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KINETICS AND MODELLING OF WATER ABSORPTION PROCESSES IN DIFFERENT TREE SPECIES

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ABSTRACT

A novel two-stage kinetic model for simulating water absorption in wood is presented, explicitly accounting for simultaneous absorption and evaporation in the longitudinal direction and addressing limitations of prior models focused primarily on drying or radial sorption. Water absorption was investigated by partial immersion of samples from three tree species – paulownia (*Paulownia in vitro*), alder (*Alnus glutinosa*), and pine (*Pinus sylvestris*). A computational experiment was conducted using parameter sensitivity analysis of the developed mathematical model. The model demonstrates high fidelity in describing sorption kinetics, with correlation coefficients reaching 85% for absorption (logarithmic dependence) and over 90% for dehydration (exponential reliance). At 20 °C, the paulownia absorption rate exceeded alder by 8% and pine by 23%. These findings enhance understanding of moisture transport mechanisms and offer practical insights for optimizing impregnation processes in wood processing.

Keywords: wood; water absorption; saturation kinetics; parameter sensitivity analysis; mathematical model.

INTRODUCTION

There is a global trend towards the cultivation of fast-growing species (crop rotation from 5 to 10 years). Their primary purpose is the production of wood fibers and biomass. But these species certainly have potential in the manufacturing of solid wood products. One of the fast-growing species is paulownia (*Paulownia in vitro*), a species under cultivation in plantations that is steadily increasing in Ukraine. However, there is still insufficient information on wood properties, and therefore doubts arise regarding the scope of use (Barbu *et al*., 2023; Huber *et al*., 2023).

The behavior of wood and wood-based materials in interaction with water is crucial during material preparation for production and during the operation of the finished product. Water in wood is present in two primary forms: as cell wall water, which interacts with polymer components (cellulose, hemicellulose, and lignin), and as capillary water, which fills the cavities in the porous structure of wood. Understanding the difference between these types of water is critically important, as each has a different impact on the physical, mechanical, and chemical properties of wood and wood-based materials (Kulman *et al*., 2019a; Kulman *et al*., 2019b; Báder and Németh, 2019; Thybring and Fredriksson, 2023). Cell wall water affects the hygroscopicity, expansion, and contraction of wood, while capillary water determines the water absorption and resistance of wood to decay and other biological processes.

These shortcomings need to be solved. The study of fluid flow (bulk and molecular) through wood has become the basis for many woodworking processes (Avramidis, 2007; Kulman *et al.*, 2021a; Tsapko *et al.*, 2022; Vaziri *et al.*, 2023). The results confirm that wood impregnation is an effective method. The principle of impregnation processes is to treat wood with an agent that, under certain conditions, diffuses into the cell walls, where it subsequently polymerizes to obtain the desired properties. Wood of various species has been impregnated with thermosetting resins (Yusof *et al*., 2019; Manabendra *et al.*, 2000; Luo *et al.*, 2021), waxes and oils (Wang *et al.*, 2017; Shiny *et al.*, 2017), monomers and polymers (Broda and Mazela, 2017; Nguyen *et al.*, 2019), acids and anhydrides (Augustina *et al.*, 2022; Horbachova *et al.*, 2024). For example, thermosetting resins, such as phenol-formaldehyde, impart wood greater rigidity and water resistance. On the contrary, waxes can reduce water absorption by forming a protective film on the surface. Oils such as linseed or tung oil penetrate the wood structure, providing additional protection against moisture and rot.

The main difficulty in modeling moisture movement in wood is that multiple mechanisms may contribute to the overall flow, and their relative contributions may vary. Modeling is also complicated by the fact that wood is a porous, anisotropic material. In these models, wood is treated as a porous medium with multiphase flow and heat transfer. The equations are derived from fundamental mathematical models of multiphase flow and heat transfer in porous media, based on conservation principles. However, such models are primarily used to quantitatively describe moisture removal from wood during drying (Ciegis and Starikovicius, 2002; Ciegis *et al.*, 2004; Avramidis *et al.*, 2023).

Existing models often overlook simultaneous absorption and evaporation during partial immersion, focusing instead on drying or non-longitudinal directions, leading to incomplete predictions for impregnation processes. This work overcomes these limitations by introducing a two-stage first-order kinetic model that explicitly accounts for both methods, thereby providing a more accurate simulation for anisotropic wood species such as paulownia.

