MATHEMATICAL MODEL OF DRYING OF DEFORMABLE MATERIALS AND NUMERICAL CALCULATION METHOD

V. A. Sychevskii

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A further development of numerical methods for calculating the nonlinear interdependent processes of heat and mass transfer in capillary-porous materials with account for their stressed-strained state is given.

Keywords: colloidal capillary-porous materials, nonlinear interconnected equations of heat and mass transfer, large deformations, stressed-strained state, finite-element method.

Introduction. The methods proposed in [1, 2] for calculating the stressed-strained state of materials in the process of their drying are based on the assumption that these materials experience small elastic deformations in each time step. This approach brings about an error in determination of the humidity deformation of a material, and, at a large shrinkage coefficient, this error can be large. If experimental data on this process were available, the indicated error could be decreased by the introduction of corresponding corrections, i.e., by fitting the theory to the experiment. However, reliable experimental data on the stressed-strained state of materials subjected to drying are absent, which generates a need for the development of a more general method for calculating large deformations and displacements arising in these materials in the process of their drying without introduction of additional simplifying assumptions. We propose such a method as well as a method for calculating the nonlinear interconnected equations of heat and mass transfer in colloidal capillary-porous materials prone to large shrinkages and deformations. The indicated methods were developed on the basis of the methods proposed in [1, 2], the generalization of which is the aim of the present work.

Mathematical Model. In the case where the processes of heat and mass transfer in a material subjected to drying proceed at a temperature lower than 100° C, a relative atmospheric humidity lower than 100° , and a rate of motion of a drying agent smaller than 7 m/sec, one can restrict oneself to the problem on the moisture stress of the material without considering the influence of its mechanical motion on the heat and mass transfer in it. We will assume that, under the indicated drying conditions, a body is at mechanical equilibrium at each instant of time, which allows us to consider the statical problem on its moisture elasticity.

Let us formulate a mathematical model of the processes being investigated, accounting for their geometrical and physical nonlinearity. The equations of heat and mass transfer are written in the curvilinear coordinates:

$$c\rho_0 \frac{\partial T}{\partial t} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^k} \left(g^{kl} \sqrt{g} \lambda_{kl} \frac{\partial T}{\partial x^l} \right) + \varepsilon Q_p \rho_0 \frac{\partial W}{\partial t}, \qquad (1)$$

$$\rho_0 \frac{\partial W}{\partial t} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^k} \left(g^{kl} \sqrt{g} a_{Wkl} \rho_0 \frac{\partial W}{\partial x^l} \right) + \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^k} \left(g^{kl} \sqrt{g} a_{Wkl} \rho_0 \delta \frac{\partial T}{\partial x^l} \right), \tag{2}$$

and the equations of motion have the form

$$\sigma_{jj}^{ij} = 0. \tag{3}$$

To determine the mechanical deformations of a material, it is necessary to know its rheology. If Hooke's law applies, we can write

A. V. Luikov Heat and Mass Transfer Institute, National Academy of Sciences of Belarus, 15 P. Brovka Str., Minsk, 220072, Belarus. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 82, No. 4, pp. 674–687, July–August, 2009. Original article submitted March 13, 2008; revision submitted June 24, 2008.

$$\sigma^{ij} = \lambda \varepsilon^{\alpha}_{\alpha} g^{ij} + 2\mu \varepsilon^{ij} - (3\lambda + 2\mu) \beta g^{ij} W.$$
⁽⁴⁾

For a plastic body, the following relations are true:

$$d\sigma^{ij} = \frac{E}{1+\nu} \left(d\varepsilon^{ij} + \frac{\nu}{1-2\nu} g^{ij} d\varepsilon^{\alpha}_{\alpha} - s^{ij} \frac{s^k_l d\varepsilon^l_k}{S} \right), \tag{5}$$

where $S = \frac{2}{3}\overline{\sigma}^2 \left(1 + \frac{2(1+\nu)H}{3E}\right)$, $\overline{\sigma} = \sqrt{\frac{3}{2}} s_j^i s_i^j$, $H = \frac{d\overline{\sigma}}{d\varepsilon^{\text{el}}}$, $\overline{d\varepsilon^{\text{el}}} = \sqrt{\frac{3}{2}} d\varepsilon_i^{\text{el}j} d\varepsilon_j^{\text{el}i}$.

An elastoviscous material adheres to the equation

$$\sigma^{ij} = \frac{\nu E}{(1+\nu)(1-2\nu)} \varepsilon^{k}_{k} g^{ij} + \frac{E}{1+\nu} \varepsilon^{ij} + \frac{E}{1-2\nu} \beta W g^{ij} - \frac{E}{1+\nu} \int_{0}^{1} R_{s} (t-\tau) \left(\varepsilon^{ij} - \frac{1}{3} g^{ij} \varepsilon^{k}_{k} \right) d\tau , \qquad (6)$$

where $R_{\rm s}(t-\tau) = \frac{E-E_{\infty}}{Et_{\rm rel}} \exp\left(-\frac{t-\tau}{t_{\rm rel}}\right)$

Equations (1)–(3) and one of the rheological equations (4)–(6) or their combination form the basis for the mathematical model of the interdependent processes of heat and mass transfer in a material and its stressed-strained state. Using the above formulas as the base, one can obtain equations of motion in displacements. By way of example we will derivate such an equation for an elastic body on the assumption that the Lamé coefficient is constant. Let us use the following relations:

$$\varepsilon_{\alpha\beta} = \frac{1}{2} \left(u_{\beta;\alpha} + u_{\alpha;\beta} + u_{k;\alpha} u_{;\beta}^k \right); \tag{7}$$

$$\varepsilon_{\alpha}^{\alpha} = g^{\alpha\beta} \varepsilon_{\alpha\beta} \,, \quad \varepsilon^{ij} = g^{i\alpha} g^{j\beta} \varepsilon_{\alpha\beta} \,. \tag{8}$$

