

HIGH TEMPERATURE EFFECT ON DIFFUSION COEFFICIENT

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ABSTRACT

The aim of the work was the investigation of the effect of high temperature on diffusion characteristics of spruce wood. Two temperatures levels of 100°C and 120°C were used. The influence of anatomical direction - longitudinal, radial and tangential was also measured. The diffusion coefficients also depend on the method used. On the basis of measured data we can conclude that all three factors mentioned had significant influence on diffusion characteristics.

KEY WORDS: spruce, poplar, black locust, oak, wood, diffusion, temperature, high temperature, diffusion coefficient, surface emission coefficient

INTRODUCTION

Diffusion is a process, describing bound water movement due to concentration differences. It is described by the first and second Ficks' laws. These equations enable to determine the amount of water, which diffuses from one surface to another, the concentration in time and space and the amount of water taken in. Because of simplification we assume that wood is non-swelling material so concentration is linearly proportional to moisture content. High temperature drying is a part of some processes for example: treatment of wood with heat, drying of wood chips for production of particleboards. Ping and Liandbai (2003) consider diffusion as a part of high temperature drying. These authors cite Miao (2000) who predicted moisture content during wood drying with small samples according Fick's second law. Some researches Stamm (1964), Choong (1963), Siau (1995) treated diffusion as an Arrhenius process. From this point of view we can suppose that diffusion is faster if temperature is higher.

The aim of this article is the description of high temperature influence on diffusion characteristics.

MATERIAL AND METHOD

The experimental material was obtained from spruce wood (*Picea abies*, L). The specimens were cut from one log. Position of the specimen in the log was chosen randomly. One run of specimen belongs to one level of temperature and to one anatomical direction. Ten specimens were chosen for one run. The specimen dimensions were $30 \times 30 \times 10 \text{ mm}^3$ in basic anatomical directions, so annual rings were parallel to one side of specimen. The specimen thickness was 10mm. The lateral sides of specimens were sealed with rubber and the direction of flux was in thickness direction. The specimens were dried at the appropriate temperature until constant mass was reached. The temperature was set at 100°C and 120°C level. The moisture uptake of specimens was performed over saturated salt aqueous solution of CaCl_2 at given temperature. The mass uptake was recorded and after it the mass and thickness of specimen were measured. Details of apparatus can be found in Hrčka and Babiak (2007).

The diffusion equation or Fick's second law is the base for description of diffusion:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial c}{\partial x} \right) \quad (1)$$

where c is concentration, x coordinate and D is diffusion coefficient.

For the description of our measurements we can use this one dimensional equation only.

If D does not depend on concentration then equation (1) has the form:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \quad (2)$$

The mean concentration \bar{c} is defined by the equation:

$$\bar{c}(t) = \frac{1}{s} \int_0^s c(x, t) dx \quad (3)$$

where s is the half thickness of the specimen. The ratio of mean concentration to the maximum mean concentration is also the ratio of the water taken up to the maximum of this water, which are easier measurable quantities. This ratio is taken as dimensionless moisture content.

The constant initial moisture content across the thickness of specimen can be taken as initial condition. The boundary condition of the first kind describes the surface concentration as a function of time. If we assume constant concentration on the surface, c_r then solution is (Požgaj et al. 1993):

$$\frac{c(x, t) - c_o}{c_r - c_o} = \sum_{n=0}^{\infty} (-1)^n \operatorname{erfc} \left[\frac{(2n+1)s - x}{2\sqrt{Dt}} \right] + \sum_{n=0}^{\infty} (-1)^n \operatorname{erfc} \left[\frac{(2n+1)s + x}{2\sqrt{Dt}} \right] \quad (4)$$

or

$$\frac{c(x, t) - c_o}{c_r - c_o} = 1 - 4 \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)\pi} e^{-\frac{(2n+1)^2 \pi^2 Dt}{4s^2}} \cos \frac{(2n+1)\pi x}{2s} \quad (5)$$

where c_o is initial concentration.

