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Reducing spatial dimensionality in a model of moisture diffusion in a solid material

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Abstract

A model of the moisture movement in solid wood under isothermal conditions taking into consideration coating (insulation) of the surface of the material, is presented in a 2-D-in-space formulation. The validity of using a corresponding 1-D model on a 2-D problem is investigated. A measure of reliability of the 1-D model is introduced. This paper presents a new technique, which adjusts the width of a material as well as the degree of coating of the edges, to ensure the relative error of the problem solution is less than the required, resulting from reducing the model from 2-D to 1-D-in-space. This technique is based on the computer simulation of 2-D diffusion to estimate the reliability of the corresponding 1-D diffusion model.

1. Introduction

The diffusion equation is widely used in modelling mass and heat transfer in solid materials [1–3]. One-dimensional-in-space (1-D) model accurately describes the diffusion process only in an extremely long and wide plate (thickness is much smaller than length and width). A two-dimensional-in-space (2-D) model accurately describes the mass and heat transfer in an extremely long stick (thickness and width are much smaller than length). However, 1-D analysis can be successfully used to predict the diffusion process for a relatively short and narrow material if four of the six surfaces are heavily coated (insulated) in order to reduce the transfer of diffusing substance from those four surfaces.

Solving a 1-D model is more efficient as it involves fewer inter-dependent parameters. This paper explores the validity of using a 1-D model of the diffusion on a 2-D problem. To predict the diffusion process accurately by using the 1-D model, we need to obtain the appropriate geometry as well as coating (insulation) of the surface of a specimen. Leaving out of consideration the level of surface coating (insulation), the influence of the geometry of a specimen on the validity of using the 1-D model on the 2-D problem, has been investigated earlier [1,4–6]. This paper describes a new technique to determine the width of a specimen as well as the degree of coating of the edges to ensure that the solution of the 1-D model is within the specified error limit. A measure of the reliability of the 1-D model was introduced. The technique was demonstrated on the modelling of wood drying.

Wood drying is usually accomplished by evaporating the moisture from the surface of wood. Moisture moves from an area of higher moisture content to an area of lower moisture content within the wood. When the surface moisture evaporates from the sides or ends, moisture moves from the interior toward these locations. This process continues until the wood reaches its equilibrium moisture content with the ambient air conditions.

From the mathematical point of view, the moisture transport process can be treated as a diffusion problem based on the Fick's second law. A drying model under isothermal conditions, can be expressed through the diffusion equation with initial and boundary conditions. The initial condition expresses an initial moisture concentration in the material, and the boundary condition describes the surface evaporation [3–5,7,8].

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Nomenclature

a	half thickness (m)
A	constant
b	half width (m)
B	constant
C	constant
D	moisture diffusivity (m^2/s)
E	fraction of total moisture content
k	ratio of width to thickness
K	minimal value of width to thickness ratio, Eq. (11)
p	relative error of half-drying time
P	relative error function, Eq. (10)
S	surface emission coefficient
t	time (s)
T	temperature (K)
$T_{0.5}$	half time of 2-D drying, half-drying time (s)
$T^*_{0.5}$	half time of 1-D drying, (s)
u	moisture content (kg/kg)
x	coordinate (m)
y	coordinate (m)
Greek symbols	
θ	dimensionless degree of coating (insulation)
Θ	minimal value of degree of coating, Eq. (12)
Subscripts	
0	initial
e	equilibrium
x	x direction
y	y direction

Moisture movement models have been also successfully used to solve the inverse coefficient problem [9–12]. In those cases, it is assumed that the type of governing equations is known. The diffusion and surface emission coefficients need to be determined by using the data from physical experiments to solve the problem. The inverse solutions are known to be sensitive to changes in input data resulting from measurement and modelling errors [2,13,14]. Hence, they may not be unique. Nevertheless, the determination of the parameters for diffusion processes in various species of solids is a current problem [15–19]. Since the multidimensional inverse methods are especially complex and use of them is problematic in practice, it is important to estimate the reliability of a 1-D model to predict the drying process accurately, i.e. to estimate an error of calculation because the model is 1-D.

The process of heat conduction, which occurs during heating of solid objects, is similar in form to the process of moisture movement in these objects. The governing Fourier equation is exactly in the form of the Fickian equation of moisture transfer, in which concentration and moisture diffusivity are replaced with temperature and thermal diffusivity, respectively. Therefore, the analysis of the validity of using the 1-D model on the 2-D problem of the moisture diffusion can be applied to the heat conduction problems as well.