Substitution of (7) and (8) into (4) gives the expression

$$\sigma^{ij} = \lambda g^{ij} u^{\alpha}_{;\alpha} + \frac{1}{2} \lambda g^{ij} g^{\alpha\beta} u_{k;\alpha} u^{k}_{;\beta} + \mu g^{i\alpha} u^{j}_{;\alpha} + \mu g^{j\beta} u^{i}_{;\beta} + \mu g^{i\alpha} g^{j\beta} u_{k;\alpha} u^{k}_{;\beta} - (3\lambda + 2\mu) \beta g^{ij} W.$$
⁽⁹⁾

Substituting, in turn, (9) into (3) and regrouping terms, we obtain

$$(\lambda + \mu) g^{ij} \left(u^{\alpha}_{;\alpha}\right)_{;j} + \mu g^{j\beta} \left(u^{i}_{;\beta}\right)_{;j} + \left(\frac{1}{2} \lambda g^{ij} g^{\alpha\beta} + \mu g^{i\alpha} g^{j\beta}\right) \left\{ (u_{k;\alpha})_{;j} u^{k}_{;\beta} + u_{k;\alpha} \left(u^{k}_{;\beta}\right)_{;j} \right\} - (3\lambda + 2\mu) \beta g^{ij} W_{;j} = 0.$$

When passing from the contravariant components to the covariant ones on condition that a covariant derivative of a scalar is equal to a partial derivative with respect to a coordinate, the following expression is obtained:

$$(\lambda + \mu) \frac{\partial}{\partial x^{i}} (u_{;\alpha}^{\alpha}) + \mu g^{j\beta} (u_{i;\beta})_{;j} + \left(\frac{1}{2} \lambda g_{ig}^{j} g^{\alpha\beta} + \mu g_{ig}^{\alpha} g^{j\beta}\right) \left\{ (u_{k;\alpha})_{;j} u_{;\beta}^{k} + u_{k;\alpha} (u_{;\beta}^{k})_{;j} \right\} - (3\lambda + 2\mu) \beta \frac{\partial}{\partial x^{i}} W = 0.$$
(10)

The covariant derivatives of covariant and contravariant vectors have, respectively, the forms

$$u_{ij} = \frac{\partial u_i}{\partial x^j} - u_m \Gamma_{ij}^m , \qquad (11)$$

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$$u_{;j}^{i} = \frac{\partial u^{i}}{\partial x^{j}} + u^{m} \Gamma_{mj}^{i} , \qquad (12)$$

and the second derivatives used in (10) are determined as

$$(u_{i;\beta})_{;j} = \frac{\partial^2 u_i}{\partial x^j \partial x^\beta} - \frac{\partial u_m}{\partial x^j} \Gamma^m_{i\beta} - u_m \frac{\partial \Gamma^m_{i\beta}}{\partial x^j} - \frac{\partial u_m}{\partial x^\beta} \Gamma^m_{ij} + u_l \Gamma^l_{m\beta} \Gamma^m_{ij} - \frac{\partial u_i}{\partial x^m} \Gamma^m_{\beta j} + u_l \Gamma^l_{im} \Gamma^m_{\beta j} ,$$
 (13)

$$(u_{;\beta}^{k})_{j} = \frac{\partial^{2} u^{k}}{\partial x^{j} \partial x^{\beta}} + \frac{\partial u^{m}}{\partial x^{j}} \Gamma_{m\beta}^{k} + u^{m} \frac{\partial \Gamma_{m\beta}^{k}}{\partial x^{j}} + \frac{\partial u^{m}}{\partial x^{\beta}} \Gamma_{mj}^{k} + u^{l} \Gamma_{l\beta}^{m} \Gamma_{mj}^{k} - \frac{\partial u^{k}}{\partial x^{m}} \Gamma_{\beta j}^{m} - u^{l} \Gamma_{lm}^{k} \Gamma_{\beta j}^{m}.$$

$$(14)$$

The divergence of the displacement vector is given by the formula

$$u_{;\alpha}^{\alpha} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^{\alpha}} \left(g^{\alpha m} \sqrt{g} u_m \right).$$
(15)

Equations (10)-(15) should be supplemented by the relations

$$g_{ij} = 2\varepsilon_{ij} + g_{0ij}, \quad g^{ij}g_{jk} = \delta^i_k, \quad g = \det g_{ik}, \quad \Gamma^l_{ik} = \frac{1}{2}g^{ml}\left(\frac{\partial g_{im}}{\partial x^k} + \frac{\partial g_{km}}{\partial x^i} - \frac{\partial g_{ik}}{\partial x^m}\right). \tag{16}$$

Thus, Eqs. (1), (2), (7), (8), and (10)-(16) form a mathematical model of the interdependent processes of heat and mass transfer in a material described by Hooke's law and its stressed-strained state.

Procedure of Numerical Solution of the Interconnected Equations of Heat and Mass Transfer. The problem on heat and mass transfer in a material will be solved by the finite element method (FEM) described in [3]. Therefore, in what follows, we will use FEM mathematical symbols. With allowance made for the initial geometry of the material being investigated, the finite element method will be realized in the Cartesian coordinate system, which suffices to construct the equations of motion and of heat and mass transfer for the problem being solved.

Let us consider the equation of mass transfer

$$\rho_{0} \frac{\partial W}{\partial t} = \frac{\partial}{\partial x} \left(a_{Wx} \rho_{0} \frac{\partial W}{\partial x} \right) + \frac{\partial}{\partial y} \left(a_{Wy} \rho_{0} \frac{\partial W}{\partial y} \right) + \frac{\partial}{\partial z} \left(a_{Wz} \rho_{0} \frac{\partial W}{\partial z} \right)$$
$$+ \frac{\partial}{\partial x} \left(a_{Wx} \rho_{0} \delta \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(a_{Wy} \rho_{0} \delta \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(a_{Wz} \rho_{0} \delta \frac{\partial T}{\partial z} \right)$$

with the boundary conditions

$$j_{\rm sur} = \rho_0 \beta_W (W - W_{\rm eq}) \,. \tag{17}$$

For the finite element method to be used, it is necessary to take into account the fact that the heat flows caused by the temperature and moisture-content gradients are independent and, consequently, the moisture-content increment arising with time consists of two parts:

