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HEAT AND MASS TRANSFER IN POROUS MEDIA

MASS TRANSFER IN THE PROCESS OF DRYING OF POROUS MATERIALS

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The mass transfer in the process of drying of deformable porous bodies was theoretically investigated and the corresponding mass-transfer equation was analytically solved. On the basis of experimental data on the drying of porous materials, the ill-posed inverse problem on determination of the region of regular change in the effective diffusion coefficient and in the porosity of a porous-material layer with time was solved.

Keywords: *drying, mass transfer, porosity, deformation, ill-posed problem, effective diffusion, deforming stress, sinuosity of pores, shear viscosity.*

Introduction. The drying of porous materials is widely used in the food and chemical industries as well as in agriculture. The process of drying of such materials, in particular of foodstuffs, was experimentally investigated in many works [1–4]. On the basis of these investigations, different empirical dependences defining the time distributions of the moisture content in porous materials subjected to drying were obtained and their diffusion coefficients were determined.

In [5–7], the mass transfer in the process of convective drying of a porous material was theoretically investigated and the convective-diffusion equation for this process was analytically solved for the purpose of determining the criteria dependence of the Sherwood Sh number on the Reynolds and Schmidt numbers in the case of molecular transfer of moisture in a porous-material layer.

The drying of a porous material occurs with fairly complex physical effects (such as the transfer of moisture in the irregular-shape capillaries of the material and its phase transformations) because many parameters of this material are determined by its humidity and porosity. In [8], the dependence of the density and porosity of a porous material on its relative humidity was experimentally investigated and the correlative dependence

$$\varepsilon = 0.038 + 0.03 \exp\left(-\frac{X}{X_0}\right)$$

was obtained for the temperature interval T = 30–60°C. Since the moisture content of a material subjected to drying is determined by the time of its treatment in a drying apparatus, in [9] the dependence of the diffusion coefficient of a material on the time of its drying was investigated in the temperature interval T = 85–105°C.

It should be noted that the drying of a porous material leads to a decrease in its volume and a change in the geometry and shape of the body because of the deformation and compaction of its layers under the action of the internal deforming stresses. Due to these effects, the porosity, density, and effective diffusion coefficient of the material change depending on the drying time. The main mechanism of drying of a porous material in its bulk is the diffusion (molecular, Knudsen) transfer of moisture to the surface of the body, and moisture is transferred from the surface of the body to the gas flow mainly due to the convective diffusion. The mass transfer in a porous material is determined by the geometry of its pores (their sinuosity, size, etc.), which is accounted for by the coefficient of effective Knudsen diffusion $D_{\text{Kn}} = 97r\left(\frac{T}{M}\right)^{1/2}\frac{\varepsilon}{\eta_{\text{d}}}$. An important stage in the drying of a porous material is the convective transfer of

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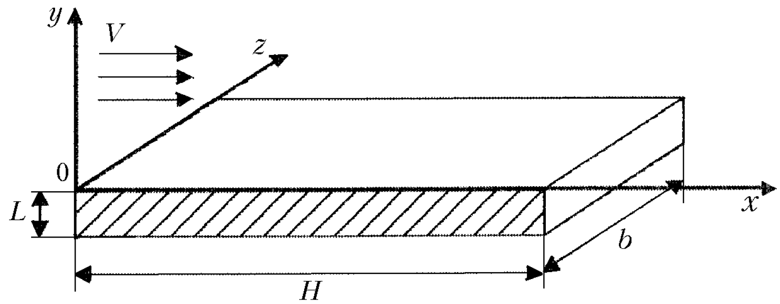

Fig. 1. Scheme of drying of a plane body.

vapor from the surface of the body to the bulk of the moving gas. In this case, the value of the mass transfer depends on the character of the gas flow (if it is laminar or turbulent). At large Reynolds numbers, the mass transfer from the surface of the material is due to the turbulent diffusion [10, 11] determined by the characteristics of turbulence (the relative dissipation energy, the scale of turbulence, and so on).