A deep understanding of the interaction between water and wood is necessary to optimize technologies for processing, storing, and using wood in various applications. It is especially true for new species, such as paulownia. This knowledge can also serve as the basis for further research in the field of wood modification (including low-density), improving performance properties, and expanding its scope of use.

The purpose of this study is to develop and improve mathematical models for the simulation of moisture movement in wood, in particular under conditions of anisotropy and the multiphase nature of this material. The study involves analyzing and optimizing mechanisms that affect moisture flux, with a focus on identifying and quantifying each mechanism's contribution to the overall process.

MATERIALS AND METHODS

The base material, lumber, was provided by Paulownia Energy Ukraine (Lutsk, Ukraine). Three species of wood were used in this study – paulownia (*Paulownia in vitro*), (density 300 kg/m^3), pine (*Pinus sylvestris*), (450 kg/m^3) and alder (*Alnus glutinosa*), (470 kg/m^3). Samples measuring 300 × 20 × 20 mm were cut from each species (Fig. 1). The areas of the radial and tangential sections are equivalent, since radially cut boards were used.

Samples were conditioned at 20°C and 65% relative humidity until reaching an equilibrium moisture content of approximately 10% (measured with an electronic moisture meter, accuracy ± 0.1%). No oven-drying was performed before experiments to simulate natural conditions. Six replicates per species were used, with measurements taken at 1-hour intervals for the first 8 hours, then every 4 hours, and statistical analysis included mean values ± standard deviation.

Paulownia is a deciduous, ring-vascular species. It has clearly defined large vessels in the early wood of the annual ring, which gradually decrease to the late wood. The main feature of paulownia is the size of the vessels – from 100 to 300 microns and beyond (especially in the early zone), which affects the low density of the wood. The walls of the vessels are thin, the rays are wide, and the parenchyma is well developed, especially the axial one, which also contributes to diffusion.

Alder is also a deciduous species, but it is diffusely vascular. The conducting elements (vessels) are small, usually 30 to 80 microns in diameter. They are evenly distributed throughout the annual ring. The vessels occupy a smaller volume than in paulownia, but are the main conducting elements. The walls of the vessels are relatively thin; the parenchyma is developed but less pronounced than in paulownia; the rays are wide. The presence of numerous small vessels provides a high diffusion rate. The smaller lumen diameter creates greater resistance to water flow than in paulownia.

Pine is a coniferous species in which the conducting elements are tracheids. Their diameter is much smaller than that of the vessels, from 20 to 50 microns. Water transport between tracheids occurs through bordered pores of a complex membrane structure with a torus, which can regulate the flow of water and prevent the spread of air emboli, but also limits the flow rate. Tracheids make up 90–95% of the volume of wood. The thickness of the cell walls is usually greater than that of the vessels, especially in late wood. The parenchyma is limited, mainly around the resin ducts; the rays are less pronounced than in hardwoods.

Fig. 1 Samples and measuring instruments.

The humidity and temperature in the room were 65% and 20°C, respectively. An electronic caliper (measurement accuracy 0.01 mm) and a thermometer (± 0.1°C) were also used. An electronic moisture meter (± 0.1%) was used to determine moisture content.

Water absorption measurements were performed by immersing one end of the sample in water. The tests were conducted in accordance with EN ISO 15148. During the tests, periodic moisture measurements were made along the fibers of the samples at a step of 19 mm, equal to the distance between the moisture meter's measuring needles. It amounted to 12 measurements per sample.

Since the speed of capillary movement directly depends on the capillary radius, wood water absorption should occur in two stages. In the first, all microcapillaries (bound water) and part of the macrocapillaries are filled, and in the second, all macrocapillaries (free water) are filled. The transition between stages is defined quantitatively as the point at which the absorption rate equals the evaporation rate, as derived from the kinetic equation (Eq. 1) as dM/dt_absorption = dM/dt_evaporation.

The total mass of water in wood, which is constantly changing due to water absorption and evaporation, was taken as the phase variable.