$$\frac{\partial W}{\partial t} = \left(\frac{\partial W}{\partial t}\right)_1 + \left(\frac{\partial W}{\partial t}\right)_2,\tag{18}$$

where $\left(\frac{\partial W}{\partial t}\right)_1$ is due to the mass flow caused by the moisture content gradient and $\left(\frac{\partial W}{\partial t}\right)_2$ is due to the mass flow caused by the temperature gradient. In this case, we can write the equation

caused by the temperature gradient. In this case, we can write the equation

$$\rho_0 \left(\frac{\partial W}{\partial t}\right)_1 = \frac{\partial}{\partial x} \left(a_{Wx} \rho_0 \frac{\partial W}{\partial x}\right) + \frac{\partial}{\partial y} \left(a_{Wy} \rho_0 \frac{\partial W}{\partial y}\right) + \frac{\partial}{\partial z} \left(a_{Wz} \rho_0 \frac{\partial W}{\partial z}\right)$$
(19)

with the boundary conditions (17) and the equation

$$\frac{\partial}{\partial x} \left(a_{Wx} \rho_0 \delta \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(a_{Wy} \rho_0 \delta \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(a_{Wz} \rho_0 \delta \frac{\partial T}{\partial z} \right) - \rho_0 \left(\frac{\partial W}{\partial t} \right)_2 = 0$$
(20)

with a constant temperature at the boundary. Then the functionals for Eqs. (19) and (20) with the corresponding boundary conditions will be as follows:

$$\chi_{1} = \int_{V} \frac{1}{2} \left[a_{Wx} \rho_{0} \left(\frac{\partial W}{\partial x} \right)^{2} + a_{Wy} \rho_{0} \left(\frac{\partial W}{\partial y} \right)^{2} + a_{Wz} \rho_{0} \left(\frac{\partial W}{\partial z} \right)^{2} + 2W \rho_{0} \left(\frac{\partial W}{\partial t} \right)_{1} \right] dV + \int_{S} \frac{1}{2} \rho_{0} \beta_{W} \left(W^{2} - 2WW_{eq} + W_{eq}^{2} \right) dS,$$
$$\chi_{2} = \int_{V} \frac{1}{2} \left[a_{Wx} \rho_{0} \delta \left(\frac{\partial T}{\partial x} \right)^{2} + a_{Wy} \rho_{0} \delta \left(\frac{\partial T}{\partial y} \right)^{2} + a_{Wz} \rho_{0} \delta \left(\frac{\partial T}{\partial z} \right)^{2} + 2T \rho_{0} \left(\frac{\partial W}{\partial t} \right)_{2} \right] dV.$$

Let us introduce the designations

$$\begin{bmatrix} D_{\text{dif}} \end{bmatrix} = \begin{bmatrix} a_{Wx} \rho_0 & 0 & 0\\ 0 & a_{Wy} \rho_0 & 0\\ 0 & 0 & a_{Wz} \rho_0 \end{bmatrix}, \quad \begin{bmatrix} H \end{bmatrix} = \begin{bmatrix} a_{Wx} \rho_0 \delta & 0 & 0\\ 0 & a_{Wy} \rho_0 \delta & 0\\ 0 & 0 & a_{Wz} \rho_0 \delta \end{bmatrix},$$

$$\{g_W\}^{\text{tr}} = \left\{ \frac{\partial W}{\partial x} \frac{\partial W}{\partial y} \frac{\partial W}{\partial z} \right\}, \quad W = [N] \{W\}, \quad \{g_W\} = [B] \{W\},$$
(21)

and write the functionals in the matrix form

$$\chi_{1} = \int_{V} \frac{1}{2} \left[\{W\}^{\text{tr}} [B]^{\text{tr}} [D_{\text{dif}}] [B] \{W\} + 2 [N] \{W\} [N] \rho_{0} \left(\frac{\partial [W]}{\partial t}\right)_{1} \right] dV + \int_{S} \frac{1}{2} \rho_{0} \beta_{W} \{W\}^{\text{tr}} [N]^{\text{tr}} [N] \{W\} dS - \int_{S} \rho_{0} \beta_{W} W_{\text{eq}} [N] \{W\} dS + \int_{S} \frac{1}{2} \rho_{0} \beta_{W} W_{\text{eq}}^{2} dS ,$$
$$\chi_{2} = \int_{V} \frac{1}{2} \left[\{T\}^{\text{tr}} [B]^{\text{tr}} [H] [B] \{T\} + 2 [N] \{T\} [N] \rho_{0} \left(\frac{\partial [W]}{\partial t}\right)_{2} \right] dV .$$

The variational formulation of the equation of mass transfer has the form

$$\frac{d\chi_1}{d[W]} = \int_V [B]^{\text{tr}} [D_{\text{dif}}] [B] dV \{W\} + \int_V [N]^{\text{tr}} [N] dV \rho_0 \left(\frac{\partial \{W\}}{\partial t}\right)_1$$

$$+ \int_{S} \rho_0 \beta_W [N]^{tr} [N] dS \{W\} - \int_{S} \rho_0 \beta_W W_{eq} [N]^{tr} dS = 0, \qquad (22)$$

$$\frac{d\chi_2}{d[W]} = \int_V [B]^{\text{tr}} [H] [B] dV \{W\} + \int_V [N]^{\text{tr}} [N] dV \rho_0 \left(\frac{\partial [W]}{\partial t}\right)_2 = 0.$$
(23)

Substituting (23) into (22), using relation (18), and performing simple rearrangements, we eventually obtain

$$\int_{V} [N]^{tr} [N] \, dV \rho_0 \frac{\partial [W]}{\partial t} + \int_{V} [B]^{tr} [D_{\text{dif}}] [B] \, dV \{W\} + \int_{V} [B]^{tr} [H] [B] \, dV \{T\} + \int_{S} \rho_0 \beta_W [N]^{tr} [N] \, dS \{W\} - \int_{S} \rho_0 \beta_W W_{\text{eq}} [N]^{tr} \, dS = 0 .$$
(24)