2. Moisture movement problem

In a two-dimensional-in-space formulation, the moisture movement, under isothermal conditions, in a symmetric piece of a porous medium (sawn board) of thickness $2a$ and width $2b$ can be expressed through the following diffusion equation as

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D_x(u)\frac{\partial u}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_y(u)\frac{\partial u}{\partial y}\right),\quad 0 < x < a,\ 0 < y < b,\ t > 0, \tag{1}$$

where $u = u(x, y, t)$ is the moisture content, expressed as the weight of water present in wood divided by the weight of dry wood substance, t is the time, x, y are space coordinates, and $D_x(u)$, $D_y(u)$ are the moisture concentration-dependent diffusion coefficients in the space directions x, y, respectively.

The initial condition ($t = 0$) is

$$u(x, y, 0) = u_0,\quad 0 \leqslant x \leqslant a,\ 0 \leqslant y \leqslant b, \tag{2}$$

where u_0 is the initial concentration in the medium. Let us assume, that the edges of the specimen may be coated (insulated), e.g. painted. The boundary conditions that describe symmetry and surface evaporation ($t > 0$) are

$$\left.\frac{\partial u}{\partial x}\right|_{x=a} = \left.\frac{\partial u}{\partial y}\right|_{y=b} = 0, \tag{3}$$

$$-D_x(u)\frac{\partial u}{\partial x} = S(u_e - u),\quad x = 0, \tag{4}$$

$$-D_y(u)\frac{\partial u}{\partial y} = (1-\theta)S(u_e - u),\quad y = 0, \tag{5}$$

where S is the surface emission coefficient, u_e is the equilibrium moisture content, and θ is the dimensionless degree of coating (insulation) of the edges ($0 \leqslant \theta \leqslant 1$). If an edge of a specimen is extremely coated, then the corresponding surface coating degree is 1; it equals 0 if the surface is not coated.

Eqs. (1)–(5) apply to sorption (water soaking) when in Eqs. (4) and (5) $u_e > u$ and to desorption (drying) when $u_e < u$.

In the calculations, discussed below, a corresponding model in one-dimensional-in-space formulation was also employed. The 1-D model can be rather easily derived from Eqs. (1)–(5) by ignoring the space coordinate y.

Analytical solutions of problems, described by partial differential equations of the diffusion type, do not usually exist in cases with variable diffusion coefficients and complex boundary conditions [1]. Therefore, the Eqs. (1)–(5) were solved numerically. The finite-difference technique was used for the discretization of the model [20], where a non-uniform discrete grid was introduced to increase the efficiency of calculations. Since moisture evaporates from the surface of a piece of wet wood, a bilinear increasing step of the grid was used in the space directions x and y from the surface to the center, while a constant step was used in the t direction [21].

3. Reliability of the 1-D moisture diffusion model

The average moisture content is usually measured at various times to predict the dynamics of sorption as well as desorption in a physical experiment. The calculated average moisture content $\bar{u}(t)$ values at any time t can be determined by numerical integration of the finite difference solutions. The relative amount of the remaining moisture content $E(t)$ in the wood during drying at time t is usually called the fraction of total moisture content in the material [4]:

$$E(t) = (\bar{u}(t) - u_e)/(u_0 - u_e). \tag{6}$$

In the case of sorption, $E(t)$ is defined as the dimensionless moisture content to be absorbed in the material.

Let k be a dimensionless ratio of the width to thickness of a material, $k = b/a$, and $T_{0.5}(a, k, \theta)$ be a function of half thickness a, ratio k, and coating degree θ as the time when the drying process reaches midst, called half-drying time, i.e. $E(T_{0.5}(a, k, \theta)) = 0.5$. Let the width be greater or equal to the thickness of the specimen, $k \geqslant 1$. The half-drying time (half-time technique) characterizes well the dynamics of substance diffusion [1,22–24]. The half-time method has been successfully employed for a solution of the diffusion problem as well as for a determination of the diffusion and surface emission coefficients in various application areas [8,24,25].