The model describes the increase in moisture content, with a constant change in the total moisture content of the wood over time. In this case, the change in total humidity will be determined by the basic kinetic equation, which reflects the law of conservation of mass:

$$dW(t) = dW^{+}(t) - dW^{-}(t) \tag{1}$$

Where: $dW^{+}(t)$ – increase in the total mass of water due to impregnation, that is, in the general case, it is diffusion (arrival), over a period of time $d(t)$, kg; $dW^{-}(t)$ – reduction in the total mass of water in wood, due to evaporation (loss) over time $d(t)$, kg.

To better understand the trend of the process, it is worth using dimensionless quantities, as they are the most informative and are not tied to reference systems (Kulman *et al.*, 2021b). To be able to compare and study the saturation kinetics of several different species (simultaneously observed) with different initial weights, we introduce new dimensionless moisture content measurements, namely, dimensionless moisture content (concentration):

$$CB(t) = \frac{W(t)}{W_0} \tag{2}$$

Given the initial conditions t = 0, the introduced dimensionless quantities can be written in the form:

$$CB(0) = 1; CA(t) = 0; CC(t) = 0 \tag{3}$$

The dimensionless moisture content was calculated as $C = (M_t - M_0)/(M_{max} - M_0)$, where M_t is moisture at time t, M_0 is the initial moisture, and M_{max} is the equilibrium moisture, justified by its ability to normalize data across species for comparative analysis.

Previously conducted water absorption experiments led to the conclusion that the wood impregnation process can be considered an analogue of a first-order chemical reaction. Therefore, the kinetic scheme of a sequential process with two elementary stages of the first order will have the form:

$$CA(t) \overset{k_1}{\rightarrow} CB(t) \overset{k_2}{\rightarrow} CC(t) \tag{4}$$

Where: *CB(t)* – current average water concentration in wood at time t; *CA(t)* – maximum water concentration inside the wood at time t, «moisture source»; *CC(t)* – minimum water concentration on the wood surface at this point in time t; k_1 – rapidity of increase in water concentration in wood due to diffusion and other impregnation mechanisms (diffusion coefficient), $g \cdot sm^{-2} \cdot s^{-1}$; k_2 – rapidity of reduction in water concentration in wood by evaporation from the surface of the detail, $g \cdot sm^{-2} \cdot s^{-1}$.

Using the new notation, we can write the basic governing equation (1) in the form:

$$\frac{dCB(t)}{dt} = k_1\big(CA(t) - CB(t)\big) - k_2(CB(t) - CC(t)) \tag{5}$$

This differential equation can be solved using the standard method of separation of variables.

$$\frac{dC}{dt} = k_1(C_m - C) - k_2(C - C_0)$$

$$\int_{C_0}^{C} \frac{1}{k_1(C_m - C) - k_2(C - C_0)} dC \rightarrow \frac{\ln[(-C)k_1 - Ck_2 + k_1C_m + k_2C_0]}{k_1 + k_2} + \frac{\ln[(-k_1)(C_0 - C_m)]}{k_1 + k_2}$$

$$\int_{t_0}^{t} \ln dt \rightarrow t \rightarrow t_0$$

$$t := \frac{(\ln(k_1C_m - k_1C - k_2C + k_2C_0)) + \ln[(-k_1)(C_0 - C_m)]}{k_2 + k_2}$$

$$C_m := 45 \quad C := 41{,}82 \quad C_0 := 10 \quad k_1 := 0{,}15 \quad k_2 := 0{,}015$$

$$\frac{(-\ln(k_1C_m - k_1C - k_2C + k_2C_0)) + \ln[(-k_1)(C_0 - C_m)]}{k_1 + k_2} float, 3 \rightarrow 59{,}2 - 19{,}0i$$

$$(59{,}2^2 + 19^2)^{0{,}5} \rightarrow 62{,}174271206022190092 \tag{6}$$

The degree of hydration was assessed by measuring the gradual saturation of the samples with water, that is, the concentration of water in the wood («moisture source»):

$$\mathrm{CA(t) = M(t)/M_0} \tag{7}$$

Where: *CA(t)* – water concentration in the sample at a point in time t, g/g; *M(t)* – weight of the impregnated sample at a point in time t, g; M_0 – sample weight at the start of testing, that is, t = 0.

