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MODELING OF TWO-DIMENSIONAL INTERRELATED HEAT AND MASS TRANSFER PROBLEMS AND STRUCTURE TRANSFORMATION

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A numerical method to solve interrelated heat and mass transfer problems with structure transformation for easily deformable disperse capillary-porous media is suggested. Structure transformations of bodies of various shape, composition, and capability of cracking during drying are analyzed.

It is known that in many natural disperse systems such as peat, sapropels, and clayey minerals their structure undergoes transformation and failure as a consequence of considerable shrinkage in dehydration and a nonuniform moisture field. Modeling of these processes under different heat and mass transfer conditions using modern computing facilities makes it possible not only to calculate temperature, moisture, and mechanical-stress fields but also to obtain visual information about changes in the structure, dimensions, and shape of samples.

Processes of heat and mass transfer involving structure transformations are of a complicated nature associated with their nonlinearity and interdependence. For such processes problems of temperature, moisture, and mechanical-stress distributions must be solved with allowance for structure transformations, changes in geometry, and the random character of cracking. It should also be taken into consideration that cracking of the open type can occur to the point of structure failure. An analysis of the literature concerned with numerical methods in fluid dynamics, heat and mass transfer theories, the mechanics of a deformable solid, and theories of material strength and destruction revealed that the problems are mainly solved by traditional methods based on the methods of finite differences and finite elements and their modifications. Recently in the domestic and foreign literature alternative methods have been discussed in which instead of a continuum use is made of point particles moving together with the medium and carrying the entire information about the mass, energy, and momentum of this medium. These methods (sometimes they are called gridless) are based on the principles of a free neighborhood of point particles carrying information about the state of the physical system. The first of them was the method of V. F. D'yachenko [1] known as "the method of free points." Later on, this approach was extended in [2-4] to numerical calculations of two-dimensional problems of gas and fluid dynamics and deformable solids. However, no works are known in which "the method of free points" is used for calculations of structure transformations in processes of dehydration of disperse systems, although for this certain prerequisites exist. It is known that many disperse materials consist of associates of macromolecules that are capable of uniting into aggregates and macroaggregates, i.e., a disperse material can be separated into certain structural elements. If we assume that the entire mass and energy of a structural element are concentrated at the center and interaction of neighboring elements is accomplished via linear links, then we can build a finite-difference grid with variable nodal connectivity to calculate processes of structure transformation of a disperse material.

An important point for adequate modeling is establishment of a correlation between heat and mass transfer characteristics, physicomechanical properties of discrete structural elements (microparameters), and analogous parameters of the body considered as a continuum (macroparameters). For hexagonal structural packing, the microcharacteristics of heat and mass transfer and the physicomechanical properties of the elements can be calculated analytically. It should be noted that a body with a regular hexagonal structure is not rigorously isotropic with respect to the physicomechanical properties.

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In the more general case of a purely isotropic structure where the structural elements are chaotic and possess a different number of links, the correspondence between the micro- and macroparameters of the heat-mass transfer and mechanical characteristics can be determined by test calculations, i.e., by prescribing certain boundary conditions on a material surface of regular shape and then comparing the calculated values obtained by a numerical method with the corresponding analytical formulas for heat and mass flows and deformation.

If a body consists of different structural elements – the case typical of composite materials – this can be reflected in the model by prescribing different heat-mass transfer and mechanical parameters of the structural elements.

The basis of the algorithm for calculation of heat and mass transfer with structure transformation is formation of a data file of dimensionality $N \times L$, where N is the number of structural elements and L is the number of parameters of each element. The parameters of the elements are their coordinates, velocity, temperature, moisture content, hydrostatic pressure, mass, heat capacity, and moisture capacity, the numbers of neighboring elements, the parameters of the links with neighboring elements, and the features of element location.

The initial parameters of the two-dimensional isotropic structure of a material are obtained by subdividing the body into structural elements by a retangular grid with a pitch Δh, the coordinates of whose nodes correspond to the location of the elements. Then the elements are enumerated, for each of them eight potential neighbors are determined, and after that an element is displaced in a random manner in an arbitrary direction by a value not exceeding 25% of the initial grid pitch. The next procedure involves elimination of cross links. Here, an advantage is given to shorter links. By this means a random isotropic structure can be obtained in which each element possesses four to eight links with neighbors. For each element the initial length of the links with its neighbors and its mass are determined proportionally to the initial area. The boundary between them is determined from the condition that the three nearest elements form a triangle, at the intersection of whose medians they have a common point.