A model of drying in a 1-D formulation can be successfully used to predict drying time for an extremely wide plate as well as for a board with heavily coated edges. Let $T^*_{0.5}(a)$ be the half-drying time of an extremely wide specimen of thickness $2a$ calculated from the appropriate 1-D model. $T^*_{0.5}(a)$ can also be described as a value of the half-drying time, when edges of a specimen of thickness $2a$ are extremely coated, i.e. $\theta = 1$,

$$E(T_{0.5}(a, k, \theta)) = 0.5, \tag{7}$$

$$E(T^*_{0.5}(a)) = 0.5, \tag{8}$$

$$T^*_{0.5}(a) = \lim_{k\to\infty} T_{0.5}(a, k, 1), \quad k = b/a. \tag{9}$$

In the case of the use of a 1-D model, the calculated half-drying time equals to $T^*_{0.5}(a)$. Therefore, the use of a 1-D model can be called as admissible for a board if the half-drying time, calculated by using the corresponding 2-D model, equals approximately also $T^*_{0.5}(a)$. Assuming $T_{0.5}(a, k, \theta)$ as the true value of the halfdrying time of 2-D medium and $T^*_{0.5}(a)$ as an approximate one, consider a function P as the relative error of the half-drying time

$$P(a, k, \theta) = \frac{T^*_{0.5}(a) - T_{0.5}(a, k, \theta)}{T_{0.5}(a, k, \theta)}. \tag{10}$$

Since $T^*_{0.5}(a)$ can be calculated by using an appropriate 1-D model, $P(a, k, \theta)$ can be called the relative error of the use of the 1-D model for a material of the half thickness a and the width k times greater than the thickness at the degree θ of coating of the edges. $P(a, k, \theta)$ may also be regarded as a level of reliability of the 1-D model to predict a drying process of a sawn board. Notice that $P(a, k, \theta) \geqslant 0$.

Assume that a 1-D model is to be used for a simulation of the moisture diffusion in a two-dimensional medium, i.e. in a specimen which is relatively long, e.g. sawn board. Because of the domain geometry it is reasonable to assume a 2-D model. In order to use a 1-D model, it is necessary to provide as far as possible a wide material or to isolate extremely the edges of a narrow material. However, a good result can be achieved also by a combination of these two ways.

Assume that Eqs. (1)–(5) can be solved numerically in 2-D as well as 1-D formulations. Using a 2-D computer simulation and the definition of the relative error of the use of a 1-D model, it is possible to adjust the width of the material as well as the degree of coating of the edges ensuring that the error of calculations is not greater than the required one in the case of use of the 1-D model.

Consider a function $K_{a,\theta}(p)$ as the minimal value of the width to thickness ratio k for which the relative error $P(a, k, \theta)$ does not exceed p at the given degree θ of coating of the edges and half thickness a, i.e.

$$K_{a,\theta}(p) = \min_{k\geqslant 1}\{k : P(a, k, \theta) \leqslant p\}. \tag{11}$$

In other words, if k is the ratio of the width to thickness of a material, such as $k \geqslant K_{a,\theta}(p)$, then the relative error of the half-drying time, calculated by using a 1-D model, does not exceed p due to the use of the 1-D model at a given degree θ of coating of the edges and thickness $2a$ of the specimen.

Consider a function $\Theta_{a,k}(p)$ as the minimal value of the degree of coating of the edges for which the relative error $P(a, k, \theta)$ does not exceed p at a given geometry of the specimen, i.e. at the given thickness $2a$ and width $2ak$:

$$\Theta_{a,k}(p) = \min_{0\leqslant\theta\leqslant 1}\{\theta : P(a,k,\theta)\leqslant p\}. \quad (12)$$

Thus, if θ is the degree of coating of the edges of a material $2a$ by $2ak$, such that $\theta \geqslant \Theta_{a,k}(p)$, then the relative error of the half-drying time, calculated by using the 1-D model, does not exceed p due to the use of the 1-D model.

Using Eqs. (11) and (12) the width as well as the degree of coating of the edges can be chosen to be sure that the error of calculations will not be greater than the required one in the case of use of the 1-D model. The kind of adjustment (width or coating of the edges) depends on possibilities.