New dimensionless quantities for measuring the degree of hydration were introduced, such as the dimensionless moisture content (moisture concentration):

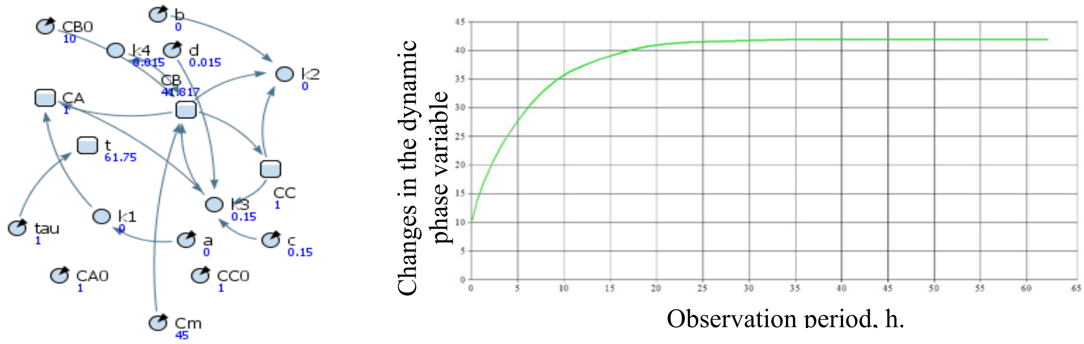
$$CA(t) = M(t)/M_0;\ \ CB(t) = (MB(t) - M_0)/M_0;\ \ CC(t) = (MC(t) - M_0)/M_0 \tag{8}$$

Where: *CA(t)* – maximum water concentration in the sample at a point in time *t,* g/g; *CB(t)* – water concentration at a point in time *t*, g/g; *MB(t)* – weight of water at a point in time t, g; *CC(t)* – minimum water concentration at a point in time *t*, g/g; *MC(t)* – weight of water in microcapillaries at a point in time *t*, g.

The computational experiment is conducted using a parametric analysis of the constructed mathematical model.

RESULTS AND DISCUSSION

A so-called parametric analysis was applied to qualitatively assess the model's ability to describe the processes occurring during hydration. To determine the logical connection between changes in parameters and the dynamics of phase variables over time, it is necessary to assess how the shape of the integral curves changes as the model parameters are varied. Since the parameters of the studied system are hydration rates, it is necessary to determine how the hydration process changes with the ratio of the process rates. Fig. 2a shows the kinetic scheme of the model under specific initial conditions. Fig. 2b shows graphs of changes in the dynamic phase variables (integral curves) in time from 0 to 62 hours.



a b

Fig. 2 Processes during hydration under conditions of changing parameters over time: a – kinetic scheme of the model at the model time of 62 h.; b – water concentration at a point time *CB(t)* (creation of a «moisture source» in the wood).

The average results of six series of experiments on the impregnation of the studied wood species are given in Tab. 1, which characterizes the dependence of changes in moisture content on time and distance (measurement number) from the «moisture source».

Tab. 1. Average moisture values (%) depending on time during impregnation of wood samples.

Time [h]	Measurement number										
	1	2	3	4	5	6	7	8	9	10	11
1	10	10	10	10	10	10	10	10	10	10	10
6	22/20.8/19	13/11/12	10	10	10	10	10	10	10	10	10
12	27/24.8/22	15/13/14	11	10	10	10	10	10	10	10	10
24	31/29/26	16/14/15	12	10	10	10	10	10	10	10	10
48	34/33/30	17/15/16	13	11	10	10	10	10	10	10	10
72	39/35.7/31	19/17/17	14	12/12/11	10	10	10	10	10	10	10
96	41/37.4/33	21/19/19	15	13/13/12	11/10/10	10	10	10	10	10	10
120	41/38.6/34	22/22/20	17/17/16	14/14/13	12/11/11	10	10	10	10	10	10
144	42/39.7/35	23/21/21	18/18/17	15/15/14	13/11/11	11/10/10	10	10	10	10	10
168	44/40.5/35	24/22/23	19/19/18	16/16/15	14/11/12	12/11/11	11/11/10	10	10	10	10
192	44/41.6/36	26/24/24	19/20/19	17/17/16	15/12/13	13/11/11	11/11/11	10	10	10	10
216	45/42.5/37	30/28/26	22/22/20	19/19/17	17/14/14	15/12/12	13/12/11	12/11/11	11/10/10	10	10

Note: The moisture content values (%) are given for the studied species in the following order: paulownia/alder/pine.