In the subsequent discussion we will use expression (24) in the more compact form

$$[C] \frac{\partial [W]}{\partial t} + [K] [W] + [F] = 0, \qquad (25)$$

where

$$[C] = \int_{V} \rho_0 [N]^{tr}[N] dV; \quad [K] = \int_{V} [B]^{tr} [D_{dif}] [B] dV + \int_{S} \rho_0 \beta_W [N]^{tr}[N] dS;$$
$$\{F\} = \int_{V} [B]^{tr} [H] [B] dV \{T\} - \int_{S} \rho_0 \beta_W W_{eq} [N]^{tr} dS.$$

Equation (25) will be solved by the finite-difference method. For this purpose, we change the derivative for the finite difference

$$\frac{\partial \{W\}}{\partial t} = \frac{1}{\Delta t} \left(\{W_{\text{new}}\} - \{W_{\text{old}}\} \right)$$

and, calculating the vectors $\{W\}$ and $\{F\}$ at the middle points of a time interval:

$$[W_{\rm m}] = \frac{1}{2} \left(\{W_{\rm new}\} + \{W_{\rm old}\} \right), \quad \{F_{\rm m}\} = \frac{1}{2} \left(\{F_{\rm new}\} + \{F_{\rm old}\} \right),$$

obtain

$$\begin{bmatrix} G_W \end{bmatrix} \{ W_{\text{new}} \} = \{ F_W \},\$$

where the following designations are used:

$$[G_W] = \frac{1}{\Delta t} [C] + \frac{1}{2} [K]; \quad \{F_W\} = \left(\frac{1}{\Delta t} [C] - \frac{1}{2} [K]\right) \{W_{\text{old}}\} - \frac{1}{2} \left(\{F_{\text{new}}\} + \{F_{\text{old}}\}\right)$$

Since the coefficients a_{Wx} , a_{Wy} , a_{Wz} , and δ are functions of W and T, we will perform an iteration process of solving the nonlinear equation of mass transfer in each time step. Iterations will be carried out as long as the modulus of the difference $|\{W_n\} - \{W_{n-1}\}|$ becomes smaller than 10^{-6} .

Let us now consider the heat-conduction equation

$$c\rho_{0}\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\lambda_{x}\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_{y}\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\lambda_{z}\frac{\partial T}{\partial z}\right) + \varepsilon Q_{p}\rho_{0}\frac{\partial W}{\partial t}$$
(26)

with the boundary conditions

$$q_{\rm sur} = \alpha \left(T_{\rm env} - T \right) - \rho_0 Q_{\rm p} \left(1 - \varepsilon \right) \beta_W \left(W - W_{\rm eq} \right) \,. \tag{27}$$

The functional for problem (26), (27) can be written as

$$\chi = \int_{V} \frac{1}{2} \left[\lambda_{x} \left(\frac{\partial T}{\partial x} \right)^{2} + \lambda_{y} \left(\frac{\partial T}{\partial y} \right)^{2} + \lambda_{z} \left(\frac{\partial T}{\partial z} \right)^{2} + 2c\rho_{0} \frac{\partial T}{\partial t} T - 2\rho_{0} Q_{p} \varepsilon \frac{\partial W}{\partial t} T \right] dV + \int_{S} \left[\frac{\alpha}{2} \left(T_{env} - T \right)^{2} - \rho_{0} Q_{p} \left(1 - \varepsilon \right) \beta_{W} \left(W - W_{eq} \right) T \right] dS .$$
(28)

Introducing the designations

$$[L] = \begin{bmatrix} \lambda_x & 0 & 0 \\ 0 & \lambda_y & 0 \\ 0 & 0 & \lambda_z \end{bmatrix}, \quad \left\{ g_T \right\}^{\text{tr}} = \left\{ \frac{\partial T}{\partial x} \frac{\partial T}{\partial y} \frac{\partial T}{\partial z} \right\}, \quad T = [N] \left\{ T \right\}, \quad \left\{ g_T \right\} = [B] \left\{ T \right\}, \tag{29}$$

we write formula (28) in the matrix form

$$\chi = \int_{V} \frac{1}{2} \left[\{T\}^{\text{tr}} [B]^{\text{tr}} [L] [B] \{T\} + 2c\rho_0 [N] \{T\} [N] \frac{\partial [T]}{\partial t} - 2\rho_0 \varepsilon Q_p [N] \{T\} \frac{\partial W}{\partial t} \right] dV + \int_{S} \frac{\alpha}{2} \{T\}^{\text{tr}} [N]^{\text{tr}} [N]^{\text{tr}} [N] \{T\} dS$$
$$- \int_{S} \alpha T_{\text{env}} [N] \{T\} dS + \int_{S} \frac{\alpha}{2} T_{\text{env}}^2 dS - \int_{S} \rho_0 (1 - \varepsilon) Q_p \beta_W (W_{\text{sur}} - W_{\text{eq}}) [N] \{T\} dS .$$

The derivative of χ with respect to $\{T\}$ has the form

$$\frac{d\chi}{d[T]} = \int_{V} [B]^{\text{tr}} [L] [B] dV[T] + \int_{V} c\rho_0 [N]^{\text{tr}} [N] dV \frac{\partial[T]}{\partial t} - \int_{V} \rho_0 \varepsilon Q_p [N]^{\text{tr}} dV \frac{\partial W}{\partial t} + \int_{S} \alpha [N]^{\text{tr}} [N] dS[T]$$
$$- \int_{S} \alpha T_{\text{env}} [N]^{\text{tr}} dS - \int_{S} \rho_0 (1 - \varepsilon) Q_p \beta_W (W_{\text{sur}} - W_{\text{eq}}) [N]^{\text{tr}} dS = 0.$$