4. Results of calculations and discussion

In order to demonstrate the accuracy and usefulness of the above technique, the moisture transfer model given by Eqs. (1)–(5) was employed to simulate the drying of materials from northern red oak (*Quercus rubra*). The experimental moisture content values for red oak by Simpson and Liu [12] were used for numerical analysis. Experimental drying conditions were 43 °C at 84% relative humidity ($u_e = 0.162$). There were two air velocities: 1.5 and 5.1 m/s. The average initial moisture content u_0 was 0.825. The size of the experimental specimen was 0.102 by 0.305 by 0.029 m, i.e. $2a = 0.029$, $2b = 0.102$ [12].

In the mathematical model (1)–(5), it was assumed that the diffusion coefficient is constant above the fiber saturation point (fsp, 0.3 for red oak) and it is equal to the coefficient at the fsp value [26]. Though the radial and tangential diffusion coefficient may be different, the transverse (in the x and y directions) diffusion below fsp for red oak was represented as

$$D_x(u) = D_y(u) = D(u) = A\mathrm{e}^{(B/T+Cu)}, \quad (13)$$

where T is the temperature, A, B and C are experimentally determined coefficients [27]. Values of the coefficients A, B, C in Eq. (13) and S in Eqs. (4) and (5) were found in [12].

The calculations showed that the half-drying time $T^*_{0.5}(a)$ of the specimen of the thickness of $2a = 0.029$ m equals 4.09×10^5 s at ambient air velocity of 1.5 m/s. This half-drying time was determined by using 1-D. The same value of the half-drying time was obtained in a case of the 2-D moisture transfer model when the edges of the material were assumed as fully isolated, i.e. $\theta = 1$, at the width of $2b = 0.102$ m.

The transverse section of a material was also modelled as a rectangle having various widths maintaining the thickness equal to $2a = 0.029$ m. Eqs. (1)–(5) were solved numerically for various values of the width to thickness ratio k ($1\leqslant k\leqslant 100$) and the coating degree θ ($0\leqslant\theta\leqslant 1$). In each board geometry and coating degree of the edges case, the drying until the half-drying time was simulated at the same drying conditions as above. Then, having the value of $T^*_{0.5} = 4.09\times10^5$ s calculated by using the 1-D model, relative error P was calculated in each specimen geometry case. Results of the calculations are depicted in Figs. 1 and 2.

It can be observed in Fig. 1 that the relative width of a material appears to be important for the relative error at different values of the degree θ of coating of the edges. This importance decreases with increase of θ. In the case of uncoated edges ($\theta = 0$), the relative error of the use of the 1-D model notably decreases with increase in the

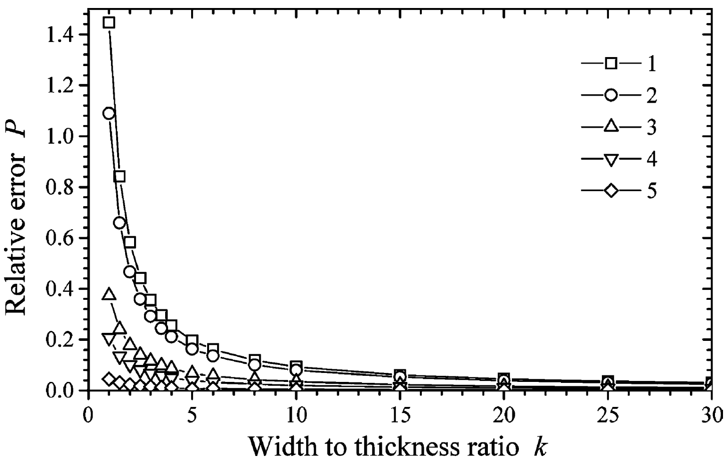

Fig. 1. Dependence of the relative error $P(a,k,\theta)$ on the width to thickness ratio k of materials of the thickness $2a = 0.029$ m at five values of the degree θ of coating of the edges: 0 (1), 0.5 (2), 0.9 (3), 0.95 (4) and 0.99 (5) for air velocity of 1.5 m/s.