A graphical presentation of all the results of fluid diffusion along the fibers is shown in Figure 3.

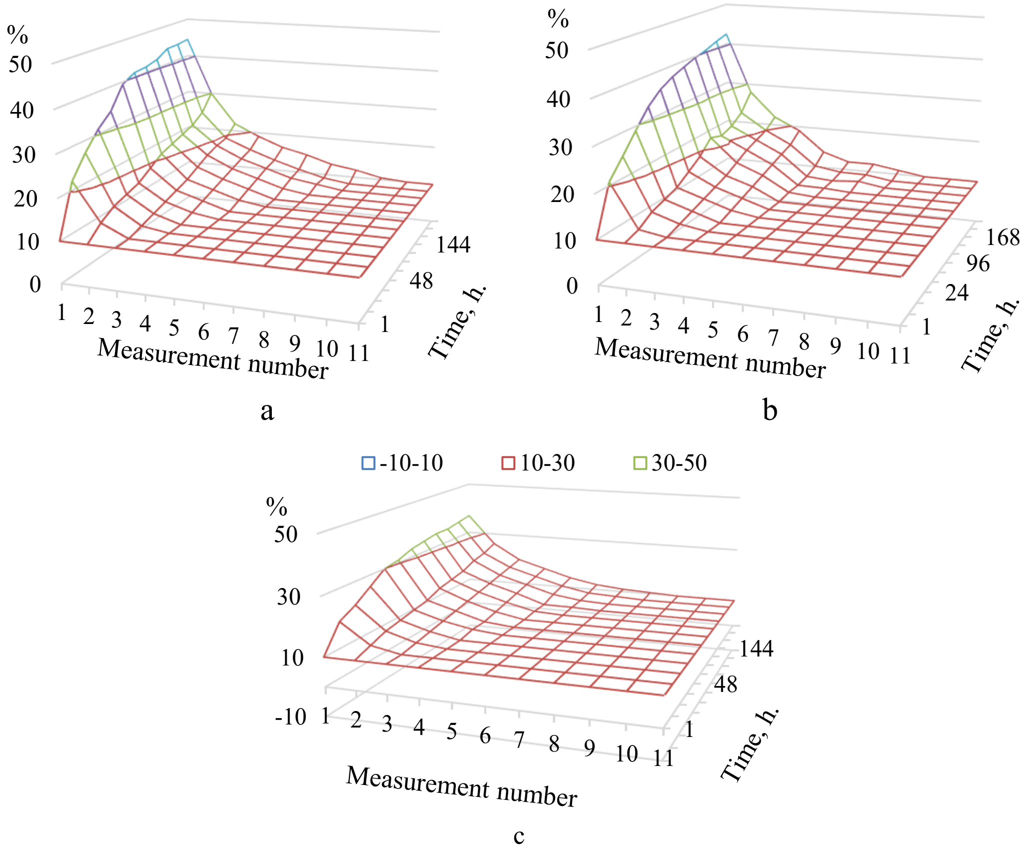
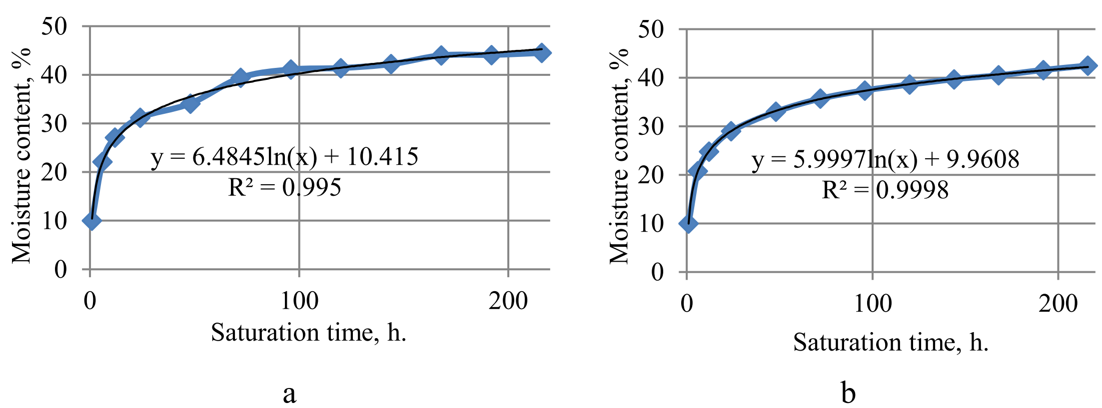
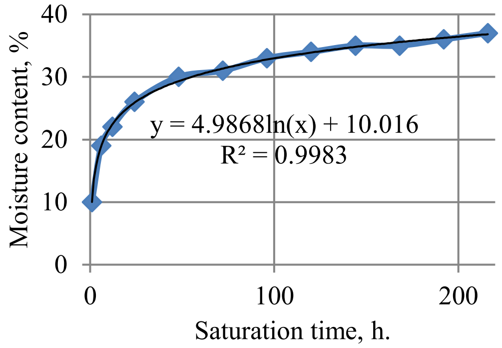


