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MATHEMATICAL MODELLING OF MOISTURE DISTRIBUTION IN POROUS MEDIA

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We propose the mathematical model for distribution of moisture in porous material during the industrial wetting process for a number of assumptions. The model is presented in form of a boundary problem for ordinary differential equation. In current article we discuss possible methods of the solution of this problem, highlight some problems, which can occur during the solution. At the end of the paper, we present some numerical results of modelling wetting process for different materials and calculation of the parameters. The model under discussion allows to understand better the influence of parameters of the problem in order to optimize the wetting process in industry.

Keywords: mathematical modelling; porous material; moisture distribution; industrial humidification; boundary value problem for ordinary differential equation; boundary value problem for ordinary differential equation.

Introduction

Nowadays, many areas of industry use the moisturization of porous media. As an example we can highlight the textile industry. This process has rather high needs and demands usage of energy-consuming systems of air conditioning. Energy effectiveness and quality of issued production highly depends on on the effectiveness of moisturization process. However, the industrial wetting processes are still underexplored due to extremely small amount of research on this area. The main reason of development gap of this area is deficiency of evidence based methods of choosing optimal parameters of wetting process. Such methods would allow us to tune an air-conditioning industrial systems in order to reach the maximum efficiency. Also, effective control of material moisture during the production process will lead to increase of production quality.

The objective of this paper is to present some reasoning on this area. Below we show useful assumption, which allows us to build a reasonable mathematical model of porous media wetting process. Then we make some analysis of experimental data and compare the modelled data with experimental in order to verify our mathematical model.

The mathematical and numerical modelling of the distribution of relative humidity of conditioned air in a porous medium, particularly within the volume of compactly formed textile semi-finished products, represents a pertinent challenge. This challenge is significant for both the development of theoretical principles and the enhancement of technological processes for the humidification and drying of textile and other materials. As noted in the literature, investigating the humidification process enables the identification of technological parameters that maximize process efficiency. For instance, in reference [1], a study on the non-stationary moisture exchange process between a stationary layer of adsorbent and an airflow passing through it was conducted. It was demonstrated that the use of industrial water absorbers effectively regulates air humidity both during the water adsorption (air drying) and desorption (air humidification) stages. By altering the nature of the adsorbent, the size of its granules, and the contact time with the airflow, the degree of drying and humidification can be deliberately modified.

In reference [2], computer modelling of moisture transfer processes in capillary-porous bodies was performed, highlighting the potential influence of technological interventions on process indicators. Works [3–5] investigated moisture transfer in porous materials within the framework of a nonlinear diffusion equation, presenting a model valid under isothermal moisture transfer conditions. Reference [6] explored the mutual influence of heat and moisture transfer in porous materials, utilizing a system of three nonlinear equations: heat conduction equations for the wet porous material temperature and diffusion equations for air and water concentrations. It is assumed therein that the temperature of the wet porous material always coincides with the temperatures of water, water vapor, and air. These equations encompass all thermophysical parameters of the porous material, dry air, water, water vapor, and transfer coefficients of water and air. Modern computational mathematics methods are applied to solve the problem of simultaneous heat and moisture transfer in porous materials. Particularly, works [7–9] investigated heat and moisture transfer issues using the finite difference method.

In article [10], numerical research results on heat and moisture transfer in porous materials are presented. The model is described by a system of equations for water concentration, water vapor, temperature, and source, as functions of spatial and temporal variables. Studies were conducted for various cases of initial and boundary conditions corresponding to drying a moist sample or humidifying a dry sample. The selection of moisture characteristics for studying the porous structure of materials as the basis for building a porous material model and the methodology for calculating characteristics of the capillary-porous building materials structure are presented in works [11, 12]. The mathematical description of mass exchange for a mixture consisting of various types of textile fibers (wool, viscose, nylon, etc.) with conditioned air is provided in reference [13]. Additionally, the concept of hygrodynamic parameters is defined therein, allowing for the selection of hygrothermal treatment modes for textile fibers depending on the directionality and cyclicality of mass exchange processes. The construction of mathematical models and numerical calculations of humidification-drying processes for porous materials enable the development of comprehensive humidification technologies for fibrous materials using new humidifier designs. These technologies ensure high uniformity of fibrous mass humidification and the necessary moisture increase [14, 15].

