.02442

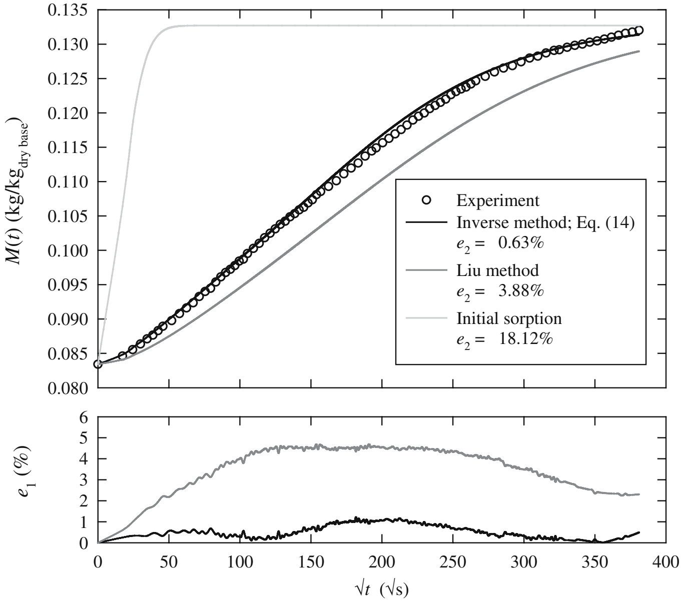

Fig. 2 Validation of the diffusion coefficient estimation, Scots pine, and radial direction

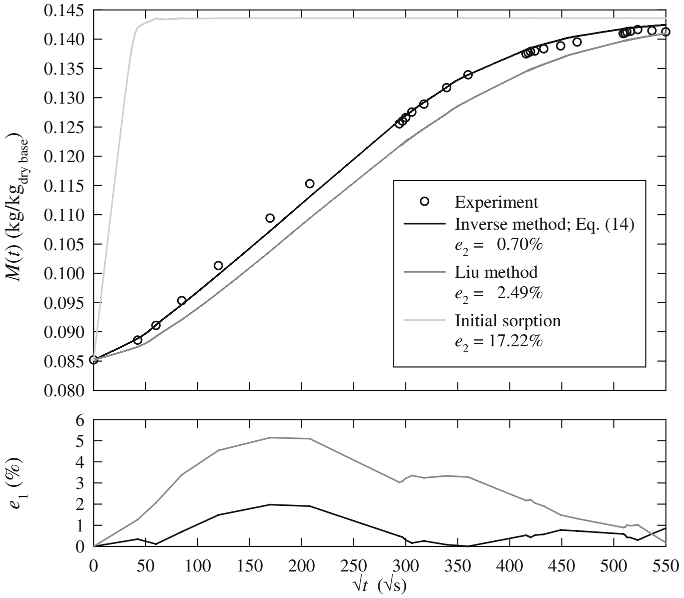

Fig. 3 Validation of the diffusion coefficient estimation, Scots pine, and tangential direction

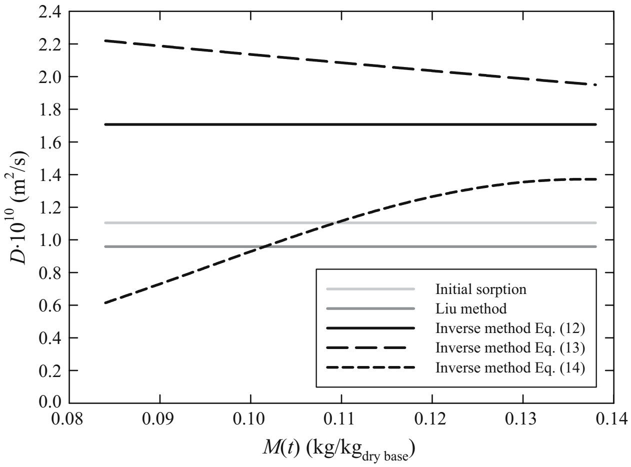

Fig. 4 Diffusion coefficient changes with moisture content, Scots pine, and radial direction

and the global relative error (e_2)

$$e_2 = 100 \frac{\sqrt{\sum_{i=1}^{NT_{\text{exp}}} \left[M_{\text{exp}}(t_i) - M_{\text{pred}}(t_i)\right]^2}}{\sqrt{\sum_{i=1}^{NT_{\text{exp}}} M_{\text{exp}}(t_i)^2}}. \tag{17}$$

For clarity, the plots (Figs. 2, 3) of the predicted values of the water content as well as the values of the local relative error (e_1) are presented for only one set of results of the inverse method identification, for which the objective function (S) had the smallest values. In both cases, the inverse identification was made for the diffusion coefficient parameterization given by Eq. 14, i.e., the three parameter submodel (Table 2). Figures 2 and 3 do not contain the values of the local relative error obtained for the diffusion prediction obtained for the coefficients identified with the use of the initial sorption method since the maximum values of the error were as high as 60%.

For the analyzed sorption processes and the empirical submodel given by Eq. 14 the obtained values of the diffusion coefficient were augmented with the increase of the bound water content. This supports the common opinion that the diffusion coefficient dependens on the bound water content (e.g., Skaar 1988). However, the results presented in Table 2 show that in case of the simplest submodel (Eq. 13) the dependency may be opposite (e.g., radial direction). Therefore, the proper selection of the empirical function describing the dependency on the water content has great importance. The changes of the diffusion coefficient values with the moisture content for all options of the identification are presented in Fig. 4 (radial direction) and Fig. 5 (tangential direction), respectively.

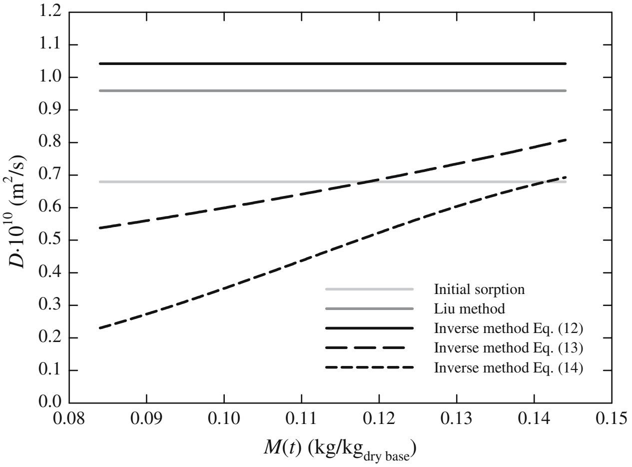

Fig. 5 Diffusion coefficient changes with moisture content, Scots pine, and tangential direction

4 Conclusions

The analysis of similarity between the diffusion modeling and the results of experiments allowed us to derive the following conclusions:

(1) Application of the initial sorption method is not acceptable from the point of view of diffusion coefficient identification in wood. The local relative error values reached as much as 60%. The assumption of the first kind boundary condition is not valid in the case of wood.

(2) The application of the analytical method which assumes the convective boundary condition, does not significantly improve the accuracy of the diffusion identification (global relative error of almost 20%). This was primarily due to the assumption of constant values of the diffusion coefficient as well as the experimental determination of the bound water content at the hygroscopic equilibrium.

(3) The best similarity was obtained for the results of the inverse identification with use of the submodel given by Eq. 14. However, a further improvement can be achieved by taking into consideration the coupling between diffusion and the heat transfer, as well as by modifying the submodel describing the diffusion coefficient's dependency on the water content.

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