Fig. 3 Three-dimensional gradient diagrams of the dependence of the change in moisture content on the time of moistening the moisture source and the impregnation time: a – paulownia; b – alder; c – pine.

Figure 4 presents the results of the saturation kinetics of a part immersed in water (creation of a «moisture source» inside the wood).





c

Fig. 4 Kinetics of hydration of a piece of wood immersed in water (formation of a moisture source): a – paulownia; b – alder; c – pine.

Figure 4 also shows the trend lines (regression equations) with the highest correlation coefficients. The general nature of all regression equations can be represented as a logarithmic dependence in the coordinates *M(t)*:

$$M(t) = a \ln t + b \tag{9}$$

The nature of the regression line, with logarithmic dependence, reflects the rate of change in the sample's weight, that is, the intensity of hydration. This means that the coefficient before the logarithm of time indicates the hydration rate. By actually differentiating the left and right sides of equation (9), it is possible to determine the rate of change of the sample weight over time:

$$\frac{d(M(t))}{dt} = \frac{d(a \ln t + b)}{dt} = \frac{a}{t} \tag{10}$$

At the same time, the constant *b* does not characterize the kinetics of the process, but depends only on the coordinate system in which the humidity value (moisture content) is determined. That is, it depends on the formula used to determine humidity (absolute or relative).

This understanding of the regression equation as a mathematical model of the hydration process enables comparison of impregnation processes under different conditions and across different species.

Based on the analysis of regression equations, it can be concluded that the hydration rate in paulownia is greater than in alder and pine, and is comparable: $V_{pl} = 6.48$; $V_a = 5.99$ and $V_{pn} = 4.99$, respectively, at a water temperature of 20 °C.

The results of the analysis of the impregnation process, that is, the movement of water inside the wood (diffusion) along the fibers from the source of moisture to the opposite section of the sample located in the air, are presented in Fig. 5.