Further we assume the effective properties of the porous media are distributed over its volume. The adsorption of water is being considered in elementary volumes. The intensity of the penetration of wet air to isolated inner parts of material is defined mainly by forced airflow parameters and diffusion process. Speed of the reaction in elementary volume also depends on air humidity and thermal conductivity of the material under investigation. Temperature of inner area of the porous media is defined by thermal diffusion and should be taken in account in case of significant temperature fluctuations of wet airflow, which penetrates to the object. In other cases, the fluctuations of temperature in- and outside investigated media could be neglected.

Consideration of porous media as a homogeneous media was offered, for example, in [16], where the kinetic reaction of adsorption was considered in each elementary volume. All kinetic parameters (such as diffusion coefficients) should be averaged over the volume. These values can sufficiently differ of real values and should be defined using the experiments together with mathematical modelling techniques.

The airflow temperature is assumed to be equal at all points of the wetting zone. Such assumption is natural in case of conditioned air, supplied to the subject has a constant temperature. This situation often arises in technical requisitions of real processes of industrial moisturization.

Due to law of perdurability of matter, the moisture φ satisfies the following equation (see [17]):

$$\frac{\partial \varphi}{\partial t} = -\nabla \cdot (j_{con} + j_{dif}) + j_{sou}, \tag{1}$$

where j_{con} is a forced wet airflow defined by initial airflow speed on the boundary of the media under investigation:

$$j_{con} = \varphi \cdot \mathbf{w},$$

$\mathbf{w} = (w_1, w_2, w_3)$ is a vector of speed of the conditioned airflow through the porous media;

$$j_{dif} = D\nabla\varphi$$

is an airflow due to diffusion of water; D is a mean diffusion coefficient, which differs from real value due to pseudohomogeneous assumption.

j_{sou} is the negative source due to wet airflow moisture loss, determined by water adsorption at each point of volume of pseudohomogeneous media:

$$j_{sou} = kF_s f(\varphi), \tag{2}$$

where k is a constant of adsorption per unit of surface, and F_s is a specific surface area of a unit of elementary volume of porous media under investigation. Density $f(\varphi)$ of the negative source of moisture adsorption j_{sou}, obviously, depends on the concrete mechanism of wetting.

Unfortunately, most of existing mathematical moisture models are devoted to private physico-chemical cases and can not be used for modelling of moisture processes in shared cases. Below we consider in details the modelling and defining the dependence $f(\varphi)$, and offering our approach to this problem. For now we assume the function $f(\varphi)$ is determined experimentally.

1. Modelling of the Equilibrium Moisture

Building of the mathematical model of wetting process, i.e. calculation of moisture distribution in volume of the material under investigation, demands knowledge of the density $f(\varphi)$ of negative source j_{sou}. Thus, it is reasonable to start consideration of moisturization process model with problem of determination and modelling of this function; In current section we also consider some parameters, affecting on it.

The function $f(\varphi)$ is equal to the equilibrium moisture of the material W_e, which depends on the relative conditioned wetting airflow humidity. This function can be measured experimentally, or it can be modelled.

In Fig. 1, graphs depicting the relationship between the equilibrium moisture content of porous textile material, W_e, and the relative humidity of air, φ, obtained experimentally and presented in the study by [18].