The aforesaid allows the conclusion that the determination of the diffusion coefficient in the bulk of a porous body subjected to drying and in the gas flow can be reduced to the estimation of the variable effective diffusion versus the porosity of the material and the time of its drying. In the present work, the mass transfer in the process of drying of deformable porous materials is considered.

Mass Transfer in the Process of Drying of a Porous Material with Consideration for Its Compaction. The drying of a porous material occurring with heat and mass transfer causes physical changes in it and a transformation of its microstructure. The main internal parameters of a porous material subjected to drying is its density and porosity related by the equation $\varepsilon = 1 - \frac{\rho}{\rho_d}$ as well as the effective diffusion coefficient dependent on the porosity of the material. These parameters are mainly dependent on the methods of drying and are determined by its rate, because, at a large rate of drying, the material is deformed and compressed under the action of the temperature-dependent internal deforming stresses, with the result that cracks and failures can appear in it [12, 13]. Experimental investigations of the influence of the moisture content of a porous material and its temperature on the parameters of the drying process have shown that, at the early stages of drying of such a material, its density and diffusion coefficient increase and reach maximum values, whereupon they decrease monotonically [14–16]. Thus, the drying of deformable porous materials leads to a change in their density, porosity, and effective diffusion coefficient.

In the case where an isotropic porous body is dried in a laminar flow at a constant temperature, the mass transfer in its plane layer is described by the equation (Fig. 1)

$$\frac{\partial M}{\partial t} + V_x \frac{\partial M}{\partial x} + V_y \frac{\partial M}{\partial y} = D_* (\varepsilon, t) \left(\frac{\partial^2 M}{\partial x^2} + \frac{\partial^2 M}{\partial y^2} \right). \tag{1}$$

As a result of the compaction of the layer under the action of the internal deforming stresses $\sigma_d(T)$, its porosity changes by the following law [17]:

$$\varepsilon = \varepsilon_0 \exp \left(-\frac{3}{4} \frac{\int_0^t \sigma_d dt}{\xi_s} \right). \tag{2}$$

On the basis of available experimental data on the effective diffusion coefficient of porous materials [18], we derived the empirical dependence

$$\frac{D_*}{D_0} = 0.62\varepsilon + 0.285\varepsilon^{4.4} . \tag{3}$$

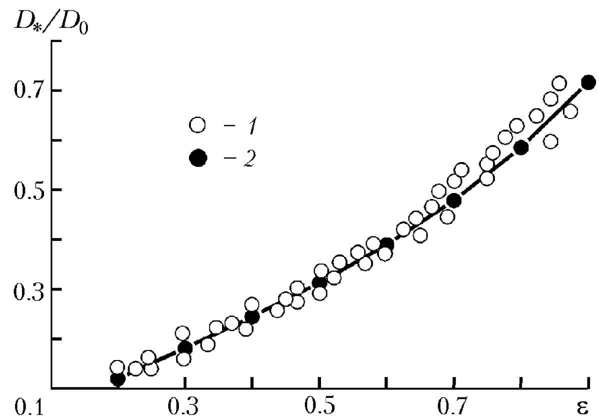

Fig. 2. Change in the effective diffusion coefficient versus the porosity of the body: 1) experimental data [18]; 2) data calculated by formula (4).

At $\varepsilon < 0.55$, expression (3) can be transformed into the linear dependence accounting for the sinuosity of the pores η_d (Fig. 2):

$$\frac{D_*}{D_0} \approx 0.62\varepsilon\eta_d \,. \tag{4}$$

In the general case, the effective diffusion coefficient of an inhomogeneous anisotropic porous material depends on the space coordinate and time.