Since

$$[C] = c\rho_0 \int [N]^{\text{tr}} [N] dV, \quad [K] = \int_V [B]^{\text{tr}} [L] [B] dV + \int_S \alpha [N]^{\text{tr}} [N] dS,$$

$$[F] = -\int_V \rho_0 \varepsilon Q_p [N]^{\text{tr}} dV \frac{\partial W}{\partial t} - \int_S \alpha T_{\text{env}} [N]^{\text{tr}} dS - \int_S \rho_0 (1 - \varepsilon) Q_p \beta_W (W_{\text{sur}} - W_{\text{eq}}) [N]^{\text{tr}} dS,$$

we obtain

$$[C] \frac{\partial [T]}{\partial t} + [K] \{T\} + \{F\} = 0.$$
⁽³⁰⁾

To solve equation (30) by the finite difference method, we change the derivative for the finite difference

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$$\frac{\partial |T|}{\partial t} = \frac{1}{\Delta t} \left(\left[T_{\text{new}} \right] - \left[T_{\text{old}} \right] \right)$$

and, calculating the vectors $\{T\}$ and $\{F\}$ at the middle points of a time interval,

$$\{T_{\rm m}\} = \frac{1}{2} \left(\{T_{\rm new}\} + \{T_{\rm old}\} \right), \ \{F_{\rm m}\} = \frac{1}{2} \left(\{F_{\rm new}\} + \{F_{\rm old}\} \right),$$

obtain

$$\begin{bmatrix} G_T \end{bmatrix} \{ T_{\text{new}} \} = \{ F_T \},\$$

where the following designations are used:

$$[G_T] = \frac{1}{\Delta t} [C] + \frac{1}{2} [K]; \quad \{F_T\} = \left(\frac{1}{\Delta t} [C] - \frac{1}{2} [K]\right) \{T_{\text{old}}\} - \frac{1}{2} \left(\{F_{\text{new}}\} + \{F_{\text{old}}\}\right).$$

Since the coefficients c, λ_x , λ_y , λ_z , and Q_p are functions of W and T, the iteration process of solving the nonlinear heat-conduction equation is performed in each time step. Iterations are carried out as long as the difference $|\{T_n\} - \{T_{n-1}\}|$ is smaller than 10^{-6} .

Since the equations of heat and mass transfer (1) and (2) are interconnected, we developed an additional iteration procedure in each time step for the purpose of verifying of the influence of the temperature on the distribution of the moisture content in the material and vice versa. The moisture-content field W is calculated by the foregoing formulas and then, with its use, the temperature field T is determined. Thereafter W and T are determined once again in the same time interval, which makes it possible to take into account the mutual influence of these fields. Iterations are carried out as long as $|\{W_n\} - \{W_{n-1}\}|$ and $|\{T_n\} - \{T_{n-1}\}|$ become smaller than 10^{-6} at a time.

Procedure of Numerical Solution of the Equation of Motion. After the distributions of the temperature and moisture-content fields have been found, the stresses and deformations corresponding to them were determined. The main distinguishing feature of the mechanical problem is that the deformation vector is not a linear function of displacements. However, the linear relation between the differentials of these quantities remains true:

$$d\left\{\mathbf{\varepsilon}\right\} = [B] d\left\{u\right\}. \tag{31}$$

In Eq. (31), the matrix [B] is a function of displacements because, as follows from (8), the dependence of the deformation vector $\{\varepsilon\}$ on the displacements is a square function. The following expression can be written:

$$d\left\{\varepsilon\right\} = \left(\left[B_{\text{lin}}\right] + \left[B_{\text{nlin}}\right]\right) d\left\{u\right\}.$$
(32)

Here, $[B] = [B_{\text{lin}}] + [B_{\text{nlin}}]$, $[B_{\text{lin}}]$ is a matrix accounting for infinitely small displacements, independent of them, $[B_{\text{nlin}}]$ is a matrix accounting for the nonlinear properties of the deformation tensor, dependent on the displacements. It follows from formulas (8) and (32) that the matrix $[B_{\text{nlin}}]$ is a linear function of the displacements.

It is known that in the case where expression (8) is among the equations of mechanical motion used in a mathematical problem, the problem becomes nonlinear. This problem can be solved using iterative calculation methods, one of which is the Newton method. Let $\{F\}$ be the vector of the total internal force. The principle of virtual internal work can be written as

$$\delta \left\{ u \right\}^{\text{tr}} \left\{ F \right\} = \int_{V} \delta \left\{ \varepsilon \right\}^{\text{tr}} \left\{ \sigma \right\} dV = 0 .$$
(33)

Using relation (31) and eliminating $\delta\{u\}^{tr}$ from (33), we obtain the following expression for the force:

$$[F] = \int_{V} [B]^{\mathrm{tr}} \{\sigma\} \, dV = 0 \,. \tag{34}$$

The vector $\{\sigma\}$ represents the true stresses dependent on the deformations attained. For an elastic material, it has the form

$$\{\sigma\} = [D] \left(\{\epsilon\} - \{\epsilon_0\}\right).$$

Here, $\{\epsilon_0\}$ is determined as

$$\left\{\epsilon_{0}\right\}^{\text{tr}} = \left\{\frac{1}{2}\left(1 + \beta\Delta W\right)^{2} - \frac{1}{2} \qquad \frac{1}{2}\left(1 + \beta\Delta W\right)^{2} - \frac{1}{2} \qquad \frac{1}{2}\left(1 + \beta\Delta W\right)^{2} - \frac{1}{2} \qquad 0 \quad 0 \quad 0\right\}.$$

According to the Newton method, to find the corrections to the predetermined initial displacements, it is necessary to solve the equation

$$\Delta\left\{u\right\} = \left[J\right]^{-1}\left\{F\right\}.$$

Here, [J] is a Jacobi matrix

$$[J] = \left[\frac{\partial[F]}{\partial[u]}\right],\tag{35}$$

that will be determined by differentiation of relation [34] with respect to the variable $\{u\}$:

$$d\left\{F\right\} = \int_{V} d\left[B_{\text{nlin}}\right]^{\text{tr}}\left\{\sigma\right\} dV + \int_{V} \left(\left[B\right]^{\text{tr}}\left[D\right]\left[B\right] d\left\{u\right\}\right) dV.$$
⁽³⁶⁾