Proceeding from the above conditions, we derived formulas to calculate the flows of transferred substances (moisture and heat) q by the links connecting the elements numbered i and k:

$$q_{ik} = \lambda (\Theta_k - \Theta_i) \left[\frac{\tan (\pi/M_k) \tan (\pi/M_i)}{\tan (\pi/M_k) + \tan (\pi/M_i)} \right] . \quad (1)$$

Calculations of test problems showed that the calculation error of the two-dimensional temperature and moisture fields using formula (1) does not exceed 2% on a grid consisting of 30 × 30 structural elements.

The changes in the moisture content and temperature on the structural elements in a time step $\Delta\tau$ are calculated by formulas of the type

$$\Delta W = \frac{\sum_{k=1}^{N} q_{ik}}{\rho_m S_i} \Delta\tau , \quad (2)$$

$$\Delta T = \frac{\sum_{k=1}^{N} q_{ik}}{\rho_m c_{sp} S_i} \Delta\tau . \quad (3)$$

The basis for calculation of mechanical stresses is the change in the length of the links between the elements l_i with respect to the equilibrium length l_0 determined by the moisture content and the temperature:

$$\Delta l_i = l_i - l_0 \, [1 + \alpha (T - T_0) + \beta (W - W_0)] . \quad (4)$$

The elastic stress on a link is calculated according to Hooke's law

$$F_e = E_{link} \frac{\Delta l_i}{l_i} . \quad (5)$$

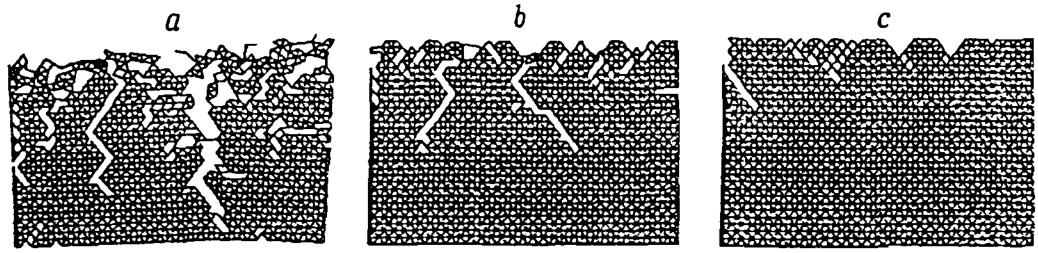


Fig. 1. Structure transformation (the final stage of the process) at $P_{\text{link}}/E_{\text{link}} =$ 0.0125 (a); 0.05 (b); 0.2 (c).

The shear stress between neighboring elements is determined as

$$F_{\text{v}} = -\eta \frac{V_i - V_{\text{n}}}{l_i}. \tag{6}$$

For a viscoelastic mechanical model it is assumed that under the action of the elastic forces on the links due to linear deformation of the links and the forces of viscous friction due to the difference in the velocities of neighboring elements displacement of element location at each time step by a value Δr at which the sum of all the forces tends to zero occurs.

To take into account the influence of hydrostatic-pressure gradients, developing under the action of the viscous forces on the links, on the processes of moisture transfer, the total hydrostatic pressure on the elements is calculated as

$$P = \frac{1}{N} E_{\text{link}} \sum_{i=1}^{N} \frac{\Delta l_i}{l_i}, \tag{7}$$

with allowance for which the moisture potential on the elements is determined in the form

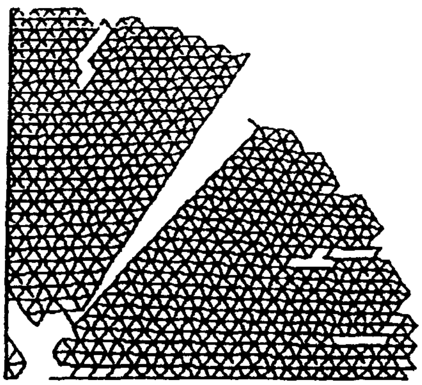
$$\Theta = \Theta_{\text{mt}}(W) + kPv. \tag{8}$$

Then the general structure of the algorithm will look as follows. First, using formulas (1)-(3) and (7)-(8) the moisture-content and temperature distributions in the body are calculated. Then formulas (4)-(6) are employed to calculate the new location of the element. Next, the condition of link breakage is checked. If it is fulfilled when the stresses attain a value exceeding the strength of the structural links, then the cracking process is modeled. Considering the random character of cracking, the strength limit is prescribed as a random quantity distributed by means of a generator of random numbers according to a certain law. This law can be represented either as uniform in a certain strength range or as normal with indication of the mathematical expectation and the root-mean-square deviation. If the force applied to a link exceeds the material strength, then new parameters (elasticity modulus, mass and heat transfer characteristics) corresponding to the conditions of crack formation are introduced. With increase in the distance between neighboring elements whose links broke, the algorithm makes provision for formation of new structural elements up to a certain value with characteristics corresponding to pore characteristics.