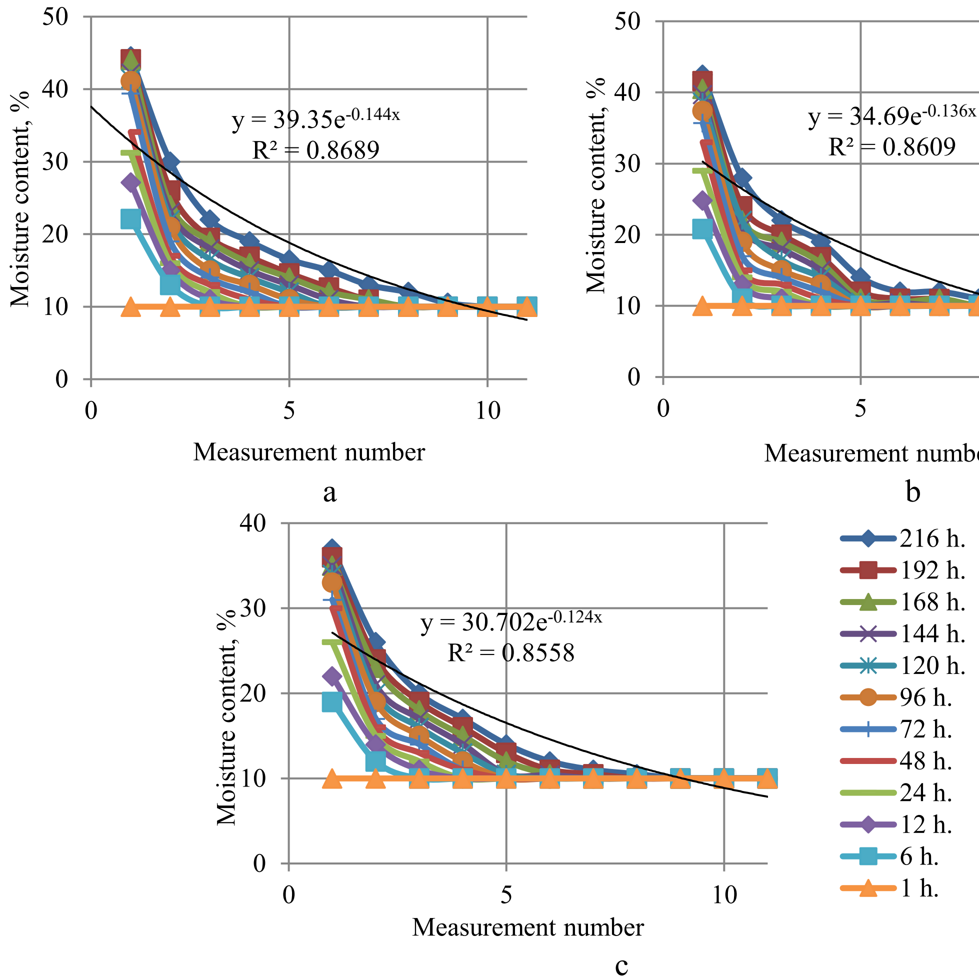


Fig. 5 Kinetics (rapidity) of water movement inside wood (diffusion) along the fibers from the source of moisture to the opposite part of the part located in the air: a – paulownia; b – alder; c – pine.

Figure 5 shows the dependence of moisture content along the fibers at different initial moisture contents of the moisture source. The regression equations and correlation coefficients are shown for the curves with the maximum initial humidity, that is, for time t = 216 h.

The curves for the three species show an exponential decrease in moisture content over time (as indicated by the presence of exponential regression equations), a pattern typical of diffusion processes. However, there are notable differences in the rate and efficiency of diffusion between species. The exponent coefficient (k = 0.144) for paulownia is the highest among the others. This indicates the fastest decrease in moisture content, i.e., the fastest rate of water diffusion along the fibers. For alder, k = 0.136, which is slightly lower than for paulownia, but higher than for pine. The lowest exponent coefficient (k = 0.124) among the three species was found in pine, which indicates the slightest decrease in moisture content and, accordingly, the lowest rate of water diffusion along the fibers.

The regression equation that most fully describes this curve is the exponential one, the equation of which, in general form, can be represented as follows:

$$M(t) = M_0\, e^{kt} \tag{11}$$

In this case, k can be both greater and less than zero. Moreover, the pre-exponential factor M_0 is equal to the value at t = 0, that is, the beginning of the process. The value of M_0 depends on the choice of the coordinate system in which the humidity value is determined and does not characterize the kinetics (speed) of the process in any way, but only determines its initial conditions. In this case, the process rapidity will be:

$$\frac{d(M(t))}{dt} = \frac{d(M_0 e^{kt})}{dt} = M_0 k e^{kt} \tag{12}$$

The coefficient k characterizes the rate of wood impregnation along the fibers. In our case, the highest impregnation rate is in paulownia, the lowest is in pine, and is $k_{pl} = 0.144$; $k_a = 0.136$; $k_{pn} = 0.124$.

The dehydration rates of paulownia and alder differ slightly at 20 °C, which may be a strong argument in favor of simultaneous drying of both species in the same chamber. It allows for improved production logistics.

High correlation coefficients for the regression equations for both hydration and dehydration confirm the hypothesis that these processes are first-order kinetics. That is, the processes can be described (modeled) in the form of ordinary first-order differential equations:

$$\frac{d(M(t))}{dt} = kM(t) \tag{13}$$

Analysis of the research results (Fig. 3) allows obtaining reliable data on the kinetics of physicochemical processes occurring during impregnation. From the point of view of chemistry, we can talk about the speed of chemical reactions (macrokinetics), and from the point of view of physics, we can talk about how water penetrates into wood due to diffusion, capillary or other pressure (Hill, 2006). To date, there is a lot of research devoted to the interaction between wood and water (Tamme *et al.*, 2013; Glass and Zelinka, 2021). However, these works reveal certain contradictions and incompatibility of individual statements. This can be explained by the fact that the physical system consisting of water and wood is extremely complex.