Setting

$$\int_{V} d\left[B_{\text{nlin}}\right]^{\text{tr}} \left\{\sigma\right\} dV = \left[K_{\sigma}\right] d\left\{u\right\}$$

and introducing the designation

$$[K_{\rm nlin}] = \int_{V} [B]^{\rm tr} [D] [B] dV, \qquad (37)$$

we write Eq. (36) in the form

$$d\{F\} = [K_{\sigma}] d\{u\} + [K_{\text{nlin}}] d\{u\} = [K_{t}] d\{u\}.$$
(38)

Here,

$$[K_{\rm t}] = [K_{\rm \sigma}] + [K_{\rm nlin}] \,. \tag{39}$$

When relations (35) and (38) are compared, it is apparent that the Jacobi matrix is a matrix of tangential stiffnesses and, consequently, the corrections to the initial displacement vector can be determined by the formula

$$[K_{t}] \Delta [u] = \{F\}.$$

$$\tag{40}$$

The iteration procedure is constructed in the following way:

1. The first approximation of the displacement vector $\{u\}$ is determined by solving the linear problem on the moisture elasticity.

2. Using the value of $\{u\}$ determined in Par. 1, the internal-force vector $\{F\}$ is calculated by formula (34). To determine the matrix [B] used in Eq. (34), according to formula (32), it is necessary to determine the matrix $[B_{\text{nlin}}]$ given by the expression

$$[B_{nlin}] = [A] [G]$$

3. The matrix $[K_t]$ is calculated by formulas (37) and (39) with the use of the expression

$$[K_{\sigma}] = \int_{V} [G]^{\text{tr}} [M] [G] dV.$$
⁽⁴¹⁾

4. The value of Δ{u} is determined from formula (40).

5. The displacement vector $\{u\}$ is refined.

6. If the components of the vector $\{F\}$ are smaller than 10^{-6} , the calculations are stopped. Otherwise, we pass to Par. 2 and continue the calculations.

To take into account the elastic properties of the material, we will use expression (6) written in the matrix form

$$\{\boldsymbol{\sigma}\} = [D] \{\boldsymbol{\varepsilon}\} - [D] \{\boldsymbol{\varepsilon}_0\} + \{r\}, \qquad (42)$$

where

$$\begin{aligned} r_1 &= -\int_0^t R_{\rm s} \left(t-\tau\right) \left[\frac{(2-\nu)E}{3\left(1-\nu^2\right)} \, \varepsilon_{11} \left(\tau\right) - \frac{(1-2\nu)E}{3\left(1-\nu^2\right)} \, \varepsilon_{22} \left(\tau\right) \right] d\tau \; ; \\ r_2 &= -\int_0^t R_{\rm s} \left(t-\tau\right) \left[\frac{(2-\nu)E}{3\left(1-\nu^2\right)} \, \varepsilon_{22} \left(\tau\right) - \frac{(1-2\nu)E}{3\left(1-\nu^2\right)} \, \varepsilon_{11} \left(\tau\right) \right] d\tau \; ; \\ r_3 &= -\frac{E}{2\left(1+\nu\right)} \int_0^t R_{\rm s} \left(t-\tau\right) \, \varepsilon_{21} \left(\tau\right) \, d\tau \; . \end{aligned}$$

The use of (42) will change the calculations of only the terms accounting for stresses, namely, the matrix [M], used for calculating the matrix $[K_{\sigma}]$, and the load vector $\{F\}$ determined by formula (34).

Once the stressed-strained state of the material has been determined, we pass to a new time layer and perform the calculation over again beginning with the determination of the temperature and moisture-content fields with consideration for the strained state of the material in the new position.

For the method proposed to be used for numerical calculations, it is necessary to specify the structure of elements. Tetrahedral elements are used in the three-dimensional case, and triangular elements are used in the two-dimensional case, which allows us to write all the above-indicated matrices in the explicit form and exactly calculate the spatial integrals. Since the presentation of these matrices for the three-dimensional and two-dimensional cases is cumbersome and these matrices are given in [3], they are not presented here. In particular, the form of the matrices [A], [G], and [M] used in the present work exactly correspond to that of [3].

Characteristics of a Material. The mathematical model proposed can be used for investigating the heat and mass transfer in colloidal capillary-porous materials with account for their stressed-strained state. This model allows one to consider the interdependence of the indicated processes, their physical nonlinearity, explained by the dependence of the properties of these materials on their moisture content and temperature, and the geometrical nonlinearity caused by the large deformations of the materials in the case of their shrinkage. For the indicated model to be used for calculating the parameters of a material, it is necessary to know the properties of this material. Let us consider wood, which is classified as capillary-porous materials. Wood is most commonly considered as an orthotropic body, the rheological and heat-and-mass-transfer characteristics of which represent tensor quantities. The orthotropic properties of the heat-and-mass-transfer processes are defined by the matrices in formulas (21) and (29). We dwell on the mechanical orthotropic properties of wood. The elastic characteristics of wood are defined by the matrix

$$[D] = \begin{bmatrix} d_{11} & d_{12} & d_{13} & 0 & 0 & 0 \\ d_{12} & d_{22} & d_{23} & 0 & 0 & 0 \\ d_{13} & d_{23} & d_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & d_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{66} \end{bmatrix},$$
(43)

where $d_{11} = \frac{1}{J}(1 - v_{23}v_{32})E_1$, $d_{22} = \frac{1}{J}(1 - v_{13}v_{31})E_2$, $d_{33} = \frac{1}{J}(1 - v_{12}v_{21})E_3$, $d_{12} = \frac{1}{J}(v_{21} + v_{23}v_{31})E_1$, $d_{13} = \frac{1}{J}(v_{31} + v_{21}v_{32})E_1$, $d_{23} = \frac{1}{J}(v_{32} + v_{12}v_{31})E_2$, $d_{44} = G_{12}$, $d_{55} = G_{13}$, $d_{66} = G_{23}$, and $J = 1 - 2v_{12}v_{23}v_{31} - v_{13}v_{31} - v_{12}v_{21} - v_{23}v_{32}$. Of the twelve elastic quantities, only nine quantities are independent because, owing to the symmetry of matrix (43), the following equalities are always fulfilled:

$$E_1 \mathbf{v}_{21} = E_2 \mathbf{v}_{12}, \quad E_2 \mathbf{v}_{32} = E_3 \mathbf{v}_{23}, \quad E_3 \mathbf{v}_{13} = E_1 \mathbf{v}_{31}.$$
 (44)