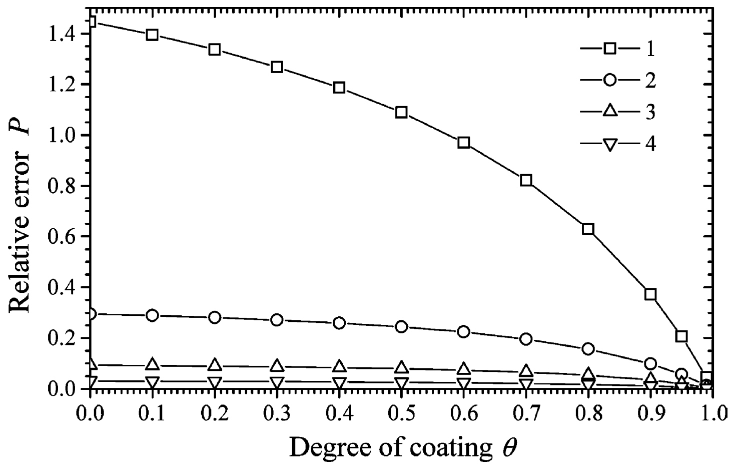

Fig. 2. Dependence of the relative error $P(a,k,\theta)$ on the degree θ of coating of the edges of materials of the thickness $2a = 0.029$ m at four values of the width to thickness ratio k: 1 (1), 3.52 (2), 10 (3) and 30 (4) for air velocity of 1.5 m/s.

width to thickness ratio k up to $k \approx 10$ (see also [6,28]). In that case ($\theta = 0$) the relative error P equals to about 0.085 at $k = 10$, while it equals to about 0.2 at $k = 5$. A similar situation appears in the case where $\theta = 0.5$. The decrease of the relative error versus k is rather slight only for values of θ greater than about 0.95. Because of the small change of the relative error P at $k > 30$, the results of calculations are depicted for $k \leqslant 30$ only. Fig. 1 shows, that function $P(a,k,\theta)$ is a non-linear monotonous decreasing function of width to thickness ratio k ($k \geqslant 1$) at given coating degree θ and half thickness a.

It can be observed in Fig. 2 that function $P(a,k,\theta)$ is a monotonous decreasing function also of the coating degree θ ($0 \leqslant \theta \leqslant 1$) at given geometry of the transverse section, i.e. width to thickness ratio k and half thickness a. However, the degree θ of coating of the edges effects the relative error P notably only in cases of relatively narrow specimens (k less than about 10). For example, if the transverse section of a specimen is a square ($k = 1$), then the hundredfold reducing of moisture transfer from the edges ($\theta = 0.99$) gives an relative error of about 0.04.

Taking into account the definition of $P(a,k,\theta)$ introduced by Eq. (10), we note that the function $T_{0.5}(a,k,\theta)$ of the half-drying time is a monotonous increasing function of k ($k \geqslant 1$) as well as θ ($0 \leqslant \theta \leqslant 1$) at given half thickness a of a material.

As was noted above, in the case of the use of the 1-D model, the accurate result of the half-drying time can be achieved by accepting a sufficiently wide material, irrespective of coating of the edges. If the 1-D model is used for a material of thickness $2a = 0.029$ m, having uncoated edges, $\theta = 0$, then the width of the material should be at least 85 times greater than the thickness ($k \geqslant 85$) to ensure the relative error of the half-drying time is not greater than 0.01 because of the use of the 1-D model, i.e. $K_{0.0145,0}(0.01) \approx 85$. This means, that the relative difference in the half-drying time calculated by using the 2-D and 1-D models does not exceed 0.01 in such a case.

On the other hand, if the geometry of a material is fixed, i.e. the geometry of the specimen can not be freely adjusted, then we can find the minimal degree $\Theta_{a,k}(p)$ of coating of the edges at which the relative error does not exceed the required value p at the given geometry (a and k) of the material due to the use of the 1-D model. The calculations showed (see Fig. 2) that use of the 1-D model for a material having a rectangle 0.029 by 0.102 m in the transverse section, $k \approx 3.52$, can result in inexact values of drying time even if the edges are coated. It is necessary to reduce moisture transfer from the edges at least about 20 times ($\theta \approx 0.95$) to ensure that the solution of the 1-D model is less than 0.05. Simpson and Liu in [12] used a 1-D model, however, the edges and ends of the specimens were heavily coated. Thus, coating the edges heavily for specimens with $k \approx 3.52$ is well justified.

In the calculations showed in Figs. 1 and 2, the dimensionless parameter k varies by varying the width of the material maintaining the thickness equal to $2a = 0.029$ m. However, similar values of k can be obtained also by varying the thickness or even both. To investigate the influence of the thickness on the relative error P Eqs. (1)–(5) were solved numerically also for various values of the thickness maintaining the width equal to $2b = 0.102$ m. In addition, the relative error of the use of a 1-D model may depend on other parameters of the model Eqs. (1)–(5). To verify if the drying conditions effect the error P, we solved the problem numerically also for the another air velocity of 5.1 m/s. Results of the calculations are depicted in Fig. 3.