Modern moisture adsorption theory does not provide an accurate analytical dependence $W_e(\varphi)$ for all interval of changing $\varphi \in [0, 1]$. There are a lot of approximate approaches (see, for example, [19]), but all of them can describe the function $W = f(\varphi)$

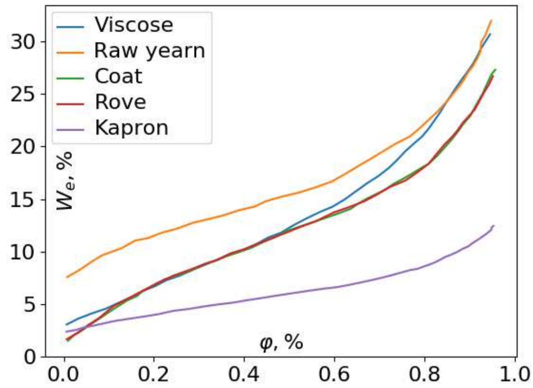


Fig. 1. Fibril equilibrium humidity dependencies $W = f(\varphi)$ on the relative humidity for viscose (blue curve), raw yarn (orange curve), coat (green), rove (red), and kapron (magenta curve)

only for some intervals of changing the relative air humidity φ. Below we consider it in details.

The form of adsorption isotherm is defined by type of connection of moisture with wet material (see [20]). The interval of relative humidity $\varphi \in [0,\, 0,15]$ on the curve is convex and defined by the monomolecular adsorption. In interval $\varphi \in [0,15,\, 0,8]$ the dependence is concave. Changing of the function character caused by changing the adsorption mechanism: this interval is defined by multimolecular adsorption. The last part $\varphi(x) > 0,8$ corresponds to very fast capillary condensation.

However, analysing the experimental curves on Fig. 1, it is seems to be reasonable for regressive descriptions to highlight only two intervals, joining together second and third part. Indeed, changing of convexity and concavity of the curve is provided by some value $\varphi_c \in (0,6,\, 0,7)$, precise value of which depends on the concrete porous material. In other words, in interval $\varphi \leq \varphi_c$ we can see the convexity of the adsorption curve, which changes to concavity in interval $\varphi > \varphi_c$. Below we derive the dependence $W_e = f(\varphi)$ for each of these intervals.

1. The adsorption mechanism of interval $\varphi(x) \leq \varphi_c$ is mainly provided by monomolecular adsorption, which lead to the set of useful assumptions. In this interval it is reasonable to assume the amount of adsorbed liquid increases in proportion to its value with current humidity φ. This assumption is due to the fact that condensed molecules of liquid become new adsorption centers and promote increase of wetting speed. In other words, $\frac{dW_e}{d\varphi} \propto W_e$. Also, this speed must be proportional to the difference $(W_m - W_e)$, where W_m is the maximum (limit) humidity of porous material, i.e., the saturating point. Summing up these words, we obtain the following equation:

$$\frac{dW_e}{d\varphi} = kW_e(W_m - W_e),$$

where k is some coefficient, which will be considered in Section 2.

Solution of the last equation depends on the constant W_n, defined with the equilibrium moisture at the initial moment of time (in sense of quasi-stationary process)

$$W_e(\varphi) = \frac{W_n}{1 + (W_n/W_m - 1)e^{-k\varphi}}. \tag{3}$$

Note that the model (3) provides that the maximum speed of changing W_e occurs when $\frac{\partial^2 W_e}{\partial \varphi^2} = 0$, i.e. when $k^2 W_e(W_m - W_e)(W_m - 2W_e) = 0$. Due to $W \in [0, W_m]$, it leads to $W_e = W_m/2$, and

$$\varphi = \frac{1}{W_m k} ln\Big(\frac{W_m}{W_n} - 1\Big). \tag{4}$$

The last expression can be useful for consideration of problems of optimization of porous material wetting in dependence of humidity of conditioned air.

2. In interval $\varphi(x) > \varphi_c$ wetting is provided by another adsorption mechanisms: poly-molecular and capillary. In this case we can assume (see [21]) that W_e is growing exponentially:

$$W_e(\varphi) = k_2 e^{k_1(\varphi - \varphi_c)}, \tag{5}$$

where k_1, k_2, and φ_c are some constants which can be chosen, for example, using the least square optimization. We consider question of determination of them in Section 2.