We now consider the solution of Eq. (1) at small Peclet numbers $\mathrm{Pe} = \frac{Vd}{D} << 1$ in the case where the deformation of a porous material is small and its diffusion coefficient changes by the general law

$$\frac{\partial M}{\partial t} = D_* (\varepsilon, t, y) \frac{\partial^2 M}{\partial y^2} \,, \quad t = 0 \,, \quad M (t, y) = M_0 \,; \quad t > 0 \,, \quad y = L \,, \quad M (t, y) = M_{eq} \,. \tag{5}$$

In the case where the effective diffusion coefficient changes only with time, it can be determined with the use of (4) as

$$D_* (\varepsilon, t) = D_0 \psi_+ (t) \,, \tag{6}$$

where $\psi_+(t) = A\varepsilon_0 \exp \left(-\frac{3}{4} \frac{\int_0^t \sigma_d(t) dt}{\xi_s} \right)$ and $A = 0.62\eta_d$. Introducing the new variables $\zeta = \zeta_0(l_0) + \int_{l_0}^{1} \frac{dy}{D_* s_0}$ and $f(\zeta) = \int_{l_0}^{1} \frac{dy}{\sqrt{D_*}}$ and performing simple rearrangement of Eq. (5) for the one-dimensional mass transfer, we obtain

$$\frac{\partial^2 M}{\partial \zeta^2} = \left(\frac{df}{d\zeta} \right)^2 \frac{\partial M}{\partial t} \,. \tag{7}$$

The independent variables ζ in (7), serving as a space coordinate, is numerically equal to the potential of the steady-state mass transfer in the tube of flow being considered at $\partial M/\partial t = 0$. For solving (7), it makes sense to approximate the function $f(\zeta)$ in the following way:

$$f(\zeta) = b\zeta^{\alpha} \,. \tag{8}$$

Then Eq. (7) can be written with the use of (8) and the Laplace transform [19] in the space of φ-representations as

$$\frac{d^2\vartheta}{d\zeta^2} - \left(\frac{df}{d\zeta}\right)^2 \lambda\vartheta = 0 \,,$$

$$\vartheta(l, \lambda) = \varphi\,[F(l, t)] = \int_0^\infty \exp(-\lambda t)\, F(l, t)\, dt \,, \quad F(l, t) = M(l, t) - M(l, 0) \,. \tag{9}$$

Substituting (8) into (9), we obtain a modified Bessel equation, and, expressing ζ in terms of f with the use of formula (8) in the form $\zeta = \left(\frac{f}{b}\right)^{\frac{1}{\alpha}}$, represent the solution (9) in the form

$$\vartheta(f, \lambda, \alpha) = \left(\frac{f}{b}\right)^{\frac{1}{2\alpha}} \left[A_1 K_{\frac{1}{2\alpha}}(f\sqrt{\lambda}) + A_2 I_{\frac{1}{2\alpha}}(f\sqrt{\lambda})\right]. \tag{10}$$

Here, $I_{\frac{1}{2\alpha}}(x)$ and $K_{\frac{1}{2\alpha}}(x)$ are first-kind and second-kind modified Bessel functions of imaginary arguments and A_1 and A_2 are coefficients. We will seek particular solutions satisfying the first-kind boundary conditions:

$$\lim_{f\to 0} \vartheta(f, \lambda, \alpha) = \vartheta(0, \lambda, \alpha) \,, \quad \lim_{f\to\infty} \vartheta(f, \lambda, \alpha) = 0 \,. \tag{11}$$

The first term of (10) satisfies the second condition of (11); therefore,

$$\vartheta(f, \lambda, \alpha) = A_1 \left(\frac{f}{b}\right)^{\frac{1}{2\alpha}} K_{\frac{1}{2\alpha}}(f\sqrt{\lambda}) \,. \tag{12}$$