For the mean concentration it follows:

$$\frac{M_t}{M_r} = 2 \sqrt{\frac{Dt}{a^2}} \left[\frac{1}{\sqrt{\pi}} + 2 \sum_{n=1}^{\infty} (-1)^n \operatorname{ierfc} \left(\frac{na}{\sqrt{Dt}} \right) \right] \quad (6)$$

or

$$\frac{M_t}{M_r} = 1 - 8 \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2 \pi^2} \cdot e^{-\frac{(2n+1)^2 \pi^2}{4} \frac{Dt}{a^2}} \quad (7)$$

where M_t is the mass of water taken up to the time t and M_r is the mass of taken water after a long time of moisture uptake. The first equation is used for the diffusion coefficient measurement in the short time as infinite sum could be neglected and the second equation is convenient for the diffusion coefficient measurement in the long times as only the first term of the sum is used.

The boundary condition of the third kind describes the surface flux as a function of concentration. We can find this condition in the form (Pożgaj et al. 1993):

$$D \left. \frac{\partial c}{\partial x} \right|_{x=s} = \alpha (c_r - c(s, t)) \quad (8)$$

where α is the surface emission coefficient.

Application of this condition in stationary method needs to know surface concentration. It can be achieved by dividing the specimen into parts. But this condition is better known from non-stationary diffusion. The solution of diffusion equation for the moisture uptake is of the form (POŻGAJ et al. 1993):

$$\frac{M_t}{M_r} = 1 - \sum_{n=1}^{\infty} \frac{2Bi^2}{\delta_n^2 (\delta_n^2 + Bi^2 + Bi)} e^{-\delta_n^2 \frac{Dt}{a^2}} \quad (9)$$

where δ_n are the positive roots of the equation $\delta_n \operatorname{tg} \delta_n = Bi$ and $Bi = \frac{\alpha s}{D}$ is Biot number.

The diffusion coefficient is determined by the least square method, where criterion Q is defined as:

$$Q = \sum_{i=1}^n (w_{\text{exp}} - w_{\text{theor}})^2 \quad (10)$$

where w_{exp} is measured moisture content and w_{theor} is moisture content defined by solutions of diffusion equation, n is number of data. The transport characteristics are parameters of this equation. The mean error can be computed as:

$$R = \sqrt{\frac{Q}{n}} \quad (11)$$

The evaluation program searches for the minimum of the sum Q while the diffusion coefficient is the independent quantity. We determined the diffusion coefficient with two and the sum of squares with four significant digits.

Temperature influence on diffusion coefficient can be assumed according to Arrhenius equation, which has the form:

$$D = D_0 e^{-\frac{E_b}{RT}} \quad (12)$$

where E_b is the activation energy, T is absolute temperature, R universal gas constant. Activation energy and D_0 are parameters of this equation. Equation (12) is often converted to linear form.

RESULTS

The next figures display average dimensionless moisture uptake of specimens in time. The x axis is designed as square root of time due to well known sigmoid shape of this curve. The dashed curve represents the solutions (6) or (7), the solid line represents the solution (9).

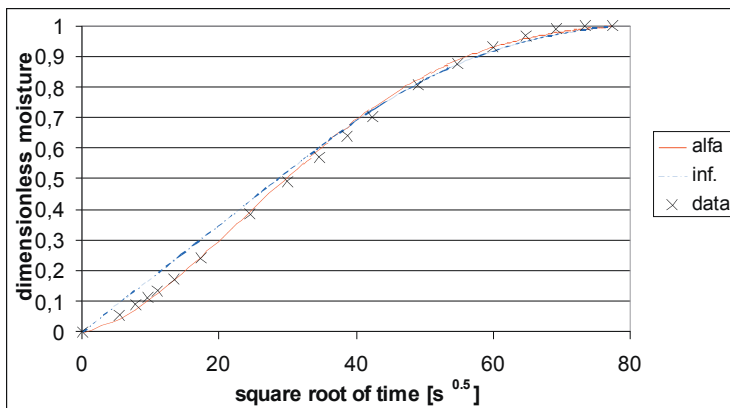


Fig. 1: The dependence of the mean dimensionless moisture uptake on square root of time in tangential direction at 100°C