Summarizing the considered cases 1 and 2, we obtain the general expression for the equilibrium moisture content as a function of the humidity of the airflow, $W_e(\varphi)$, over the entire range of variation of relative air humidity, $0 \leq \varphi \leq 100$ %

$$W_e(\varphi) = k_2 e^{k_1(\varphi - \varphi_c)} + \frac{W_m}{1 + \big(\frac{W_m}{W_n} - 1\big)e^{-k\varphi}}. \tag{6}$$

On Fig. 2 we show an example of such curve:

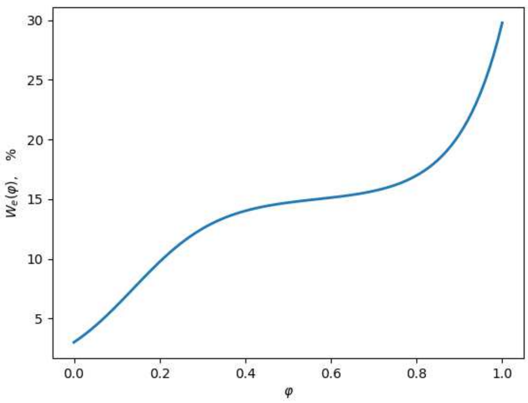


Fig. 2. Example of the hysteresis branch, calculated using 6 with the parameters: $k_1 = 0,1, k_2 = 2, \varphi_c = 0,8, W_m = 15, W_n = 3, k = 0,1$

2. Parameters of the Process and Ways to Obtain Them

Objective of this section is the discussion of physical constants and other parameters of cost mathematical model.

Consider firstly a sponginess ε of the wetting material. This parameter affects on the square S of surface of the material under reaction, on line speed of movement of conditioned air inside pseudohomogeneous media, on the constant of maximum humidity of the material (W_m) and other parameters. The sponginess (or porosity coefficient) can be determined using the porous sample mass M, its volume V_s, and density ρ of fibrils of the material

$$\varepsilon = 1 - \frac{M}{V_s\rho}. \tag{7}$$

Note that $\varepsilon \in [0,1]$. It is easy to see that compression of the material twice is decreasing the sponginess by $3-8\%$. Values of the textile materials under consideration can vary in interval $\varepsilon \in [0,6,\ 0,9]$.

According to wetting process, the specific response surface S is also very important parameter. Obviously, increase of this parameter caused more effective wetting process due to major amount of adsorbed on this surface liquid. The value S is defined mostly with fibril radius r, density ρ of material, and sponginess ε. In the simplest case, assuming regular fibril structure and ignoring its roughness and dependence on ε, the specific surface can be calculated as follows:

$$S = \frac{2p_e}{\rho r}, \tag{8}$$

where p_e is a specific mass of the material.

In order to determine values of specific surface, approximated to real conditions, we need to collect and process the experimental data of dependence of S on r and ε using the least square method:

$$S = a_0 + a_r r + a_2\varepsilon + a_3 r\varepsilon. \tag{9}$$

Numerical experiments show that S can be approximated within tolerable error as follows:

$$S = 3066,9 - 574,9r + 24,5\varepsilon \tag{10}$$

for units cm^2/cm^3. Note that model (9) demands consideration only linear dependencies between S, r and ε.

According to speed of movement of wetting air we note the following. Assuming the volume velocity w_0 on the boundary of a sample is known, the linear speed w in equation (13) can be calculated from the formula $w = \varepsilon w_0$. During the wetting process the linear volume speed w can change. It increases due to decrease of the pores volume and decreases due to stagnation of the airflow in porous media. Some very accurate calculations and models demand some coefficients, depending on current humidity of porous media, but in practical cases we rarely need them.