Using the asymptotic equality $K_\nu(z) = 2^{\nu-1}\Gamma(\nu)z^{-\nu}$ that is true at small values of z and the first boundary condition of (11), we obtain

$$A_1 = \frac{2^{1-\frac{1}{2\alpha}}}{\Gamma\left(\frac{1}{2\alpha}\right)}\, \vartheta(0, \lambda, \alpha)\, (b\sqrt{\lambda})^{\frac{1}{2\alpha}} \,,$$

and represent solution (12) in the form

$$\vartheta(f, \lambda, \alpha) = \lambda\vartheta(0, \lambda, \alpha)\, \omega(f, \lambda, \alpha) \,, \quad \omega(f, \lambda, \alpha) = 2^{1-\nu} f^{\nu} \lambda^{\frac{\nu}{2}-1} K_\nu(f\sqrt{\lambda}) \,. \tag{13}$$

The original of $\omega(f, \lambda, \alpha)$ is the incomplete gamma function

$$\Gamma\left(\frac{f^2}{4t}, \nu\right) = \varphi^{-1}[\omega(f, \lambda, \nu)] = \int_\delta^\infty \exp(-y)\, y^{\nu-1} dy \,, \quad \delta = \frac{f^2}{4t} \,.$$

Thus, on condition that $\nu = \frac{1}{2\alpha}$, original (13) can be determined using the inverse-transformation theorem [19] as

$$F(l, t) = F(f, t, \alpha) = \frac{\partial}{\partial t} \int_0^t F(0, t - \tau, \alpha)\, \psi\left(\frac{f^2}{4\tau}, \alpha\right) d\tau\,, \tag{14}$$

$$\psi\left(\frac{f^2}{4\tau}, \alpha\right) = \frac{1}{\Gamma\left(\frac{1}{2\alpha}\right)} \int_\delta^\infty \exp(-y)\, y^{\frac{1}{2\alpha}-1} dy\,. \tag{15}$$

Making the substitution $x = y^{\frac{1}{2\alpha}}$ in (15) and using the relation $z\Gamma(z) = \Gamma(1 + z)$ for the gamma function, we obtain

$$\psi\left(\frac{f^2}{4\tau}, \alpha\right) = \frac{1}{\Gamma\left(1 + \frac{1}{2\alpha}\right)} \int_x^\infty \exp(-x^{2\alpha})\, dx\,, \quad x = \left(\frac{f^2}{4\tau}\right)^{\frac{1}{2\alpha}}.$$

Differentiation of (14) with respect to t gives, in view of (15), the expression

$$F(f, t, \alpha) = \frac{1}{\Gamma\left(\frac{1}{2\alpha}\right)} \int_0^t F(0, t - \tau, \alpha) \left(\frac{f^2}{4\tau}\right)^{\frac{1}{2\alpha}} \exp\left(-\frac{f^2}{4\tau}\right) \frac{d\tau}{\tau}\,. \tag{16}$$

It is easy to verify that solution (16) satisfies equation (7) and the boundary conditions (12). Then solution (5), by analogy with (16), can be represented, with the use of the boundary conditions (4), in the form

$$\Delta M(f, t, \alpha) = \frac{1}{\Gamma\left(\frac{1}{2\alpha}\right)} \int_0^\infty \Delta M(0, t - \tau, \alpha) \left(\frac{f^2}{4\tau}\right)^{\frac{1}{2\alpha}} \exp\left(-\frac{f^2}{4\tau}\right) \frac{d\tau}{\tau}\,, \tag{17}$$

where $\Delta M(f, t, \alpha) = M(l, t) - M(l, 0)$, $M(l, 0) = M_0$. Equation (17) defining the moisture transfer in a porous body in the general case is fairly complex, and, in the case where $f(\zeta)$ is an arbitrary function, it can be solved numerically or with the use of exponential series. However, if at $l = L$ the moisture content in a porous material is constant and equal to $M(L, t, \alpha) = M_{eq}$, solution (17) can be written as

$$M_r(f, t, \alpha) = \frac{M(f, t, \alpha) - M_0}{M_{eq} - M_0} = 1 - \psi\left(\frac{f^2}{4\tau}, \alpha\right). \tag{18}$$