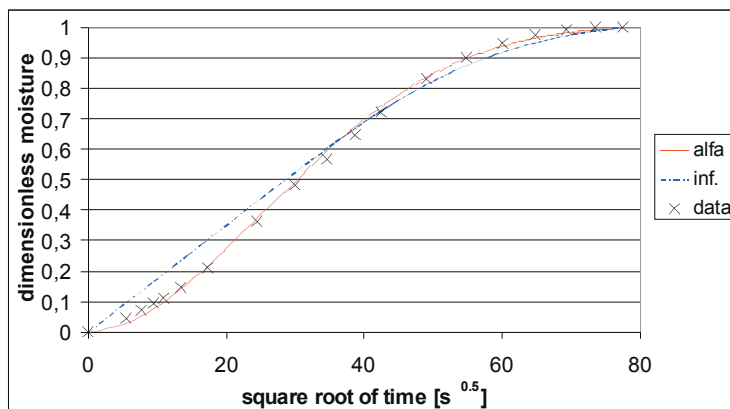


Fig. 2: The dependence of the mean dimensionless moisture uptake on square root of time in radial direction at 100°C

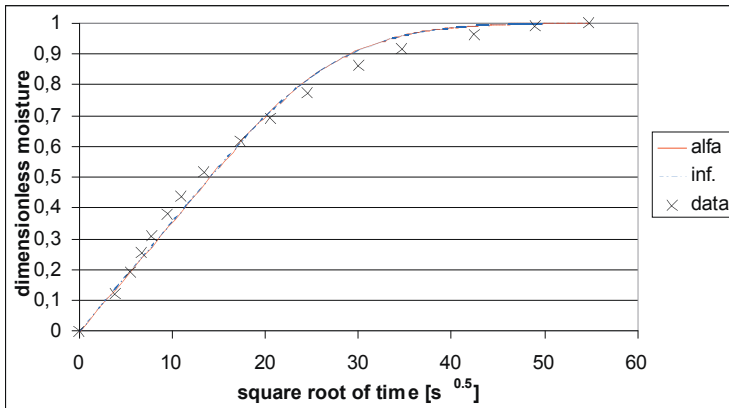


Fig. 3: The dependence of the mean dimensionless moisture uptake on square root of time in longitudinal direction at 100°C

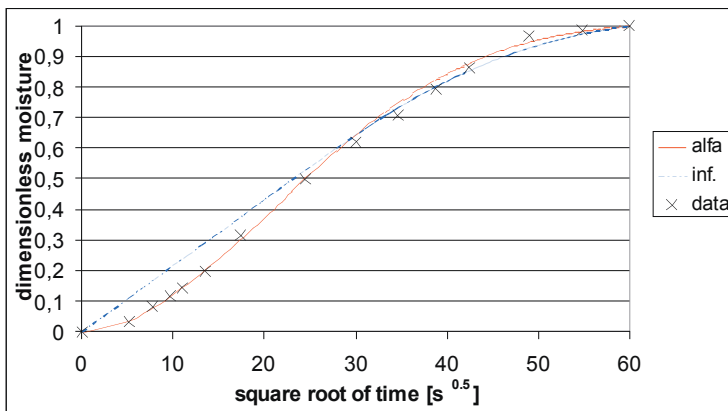


Fig. 4: The dependence of the mean dimensionless moisture uptake on square root of time in tangential direction at 120°C

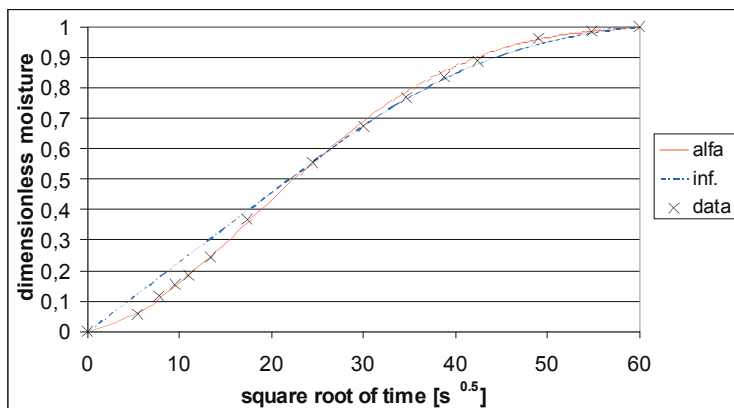


Fig. 5: The dependence of the mean dimensionless moisture uptake on square root of time in radial direction at 120°C