For the two-dimensional stressed state, we have

d

$$[D] = \begin{bmatrix} d_{11} & d_{12} & 0 \\ d_{12} & d_{22} & 0 \\ 0 & 0 & d_{33} \end{bmatrix},$$
(45)

where

$$\begin{split} d_{11} &= \frac{E_1}{J} \frac{(1 - \mathsf{v}_{12} \mathsf{v}_{21})(1 - \mathsf{v}_{23} \mathsf{v}_{32}) - (\mathsf{v}_{31} + \mathsf{v}_{21} \mathsf{v}_{32})(\mathsf{v}_{13} + \mathsf{v}_{12} \mathsf{v}_{23})}{1 - \mathsf{v}_{12} \mathsf{v}_{21}}; \\ d_{22} &= \frac{E_2}{J} \frac{(1 - \mathsf{v}_{12} \mathsf{v}_{21})(1 - \mathsf{v}_{13} \mathsf{v}_{31}) - (\mathsf{v}_{32} + \mathsf{v}_{12} \mathsf{v}_{31})(\mathsf{v}_{23} + \mathsf{v}_{21} \mathsf{v}_{13})}{1 - \mathsf{v}_{12} \mathsf{v}_{21}}; \\ _{12} &= \frac{E_1}{J} \frac{(1 - \mathsf{v}_{12} \mathsf{v}_{21})(\mathsf{v}_{21} + \mathsf{v}_{23} \mathsf{v}_{31}) - (\mathsf{v}_{31} + \mathsf{v}_{21} \mathsf{v}_{32})(\mathsf{v}_{23} + \mathsf{v}_{21} \mathsf{v}_{13})}{1 - \mathsf{v}_{12} \mathsf{v}_{21}}; \ d_{33} = G_{12}. \end{split}$$

To determine the characteristic matrix [D] of the plane stressed state, it is necessary to know the following seven quantities: E_1 , E_2 , E_3 , v_{12} , v_{13} , v_{23} , G_{12} . In [4–7], a complete set of anisotropic characteristics of wood has been obtained. The dependence of the rheological properties of wood on its moisture content and temperature was investigated in [8–10], where the corresponding data are presented. The elastoviscous properties of wood were determined in [11, 12].

The density of wood depends critically on the content of moisture in it. The moisture content of different kinds of wood can be found in [6, 13, 14]. The heat capacity of wood was discussed in [6, 9, 13]. Taking into account the results obtained in these works, we constructed the dependences of this quantity on the temperature and moisture content. As already noted, the heat conductivity of wood depends substantially on the direction of heat transfer in it. In the literature [6, 9, 13, 14] there are data on the heat conductivity of wood in the mutually perpendicular radial, tangential, and longitudinal directions as well as the functional dependences of the heat conductivity on the temperature and the moisture content. The diffusivity of wood as well as its heat-conductivity coefficient are dependent on the spatial direction of heat flow in it. Its description can be found in [6, 9, 15, 16]. According to [16], the diffusion



Fig. 1. Typical temperature distribution in the material at different instants of time: a) 0.1 h; b) 0.3 h; c) 0.5 h; d) 1.4 h. *T*, $^{\circ}$ C; *x*, *y*, m.

differs from the heat conduction in that the influence of the humidity on the diffusivity can be disregarded as compared to the temperature effect. The temperature-gradient coefficient is calculated by its functional dependence on the temperature and the moisture content, proposed in [9]; this dependence agrees well with the results obtained in [16, 17]. The phase-transition criterion ε characterizing the amount of moisture evaporating inside the material was determined in [17–20]. In accordance with the results of the indicated works, this criterion is taken to be a constant equal to 0.15. To perform numerical calculations, it is necessary to know the dependence of the equilibrium moisture content on the temperature and the relative humidity. Such functional dependences can be found in [6, 9]. With the use of the functions $W_{eq} = W_{eq}(T, \phi)$ we can determine the energy of binding of water with a material that can be high at a small content of moisture in it. The quantity W_{eq} is also necessary for formulation of boundary conditions.

For numerical calculations, in addition to the characteristics of the heat and mass transfer in wood, it is necessary to know the characteristics of the heat and mass exchange between the wood and the environment (a drying agent). The calculations are carried out on the assumption that the parameters of the drying agent (temperature, velocity, relative humidity) remain unchanged during the drying process or change only when passing from one stage to another (the number of these stages is most often not larger than three) in accordance with a definite drying regime. Therefore, unlike the internal properties of wood, the coefficients of heat and moisture exchange are determined in advance. They can be obtained from the functional and graphical data presented in [6, 9, 16].

Results of Calculations. The processes of heat and mass transfer in wood and its stressed-strained state were calculated on the basis of the physical and mathematical models, numerical methods, algorithms, and programs, developed by us. A sample of width 0.15 m and thickness 0.075 m was considered. The heat and mass exchange between all the surfaces of the sample and the environment was carried out by the conductive-convective mechanism. Let the



Fig. 2. Typical distribution of moisture content in the material at different instants of time: a) 6 h; b) 36 h; c) 80 h; d) 160 h. W, kg/kg; x, y, m.

mass-transfer coefficient $\beta_W = 2.7 \cdot 10^{-6}$ m/sec, the heat-transfer coefficient $\alpha = 33$ W/(m²·K), the initial humidity $W_0 = 0.5$ kg/kg, the equilibrium moisture content $W_{eq} = 0.03$ kg/kg, the ambient temperature $T_{env} = 80^{\circ}$ C, the initial temperature of the material $T_0 = 20^{\circ}$ C, the density of the dry pine $\rho_0 = 470$ kg/m³, the coefficients of linear shrinkage in the radial and tangential directions $\beta_r = 0.17$ and $\beta_t = 0.28$, respectively, and the Poisson coefficients $v_{12} = 0.4$, $v_{23} = 0.02$, and $v_{13} = 0.03$. Note that, with allowance made for the symmetry of the problem, the calculations were performed for a fourth of the sample.