Coefficients k, k_1 and k_2 also sufficiently affect on the approximation quality of the model under consideration. Most important of these coefficients is k due to location in the part of equation (6), which mostly affects on initial and middle intervals of $\varphi(x)$. This coefficient can be found using modified representation (3):

$$e^{-k\varphi} = \frac{W_n\big(W_n - W_e(\varphi)\big)}{W_e(\varphi)\big(W_n - W_m\big)}. \tag{11}$$

From the latter equation, the coefficient k can be easily obtained using the least-squares method on experimental data. Importantly, equation (11) is meaningful only when $W_n < W_e(\varphi)$; however, this condition holds true and can be inferred from the experimental data depicted in Fig. 1.

On Fig. 3 we compare the modelled curves with experimental curves, shown on Fig. 1. The models were created with the parameters, calculated using least-square method, as it

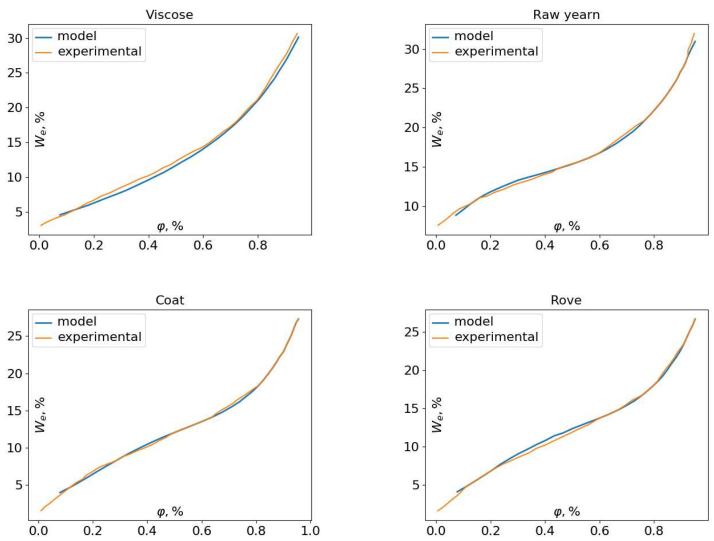


Fig. 3. Modelled curves (orange) built with parameters, calculated with least-square method, compared with experimental curves (blue). The parameters are presented in Table

is described abowe. Calculated parameters are presented in Tabel. Note that the "Error" field in this tabular means the error of modelling curve according to the experimental one, i.e. the descripancy.

Table

The parameters for materials, calculated via least-square method

Material	W_m	W_n	k	k_1	k_2	φ_c	Error (%)
Viscose	14, 9	3, 5	3	4, 4	3, 3	0, 55	7
Raw yearn	13	6	3	4, 5	10	0, 55	5
Coat	13	2, 7	2	6, 6	6, 5	0, 65	7
Rove	13	2, 7	2	6, 5	7	0, 65	7

3. Mathematical Model of Moisture Distribution in Volume of Porous Media

The equation (1) can be written as follows:

$$\frac{\partial \varphi}{\partial t} = \left(w_1 \frac{\partial \varphi}{\partial x} + w_2 \frac{\partial \varphi}{\partial y} + w_3 \frac{\partial \varphi}{\partial z} \right) - D \left(\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} \right) + kF_s f(\varphi). \qquad (12)$$

Firstly, we assume the vector **w** to have a constant coefficients.

Besides this, we assume the process of moisture distribution in volume to be quasi-stationary. In other words, the humidity of wet airflow, coming to the material, assumed to be constant for big time intervals, which means $\frac{\partial \varphi}{\partial t} = 0$ inside these intervals.

Also, we assume that the three-dimensional equation (12) can be reduced to one-dimensional. The possibility of such reduction is defined by wet airflow. For example, such reduction can be done in cases of stream-line airflow with speed vector perpendicular to the boundary of material under investigation. Such situation is common for wetting process and, thus, assumption is reasonable.