In the case where $\alpha = 1$, i.e., the linear dependence $\Gamma\left(\frac{1}{2}\right) = \frac{\pi}{a}$ is true, the expression in the right side of Eq. (18) is transformed into the probability integral and the solution takes the form

$$M_r(y, t) = \frac{2}{\pi} \int_0^x \exp(-\lambda^2)\, d\lambda = \operatorname{erf}\left(\frac{y}{2\sqrt{D_* t}}\right) = \operatorname{erf}\left(\frac{y}{2L\sqrt{\mathrm{Fo}}}\right) = \Phi(\eta)\,, \tag{19}$$

where $\mathrm{Fo} = D_* t/L^2$, $\eta = y/(2\sqrt{D_* t})$, and the effective diffusion coefficient is determined in accordance with Eq. (7). It is apparent that at $\alpha \neq 1$ the moisture-content distribution can differ from (19) because of the nonlinearity of solution

(17). It should be noted that, if the effective diffusion coefficient depends only on time, Eq. (5) can be written with the use of (6) as

$$\frac{\partial M}{\partial t_*} = \frac{\partial^2 M}{\partial y^2}, \tag{20}$$

where $t_+ = D_0 \int_0^1 \psi_+(\tau) d\tau$. We introduce the variable $\zeta = y/2\sqrt{t_+}$ and transform Eq. (20) into an ordinary differential equation analogous to (19) with the solution $M_r(y) = \text{erf}\ (\zeta)$. With the use of solution (19), the vapor-mass transfer from the surface of a layer S is determined as

$$J = -SD_* \left.\frac{\partial M}{\partial y}\right|_{y=L} \approx \frac{bH}{L}\frac{D_* (M_{eq} - M_0)}{\sqrt{\pi \text{Fo}}} .$$

Then, the dimensionless vapor flow or the Sh number and its average value will take the form

$$\text{Sh} = \frac{\frac{H}{L}}{\sqrt{\pi \text{Fo}}}, \quad \text{Sh} = \frac{1}{t}\int_0^t \text{Sh}\ (\tau)\ d\tau .$$

Clearly this expression for calculating the Sh number takes no account of the convective vapor transfer from the surface of the material to the gas flow because, in this case, a large number of parameters of the gas flow and vapor (temperature, humidity, turbulent diffusion and molecular-diffusion coefficients, viscosity, etc.) and other dependences should be taken into account [5–7].

Solution of Ill-Posed Inverse Problem. The problem on determination of the diffusion coefficient or the general variable η by the measured and calculated values of $M_r(y, t)$ is an ill-posed inverse problem [20]. The inverse problem on estimation of the effective diffusion coefficient with the use of (19) in the form

$$\eta = \Phi^{-1}\ (M_r) \tag{21}$$

is an ill-posed problem because very small errors in the experimental measurements and calculations of the moisture content can cause large errors in the estimation of η or the variable diffusion coefficient. In solving the inverse problem, the main criterion for estimation of the effective diffusion coefficient is the relative squared error calculated by the formula

$$I = \int_0^t \left[\frac{\tilde{M}_r - M_r\ (y, t)}{\tilde{M}_r}\right]^2 dt , \tag{22}$$

where $\tilde{M}_r$ are experimental values. At the same time, there is a need for determination of the region of regularity of the inverse-problem solution, i.e., determination of the sensitivity of the η values to the errors in the measurement of the moisture content and to its deviations. Differentiation of expression (21) with respect to the moisture content gives

$$\frac{\partial \eta}{\partial M} = \frac{\partial \Phi^{-1}\ (M)}{\partial M} = \frac{\partial M_r}{\partial M}\left(\frac{\partial \Phi}{\partial \eta}\right)^{-1} . \tag{23}$$

Taking into account the small changes in the moisture content and determining the derivative $\frac{\partial \Phi}{\partial \eta} = \frac{1}{\sqrt{2\pi}} \exp\ (-\eta^2)$ from (19), on simple rearrangements of (23), we obtain