It can be observed in Fig. 3 that in the case of uncoated edges ($\theta = 0$), the relative error P of the

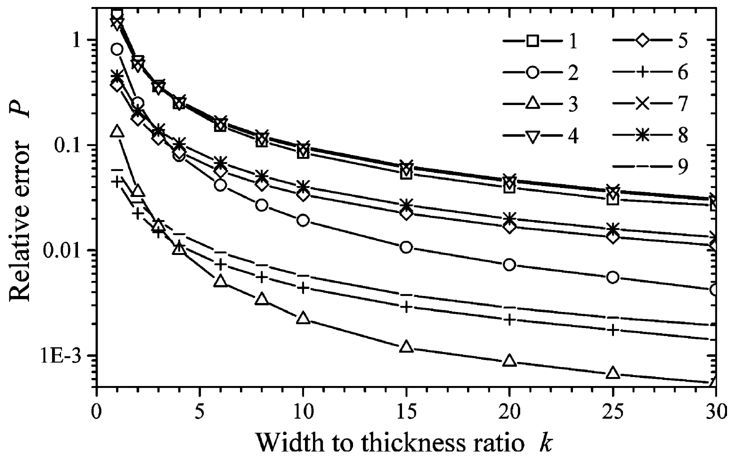

Fig. 3. Dependence of the relative error $P(a,k,\theta)$ on the width to thickness ratio k at two air velocities: 1.5 (1–6), 5.1 (7–9) m/s, three values of the degree θ of coating of the edges: 0 (1, 4, 7), 0.9 (2, 5, 8), 0.99 (3, 6, 9), holding the width $2b = 0.102$ m (1–3) as well as the thickness $2a = 0.029$ m (4–9) constant.

half-drying time depends on the width to thickness ratio k only. There is no notable difference between three upper lines in Fig. 3. Consequently, the influence of the drying conditions as well as the concrete thickness of the material on the error P is insignificant in the case of $\theta = 0$ at given k. When the edges are coated ($\theta > 0$) faster drying (higher air velocity) corresponds to a slightly greater error at the same geometry of the materials. The error of calculation decreases with decrease of the thickness at the same ratio k. A few lines intersect because of the same thickness at $k \approx 3.52$.

In the modelling of water-vapour diffusion during drying, the flow in the direction of the width of a board is frequently negligible in comparison to that in the thickness direction if the width to thickness ratio k is equal to or greater than 5 [4]. However, Figs. 1 and 3 show that in the case of uncoated edges the relative error of the half-drying time calculated from the 1-D model may be equal to about 0.2. The error of such magnitude can be unacceptable in various applications, and especially in solving the inverse coefficient problem. When the edges are coated, the error depends on the drying conditions as well as on the concrete geometry of the material. Therefore, having concrete values of the parameters of the model, using the computer simulation based on the 2-D model is highly reasonable to evaluate applying the corresponding 1-D model on the given 2-D problem for the following investigation based on the 1-D model.

5. Conclusions

Using a computer simulation of a substance diffusion, expressed by a 2-D-in-space model, a reliability of the corresponding 1-D model can be efficiently estimated by applying a concept of the relative error which was introduced in this paper. The relative error $P(a,k,\theta)$ of the use of a 1-D model in comparison with the corresponding 2-D model for a material of thickness $2a$ and width $2ak$ at the degree θ of coating (insulation) of the edges was defined by Eq. (10).

The proposed error estimation procedure can be successfully used to adjust the width of the material (e.g., long sawn board) as well as the degree of coating of the edges to ensure the relative error less than the required resulting from reducing the model from 2-D to 1-D-in-space.

The 2-D model guarantees perceptibly better prediction of the drying process of a sawn board than the corresponding 1-D model if the ratio k of the width to thickness of the material is rather small (less than about 10) or the degree θ of coating of the edges is not very high (less than about 0.95).

In the case of coated edges ($\theta > 0$), in addition to the ratio k, the drying conditions as well as the thickness of the material have a notable effect on the error of the use of the 1-D model on the 2-D problem.

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