In these assumptions, the equation (12) is being simplified as follows:

$$D\frac{\partial^2\varphi}{\partial x^2} + w\frac{\partial\varphi}{\partial x} = F_s \cdot f(\varphi). \tag{13}$$

To solve the last equation with finite-difference approach, we need to know the form or values of the function $f(\varphi)$, mean value of the diffusion coefficient D, linear volume speed of the flow w, specific surface F_s, and boundary conditions for the function $\varphi(x)$. Now we derive these conditions.

Obviously, the humidity value on the bound at the point $x = 0$ is equal to wet airflow humidity φ_0, i.e.

$$\varphi(0) = \varphi_0. \tag{14}$$

In order to obtain $\frac{\partial\varphi}{\partial x}|_{x=0}$, consider in porous media an elementary volume V_m of unit cross-section square and small thickness. Respective humidity of airflow $\varphi(x)$ in this volume is decreasing with distance from the boundary due to the deposition of moisture in pores of media under investigation. Denoting the humidity on distance Δx from the boundary as φ_Δ, we can write for changing of moisture:

$$(\varphi_0 - \varphi_\Delta) = \frac{Q_p^0 - Q_p^\Delta}{Q_{max}},$$

where Q_p^0 and Q_p^Δ are amounts of aqueous vapor in the unit volume of wet airflow before and after wetting the volume V_m of porous media; Q_{max} is the maximum amount of aqueous vapor in unit volume of wet airflow. In this case, the value $Q_{max}(\varphi_0 - \varphi_\Delta) \cdot V_m/V_e$ is the adsorbed moisture content in the volume V_m. V_e is a unit value.

$$\rho S_m \int\limits_0^{\Delta x} \big[f(\varphi(x)) - W_0\big] dx,$$

where S_m is a square, covered with material under investigation, ρ is the density of porous media, W_0 - specific humidity of the investigated material before wetting. Thus, we obtain:

$$Q_{max}(\varphi_0 - \varphi_\Delta)\frac{V_m}{V_e} = \rho S_m \int\limits_0^{\Delta x} \big[f(\varphi(x)) - W_0\big] dx.$$

Dividing the last equation by Δx and calculating and pass on to the limit $\Delta x \to 0$. We assume the area V_m after passage to limit will be a part of unit surface S_m equal to the square of the pores: εS_e. S_m in this case is the rest part of unit surface, i.e. part which is not covered with porous material: $S_m = (1-\varepsilon)S_e$. Thus, we obtained the Neumann boundary condition for the function $\varphi(x)$:

$$\frac{d\varphi}{dx}(0) = -\frac{1-\varepsilon}{\varepsilon} \cdot \frac{\rho}{Q_{max}}\Big[f\big(\varphi(0)\big) - W_0\Big]. \tag{15}$$

Also, without lost of generality, we assume that exists a distant of a boundary point, in which the humidity of air is constant in pores. Thus, denoting this distance as δ, we can produce also the left boundary condition, which can be used for controlling the numerical solution:

$$\left.\frac{d\varphi(x)}{dx}\right|_{x\geq\delta} = 0. \tag{16}$$

Thus, we described the problem under investigation as a Cauchy problem for ordinary differential equation, written with expressions (13) – (16). This mathematical model is only an approximation of the wetting process, but, with correct choosing of process parameters, it gives a possibility to calculate water distribution in pores of the material under investigation in rather accurate way.

Despite the fact that Cauchy problem for ordinary equations is well-developed, numerical solution of it has some difficulties due to classical instability of the equation (13). In order to show this problem, we transform the equation (13) to the system of two differential equations, considering the function $\psi(x) = \dfrac{d\varphi}{dx}$:

$$D\frac{d\psi}{dx} + w\frac{d\varphi}{dx} = F_s f(\varphi), \quad \frac{d\varphi}{dx} = \psi. \tag{17}$$

In order to show the instability of this system, we simplify it in assumption of $w \approx 0$, i.e. amount of air, which penetrates to the porous media is small. The last system can be written as follows:

$$\begin{aligned} &D\frac{d\psi}{dx} = F_s f(\varphi), \\ &\frac{d\varphi}{dx} = \psi. \end{aligned} \tag{18}$$