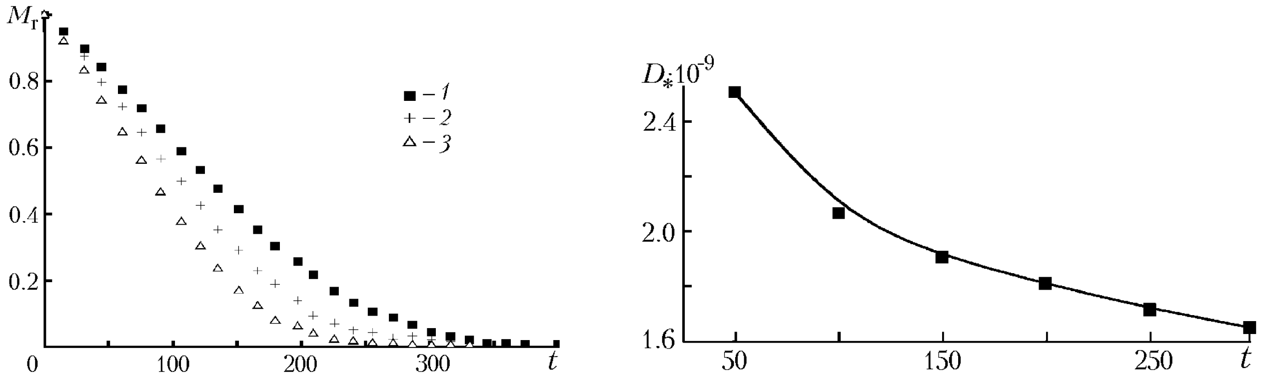

Fig. 3. Dependence of the relative moisture content on the drying time at a velocity of the gas flow V = 1 m/sec and different temperatures: T = 40 (1), 45 (2), and 50°C (3). t, min.

Fig. 4. Change in the calculated effective diffusion coefficient versus the drying time. D_*, m²/sec. t, min.

$$\delta(\eta) = \frac{\Delta\eta}{\eta} = K(\eta)\frac{\delta M_r}{M_0 - M}. \tag{24}$$

where $K(\eta) = \frac{\sqrt{2\pi}}{\eta}$ erf (η) exp (η^2) and δM_r is the absolute error. Thus, expression (24) determines the region of regularity of expression (21) on condition that the relative error δ_η is fairly small. Assuming that $\eta = y/(2\sqrt{D_* t})$, from (24) we estimate the error in determining the effective diffusion coefficient:

$$\frac{\Delta D_*}{D_*} \approx K^{-2}(\eta)\left(\frac{\Delta M}{M_0 - M_{eq}}\right)^2, \tag{25}$$

in this case, the values of $K^{-1}(\eta)$ vary within the range 0–1:

$$\lim_{\eta\to 0} K^{-1}(\eta) \to 1, \quad \lim_{\eta\to\infty} K^{-1}(\eta) \to 0.$$

As follows from (25), the error in determining the effective diffusion coefficient depends on the squared error in the measurement of the moisture content. Since the relative error $\delta(M) = \Delta M/(M_0 - M_{eq}) < 1$, $K(\eta) \le 1$, and $\delta(D_*) = \Delta D_*/D_* \to 0$ at $\delta(M) \to 0$, to infinitely small variants in $\delta(M)$ correspond infinitely small increments $\delta(D_*)$, i.e., the solution of the inverse problem on estimation of the effective diffusion coefficient is conditionally correct or correct according to Tikhonov [20].