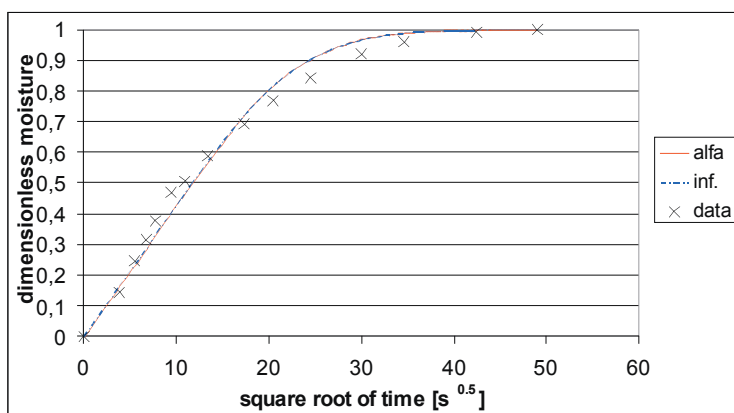


Fig. 6: The dependence of the mean dimensionless moisture uptake on square root of time in longitudinal direction at 120°C

The next tables contain the values of diffusion characteristics as were computed by least square method from data shown at previous figures. The first line with numbers is average and the second one is standard deviation.

Tab. 1: The diffusion coefficient and mean error for the boundary condition of the first order

Temp. [°C]	D [m ² s ⁻¹]			R [%]		
	Tangential	Radial	Longitudinal	Tangential	Radial	Longitudinal
100	5,6E-09	6,2E-09	2,6E-08	0,1884	0,1993	0,1258
	5,1E-10	9,9E-10	5,1E-09	0,0372	0,0516	0,0320
120	8,5E-09	1,1E-08	3,8E-08	0,2310	0,1657	0,1193
	1,2E-09	2,3E-09	1,2E-08	0,0515	0,0423	0,0470

Tab. 2: The diffusion coefficient and mean error for the boundary condition of the third order

Temp. [°C]	D [m ² s ⁻¹]			R [%]		
	Tangential	Radial	Longitudinal	Tangential	Radial	Longitudinal
100	9,1E-09	2,0E-08	2,6E-08	0,0864	0,0783	0,1257
	1,3E-09	8,6E-09	5,1E-09	0,0240	0,0413	0,0320
120	2,8E-08	2,3E-08	3,9E-08	0,0848	0,0654	0,1184
	1,0E-08	1,1E-08	1,4E-08	0,0629	0,0140	0,0479

Tab. 3: The surface emission coefficient and Biot number

Temperature [°C]	α [ms ⁻¹]		Bi	
	Tangential	Radial	Tangential	Radial
100	1,1E-05	6,7E-06	6,1	2,1
	2,7E-06	2,0E-06	2,1	1,4
120	1,7E-05	1,7E-05	2,0	4,6
	2,4E-05	4,9E-06	1,2	2,4

The average equilibrium moisture content of all specimens was 3%.

DISCUSSION

We studied three factors, which influence the diffusion coefficient: high temperature, anatomical direction and method. High temperature had two levels: 100°C and 120°C, anatomical direction had three levels: tangential, radial and longitudinal and method had two levels according to the type of boundary conditions.

From results we can conclude that the value of diffusion coefficient is higher if temperature is higher. At all cases we determined that the diffusion coefficient had the smaller value for 100°C then for 120°C. The value is of order from 10^{-9} to 10^{-8} m²s⁻¹. The diffusion coefficient has the largest value in longitudinal direction. Differences in transverse directions are not so clear, but we suppose that the value must be higher in radial then tangential direction due to presence of wooden rays.

The solution (9) is more complex then solution (6). It describes the change of flux as a function of surface concentration. If surface concentration is constant then the two solutions are equal. We observed this phenomenon at high temperatures for longitudinal direction. It can be seen that the values of diffusion coefficient and mean error are almost the same for longitudinal direction at given temperature. Also we can see at the beginning of fig. 3 and 6 straight line. These facts are not valid for radial or tangential directions at high temperatures. The values of diffusion coefficient differ and the graphs have the characteristic sigmoid curve. The solution (9) is more suitable then solution (6) for radial or tangential direction at high temperatures. The value of surface emission coefficient depends on temperature. Its value is higher if temperature is higher. The Biot number does not depend on temperature. But we must put stress on the high variability of results.