The secular equation for the last system:

$$\lambda^2 - F_s\frac{df}{d\varphi} = 0, \tag{19}$$

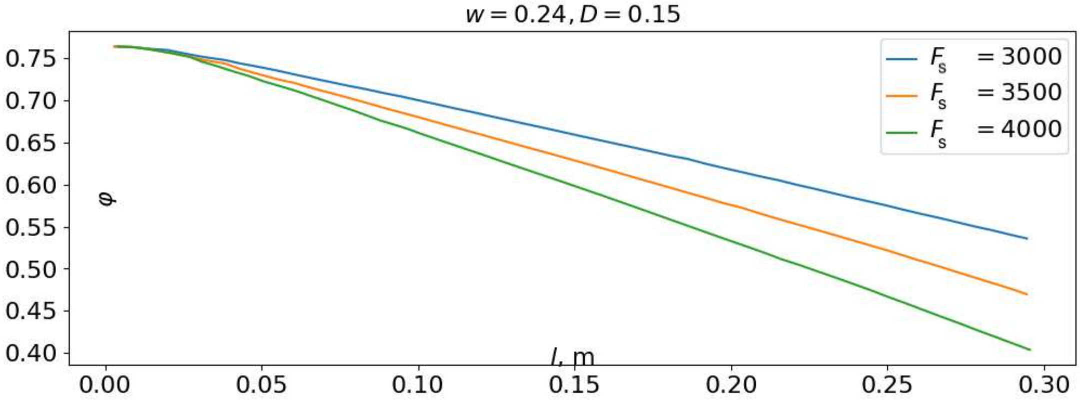
where λ is some formal unknown value ([22]). Since the function $f(\varphi)$ is an adsorption curve, it is a monotonic function with the positive everywhere derivative. Thus, the equation (19) has a positive root. This fact shows the possible instability of the solution of the system (18), and, obviously, of more complicated system (17).

Numerical experiment shows that, despite this fact, the finite-difference Runge–Kutta method can be used for solving this system. In this case, integrating step is being chosen authomatically with a numerical solution control by the condition (16).

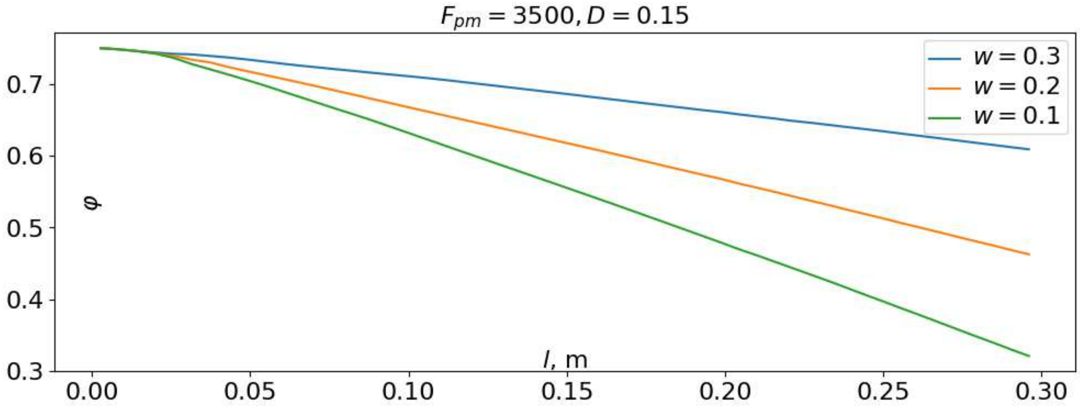
4. Numerical Results

Fig. 4 demonstrates results of calculation of distribution of the humidity over the distance l from the boundary.