Figure 1 shows a typical temperature distribution in the material at the instants of time 0.1, 0.3, 0.6 and 1.4 h, and, in Fig, 2, a typical moisture-content distribution in the material at the instants of time 6, 36, 80, and 160 h is given. Figure 3 presents typical distributions of stresses in the material; it is evident from this figure that they are complex in character. However, one regularity follows from the graphs: the maximum values of the quantities σ_{xx} , σ_{yy} , and σ_{int} are attained near the surface of the material, and they have smaller values at all the other points. Figure 4 presents a graphic pattern of possible crack formation and destruction of the material. The values of σ_{int} and σ_{str} were determined at the center of the upper surface of the material dried. It is seen from Fig. 4a that the intensity curve intersects the strength curve. This means that the stresses in the material exceeded its strength, which gave rise to the formation of cracks on the surface. In Fig. 4b, it is shown that the stresses developing in the material do not exceed its strength and, therefore, it will dry without cracks and destruction. To provide this condition, we decreased, as compared to the data presented in Fig. 4a, the thickness of the material to 0.015 m and the mass-transfer coefficient β_W to $1 \cdot 10^{-6}$ m/sec.

Conclusions. The mathematical model and the numerical calculation method proposed as well as the nonlinear characteristics of the internal and external heat and mass transfer in colloidal capillary-porous materials and their rheological properties allow one to simulate and investigate various processes of heat and mass transfer in these mate-



Fig. 3. Typical distribution of stresses in the material within 18 h after the beginning of drying: a) σ_{xx} ; b) σ_{yy} ; c) σ_{xy} ; d) σ_{int} . x, y, m; σ_{xx} , σ_{yy} , σ_{xy} , σ_{int} , Pa.



Fig. 4. Change in the intensity of the normal stresses (1) and in the strength (2) at the center of the upper surface: a) width 0.15 m, thickness 0.075 m; b) width 0.15 m, thickness 0.015 m. σ_{int} , σ_{str} , Pa.

rials and their stressed-strained state under natural and artificial technological conditions. The model proposed makes it possible to calculate the interdependent, nonlinear processes arising in materials in the process of drying as a result of their large deformations and shrinkages, the appearance of displacements in them, and the change the rheological and heat-and-mass-transfer characteristics of the materials with change in their temperature and moisture content. The only

limitation of this model is that it cannot give an accurate experimental determination of the properties of the material and the drying agent.

NOTATION

 a_W , diffusion coefficient, m²/sec; a_{Wii} , components of the diffusion tensor, m²/sec; [A], matrix presented in [3]; [B], gradient matrix; c, specific heat capacity, $J/(kg \cdot K)$; d_{11} , d_{12} , d_{13} , d_{22} , d_{23} , d_{33} , d_{44} , d_{55} , d_{66} , elements of the matrix [D]; [D], $[D_{diff}]$, characteristic matrices of a material; E, modulus of elasticity, Pa; $\{F\}$, force vector from formula (33) or load vector from formulas (25) and (30); G rigidity modulus, Pa; [G], matrix presented in [3]; g, determinant of the metric tensor; g^{ij} , components of the metric tensor; [H], characteristic matrix of the material; j, moisture flow, kg/(m²·sec); [J], Jacobi matrix; [K_t], tangential-rigidity matrix; [K_{nlin}], matrix of large displacements; [K_{σ}], matrix of initial stresses; [L], characteristic matrix of the material; [M], matrix presented in [3]; [N], shape-function matrix; $Q_{\rm p}$, heat of evaporation of moisture from the material, J/kg; $q_{\rm sur}$, heat flow, W/m²; {r}, vector accounting for the initial properties of the material; r_1 , r_2 , r_3 , components of the vector r; s^{ij} , components of the deviator stress tensor, Pa; S, area, m²; T, temperature, K; $\{T\}$, temperature vector; t, time, sec; $\{u\}$; displacement vector; u_m , u^m , covariant and contravariant components of the displacement vector, m; V, volume, m^3 ; W, moisture content; kg/kg; {W}, moisture-content vector; x, y, z, coordinates, m; α , heat-transfer coefficient, W/(m²·K); β , shrinkage coefficient; β_{W} , mass-transfer coefficient, m/sec; β_r , β_t , coefficients of linear shrinkage in the radial and tangential directions respectively; Γ'_{jk} , Christoffel symbols; δ , thermal-gradient coefficient, 1/K; δ'_{j} , Kronecker symbol; ε , phase-transition criterion; ε_i^i , components of the deformation tensor; { ε_i }, deformation vector; { ε_0 }, humidity-deformation vector; λ , heat-conductivity coefficient, W/(m·K), or the Lamé coefficient; λ_{ii} , components of the heat-conductivity tensor, W/(m·K); μ , Lamé coefficient; v, Poisson coefficient; ρ_0 , density of the dry material, kg/m³; σ^{ij} , σ_{xx} , σ_{yy} , σ_{xy} , components of the stress tensor, Pa; { σ }, stress vector; σ_{int} , intensity of normal stresses, Pa; σ_{str} , strength, Pa; τ , integration variable, sec; φ , relative humidity of air; χ , functional. Subscripts: dif, diffusion; *i*, *j*, *k*, *l*, *m*, α , β , tensor components; *n*, number of iterations; r, radial; s, shift; T, heated; tr, transposition of matrix; t, tangential; int, intensity; lin, linear; nlin, nonlinear; new, new; el, elasticity; sur, surface; str, strength; eq, equilibrium; rel, relaxation; env, environment; m, middle; old, old; p, phase; W, moist; 0, zero or initial; 1, 2, part of the mass flow in formula (18); 1, 2, 3, vector components in formula (42) or spatial directions in formulas (43)-(45); ; , covariant derivative.

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