Sergovskij and Rasev (1987) published the value for diffusion coefficient $2,5 \cdot 10^{-9}$ m²s⁻¹ and for surface emission coefficient the value less then 10^{-6} ms⁻¹ for spruce wood at 100°C

in directions perpendicular to grain. Siau (1995) assumed diffusion as activated process. He published relationship among diffusion coefficient, temperature and moisture content. We gain the value $4,5 \cdot 10^{-11} \text{ m}^2\text{s}^{-1}$ from this relationship for 100°C and 5% moisture content for direction perpendicular to grain. All the mentioned values found in literature are lower than our values. The diffusion characteristics values of Sergovskij and Rasev (1987) are closer to our values especially for tangential direction and for method of immediately equilibrated the surface moisture content with the equilibrium moisture content. Also we assumed diffusion of water in wood as activated process. If we took value for diffusion coefficient at 20°C in radial direction for spruce from other data (Babiak and Hrčka 2007) then activation energy is 74 kJmol^{-1} . It is more than values obtained for other species: $30,4 \text{ kJmol}^{-1}$ for black locust, $39,4 \text{ kJmol}^{-1}$ for oak and $27,4 \text{ kJmol}^{-1}$ for poplar from other data (Babiak and Hrčka 2007). Then the calculated values of diffusion coefficient for this species at 100°C are $2,4 \cdot 10^{-10} \text{ m}^2\text{s}^{-1}$ for black locust, $1,0 \cdot 10^{-9} \text{ m}^2\text{s}^{-1}$ for oak and $1,2 \cdot 10^{-9} \text{ m}^2\text{s}^{-1}$ for poplar. These values are also lower than the values obtained in this work.

CONCLUSIONS

Diffusion coefficient is an anisotropic quantity which value depends on temperature even the temperature is high ($100\text{-}120^\circ\text{C}$). Diffusion coefficient reached the highest value in longitudinal direction for higher temperature. The results are not so clear in transverse directions.

The method with surface emission factor was the best description of diffusion as the mean error was the smallest.

Also surface emission factor is anisotropic quantity. It gains high value in longitudinal direction that we can adapt the fact that the method with surface emission factor is on the same qualitative level as the method of immediately equilibrated surface concentration with equilibrium concentration. Surface emission factor has higher value for higher temperature. Biot number for transverse directions does not depend on temperature. The results showed large variability.

Activation energy obtained for spruce wood in radial direction was 74 kJmol^{-1} .

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REFERENCES

1. Babiak, M., Hrčka, R. 2007: Modelling of transport processes in wood. In: Modelling the wood chain: Forestry-Wood Industry-Wood product markets. Helsinki, Ghent University, Pp. 125-133
2. Hrčka, R., Babiak, M. 2007: A method of the diffusion coefficient determining during high temperature acting. Wood Research, 52(2): 99-104
3. Choong, E. T. 1963: Movement of moisture through a Softwood in the Hygroscopic Range. For. Prod. Journal, 13: 489-498
4. Miao, P. 2000: Water movement and heat transfer of Masson Pine lumber during high temperature drying. Ph.D. thesis, University of Nijing forestry, China
5. Ping, M., Liandbai, G. 2003: Water transfer of Masson pine lumber during high temperature drying. Holz als Roh- und Werkstoff, 61: 349-354
6. Požgaj, A., Chovanec, D., Kurjatko, S., Babiak, M. 1993: Štruktúra a vlastnosti dreva. Bratislava, Príroda, Pp. 486
7. Sergovskij, P. S. – Rasev, A. I. 1987: Gidrotermičeskaja obrabotka i konservirovanie drevesiny. 4. izd. Moskva, Lesnaja Promyšlennost': Pp. 360
8. Siau, J. F. 1995: Wood: Influence of moisture on physical properties. Department of Wood Science and Forest Products, Virginia Polytechnic Institute and State University, Pp. 227
9. Stamm, A. J. 1964: Wood and Cellulose Science. New York, Ronald, Pp. 549

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