Analysis of the research results (Fig. 3) allows obtaining reliable data on the kinetics of physicochemical processes occurring during impregnation. From the point of view of chemistry, we can discuss the rate of chemical reactions (macrokinetics), and from the point of view of physics, we can discuss how water penetrates wood through diffusion, capillary pressure, or other forces (Hill, 2006). To date, much research has focused on the interaction between wood and water (Tamme *et al.*, 2013; Glass and Zelinka, 2021). However, these works reveal certain contradictions and incompatibility of individual statements. This can be explained by the fact that the physical system consisting of water and wood is highly complex.

Based on the obtained regression equations (Figs. 4 and 5), it was established that when the coordinate system for moisture estimation is changed, the equations for the same species differ only in the values of the constant coefficients, which do not affect the nature of the hydration kinetics at all. However, the structure of the conductive elements of wood has a significant effect on the rate of water diffusion along the fibers. Paulownia, with its large vessels, exhibits the fastest diffusion, alder, with its smaller vessels, is in between, and pine, which contains tracheids, has the lowest diffusion rate. This is an essential factor to consider when selecting wood species for various applications where moisture content control is critical. At the same time, it is known that during the impregnation of wood along the fibers, provided it is partially immersed in water, three kinetic processes co-occur. Hydration of the part that is in water – creation of a source of moisture inside the wood; diffusion (movement) of water inside the wood towards the free end under the action of a concentration gradient; evaporation (dehydration) of liquid from the surface of the sample depending on the temperature gradient and the speed of thermal convection of air around the sample (Kulman *et al.,* 2019c; Augustina *et al.*, 2023).

The model's plausibility is assessed by comparing the experimental absorption (Figs. 3 and 4) with the theoretical results of the kinetic parameters (Equations 7 and 8). Under these conditions, the analytical solution and the numerical model yield the same curves. A high degree of correlation between theoretical and experimental kinetics was observed, confirming the validity of the model. Fig. 3 shows the profiles of water saturation in the samples as a function of wetting time and distance from the moisture source. These concentration profiles are intended to provide qualitative information about the water within the wood, depending on the species at each sample point. This result is consistent with other studies (Amardo *et al.*, 2013; Mahhate *et al*., 2014).

Species differences in absorption and diffusion behavior can be attributed to anatomical features: Paulownia has numerous small vessels (30-80 μm), which provide moderate resistance, while pine tracheids (20-50 μm) with bordered pits limit flow, accounting for its slower rates.

The knowledge gained can serve as a basis for optimizing wood processing, storage, and use technologies, as well as for further research into wood modification techniques to obtain a material with planned properties. In addition, the measurement results enabled us to model the wood-drying process, which can serve as a direction for further research. In future studies, it is worth analyzing the dimensional changes in axial deformation of wood under different immersion conditions in the solution. Acetylation and impregnation of wood with salt solutions also remain promising from the perspective of process kinetics. After all, improved wood processing and storage technologies can reduce material and energy costs, which, in turn, will have a positive impact on the environment and the economy, ensuring more efficient use of natural resources.

CONCLUSION

A novel two-stage kinetic model for longitudinal water absorption in wood is introduced, marking the first application of a first-order sequential scheme that simultaneously accounts for absorption, diffusion, and evaporation during partial immersion. Model verification using computational and experimental data confirms its accuracy in describing the dynamics of paulownia, alder, and pine, with correlation coefficients of 85% for absorption (logarithmic) and >90% for dehydration (exponential). Alder exhibits intermediate absorption rates, 8% slower than paulownia but faster than pine, with dehydration kinetics similar to paulownia, suggesting potential for co-drying these species to optimize processes. Compared to existing models (e.g., those in Ciegis *et al*., 2004), our approach better handles anisotropy by quantifying stage transitions using rate-equality criteria, yielding superior predictions of impregnation duration. In practice, these insights enable optimized impregnation for fast-growing species like paulownia, thereby enhancing product quality in wood-based materials. Limitations include single-temperature testing (20 °C) and a fixed initial moisture content (10%); future work should explore temperature dependence, alternative liquids (e.g., salts), and associated dimensional changes to broaden applicability.

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