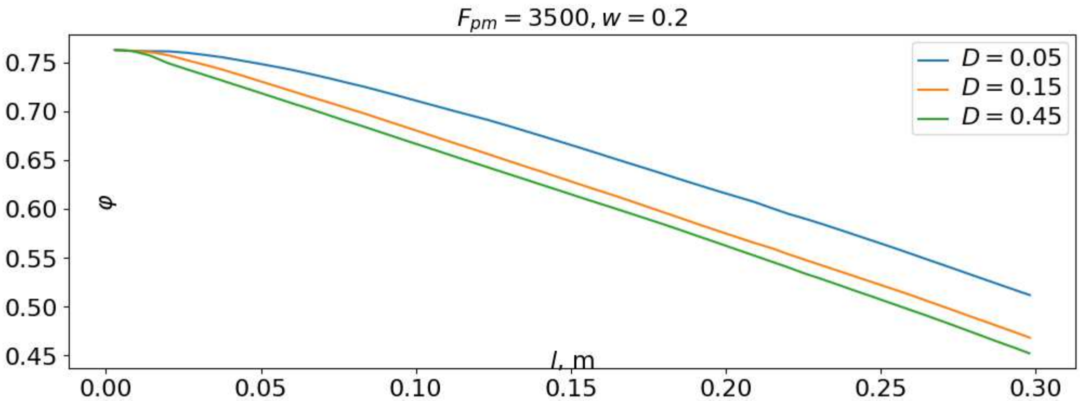
Analysing numerical results one can see, that value φ decreases monotonically with increasing of the distance of boundary until it reaches some limit value. As it follows from Fig. 4 a), increase of specific surface of media leads to more intensive decrease of wetting airflow humidity φ with the distance of boundary. Analyzing Fig. 4 b) allows to conclude



a)



b)



c)

Fig. 4. Calculated distribution of the relative humidity $\varphi, \%$ of conditioned airflow over the thickness of the pmous material under investigation: a) $w = 0,24, D = 0,15$: 1st curve – $F_s = 3000$, 2nd curve – $F_s = 3500$, and 3rd curve – $F_s = 4000$; b) $D = 0,15, F_s = 3500$: 1st curve – $w = 0,3$, 2nd curve – $w = 0,2$, 3rd curve – $w = 0,1$; c) $w = 0,2, F_s = 3500$: 1st curve – $D = 0,05$, 2nd curve – $D = 0,15$, 3rd curve – $D = 0,45$

that decrease of flow speed also leads to more effective wetting process; Fig. 4 c) also shows the same situation with increase of diffusion coefficient D.

As a conclusion, we can highlight the following. Using the pseudo-homogeneous approximation of the material under research, we can use averaged values of physical and technological parameters. Together with some physico-mathematical descriptions of the wetting process of capillary media, this approach allows us to construct a solid mathematical model and formulate the boundary problems for humidity of the conditioned air inside the target porous object. On the base of discussed methods of solution of these problems, we calculated and presented the solutions for different technological and physical parameters.

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МАТЕМАТИЧЕСКОЕ МОДЕЛИРОВАНИЕ РАСПРЕДЕЛЕНИЯ ВЛАЖНОСТИ В ПОРИСТОЙ СРЕДЕ

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Мы предлагаем математическую модель распределения влаги в пористом материале в процессе промышленного увлажнения. С использованием ряда предположений, модель может быть представлена в виде граничной задачи для обыкновенного дифференциального уравнения. В данной статье мы обсуждаем возможные методы решения этой задачи, выделяем некоторые проблемы, которые могут возникнуть в процессе решения. В конце статьи мы представляем некоторые численные результаты моделирования процесса увлажнения для различных материалов и параметров процесса. Модель, рассматриваемая в статье, позволяет лучше понять влияние параметров задачи с целью оптимизации процесса увлажнения в промышленности.

Ключевые слова: математическое моделирование; пористый материал; распределение влаги; промышленное увлажнение; граничная задача для обыкновенного дифференциального уравнения.

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