Discussion of Results. In the present investigation, the process of drying of a deformable porous material was calculated. It was established that the effective diffusion coefficient and the porosity of a layer of this material are functions of time in the case where the drying of the material is accompanied by compaction and deformation of its structure. The analytical solutions (19) of the mass-transfer equation were obtained and the effective-diffusion and porosity coefficients were estimated. It should be noted that the inverse problem on estimation of the effective diffusion coefficient can be considered as conditionally correct at a minimum square criterion (22). The values of the effective-diffusion coefficient estimated by criterion (22) and the experimental data on the drying of compacted sawdust (Fig. 3) of thickness 2.5–3.0 mm at different temperatures were very different, which can be due to the linearity of the function $f(\alpha = 1)$ (7) or the deformation of the structure of the material subjected to drying for a long time. Because of this, the empirical dependence of the distance along the line of flow in the layer being dried on the drying time $y = L_0 \exp(-1.413\cdot 10^{-8} t^{1.92})$ ($L_0 = 2.78\cdot 10^{-3}$ is the average thickness of the layer) was introduced into the main solution

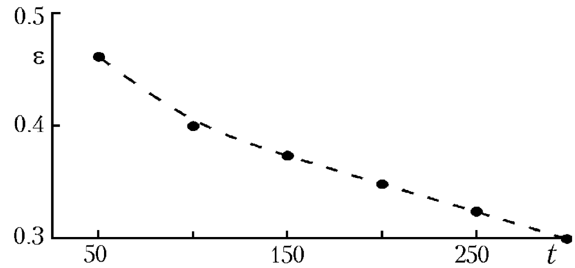

Fig. 5. Change in the porosity of the body versus the drying time. t, min.

(20). The calculated dependences of the effective-diffusion coefficient on the time are presented in Fig. 4. By these data we estimated the dependence of the porosity of a porous-material layer on the drying time (Fig. 5):

$$\varepsilon(t) = 0.459 \exp\left(-\frac{3\sigma_d t}{4\xi_s}\right). \qquad (26)$$

The relation between the internal deforming stress and the shear viscosity was obtained in the form $\sigma_d/\xi_s = 1.28 \cdot 10^{-5}(1 + 0.035T)$ and determined for different drying temperatures (T = 40–50^{o}C). Using this dependence and Eqs. (2) and (6), one can estimate the dependence of the effective-diffusion coefficient, the density, and the porosity of a material on the temperature of its drying.

Conclusions. Porous bodies subjected to drying can take fairly complex internal and external configurations determining their porosity and effective diffusion coefficient. This is explained by the fact that the anisotropy of the geometry of these bodies, arising as a result of the drying, breaks the symmetry of their shape, which cannot be described by the ordinary equation of mass transfer.

NOTATION

b, width of a layer, m; D_0, initial value of the diffusion coefficient, m^2/sec; D_{Kn}, Knudsen diffusion coefficient, m^2/sec; D_*, effective diffusion coefficient, m^2/sec; d, diameter of pores, m; $F(l, t)$, function of an independent variable or an original; Fo, Fourier number; H, length of the layer, m; L, thickness of the layer, m; l, distance along the line of flow, m; M, moisture content, kg/m^3; M_0, initial moisture content in the porous material, kg/m^3; M_{eq}, moisture content equilibrium with the flow, kg/m^3; M_r, relative moisture content, kg/m^3; Pe, Peclet number; r, radius of pores; S, area of the evaporation surface, m^2; Sh, Sherwood number; s_0, area of the cross section of the pore channel, m^2; T, temperature, ^{o}C; t, time, sec; V, velocity of the flow, m/sec; V_x, V_y, velocity components of the flow along the coordinates x and y; X, X_0, current and initial moisture contents; x, y, z, Cartesian coordinates; α, constant; δ, relative error; ε, porosity of the layer; η, dimensionless coordinate; η_d, sinuosity of pores; λ, complex variable; ξ_s, shear viscosity, N·sec/m^2; ρ, density of the material, kg/m^3; ρ_d, density of the solid phase of the porous material, kg/m^3; σ_d, internal deforming stress, N/m^2; $\vartheta(l, \lambda)$, function representation; Φ^{-1}, inverse operator function. Subscripts: 0, initial value; eq, equilibrium value; d, parameters of the solid phase; r, relative values; s, solid phase.

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