The algorithm can involve a change of the neighboring elements connected with a given element, which makes it possible to solve problems of viscoelastic flow of a material.

Prescribing certain boundary conditions on a material surface of various shape, one can solve a number of heat and mass transfer problems with structure transformation of the material up to disruption of structure continuity.

We conducted a series of numerical calculations of the drying process for bodies of different configuration and strength. On the upper surface of the sample boundary conditions of the third kind were prescribed. On the lateral and lower surfaces conditions of isolation from the external medium were adopted. The drying intensity was prescribed by means of the Biot mass-transfer number, equal to 50, 2, and 0.2. The moisture content of the material was varied from 6 to 1 kg/kg, which corresponded to twofold linear material shrinkage during drying. The



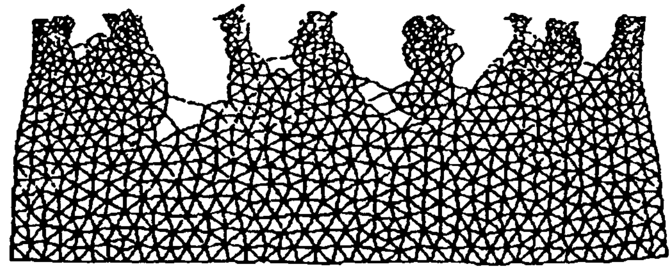


Fig. 2. Structure transformation of a cylindrical sample (1/4 of the sample cross section is depicted), Bi = 2; $P_{\text{link}}/E_{\text{link}}$ = 0.05.

Fig. 3. Structure transformation with the possibility of cracking at Bi = 100, $P_{\text{link}}/E_{\text{link}}$ = 0.2.

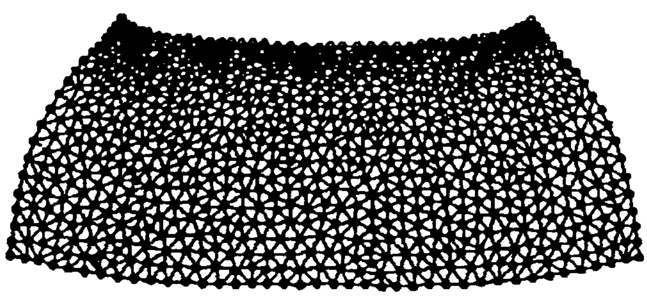


Fig. 4. Change in the sample shape without cracking at Bi = 100.

viscoelastic state of the body was modeled by prescribing the linear-elasticity modulus E_{link} and the limiting rupture strength of the links P_{link}. With account for the fact that the character of structure transformation is mainly determined by the state of the rupture strength of the links and the linear-elasticity modulus E_{link}, Fig. 1 presents typical structure transformations for flat samples at Bi = 50.

An analysis of structures for different strength characteristics, intensity of external mass transfer, and geometry reveals the following regularities in structure transformation of the material during drying. At the beginning of drying, samples in form of a plate exhibit cracks of the open type and their penetration into the material from the surface being dried. As a result, the sample edges undergo bending. As sample drying proceeds, cracks of the closed type appear. In the last stage of the process the sample unbends. The upper part of the most cracked samples becomes broader than their lower part, as noticed in laboratory experiments and full-scale observations, which corresponds to elevated porosity and cracking of the sample surface. With increase in Bi, the internal stresses in the body increase, thus causing enhancement of cracking [5]. A change in the strength limit also influences the amount of cracks in the sample. With decrease in P_{link}, their amount and size increase.

As concerns the influence of shape on the structure-formation process, it should be noted that the picture of cracking in semicylindrical samples is rather similar to that in flat samples. At the same time cylindrical samples are characterized by more intensive cracking, which in some cases leads to complete destruction of the sample (Fig. 2). This can be attributable to the lesser possibility of relaxation of the stressed state in cylindrical samples as compared to flat or semicylindrical samples, in which due to bending deformation the stressed state undergoes partial relaxation. In cylindrical samples all-sided drying precludes such a possibility. The suggested model also allows calculation of the moisture content, mass-transfer potential, and hydrostatic pressure distributions in a sample. Calculations of the processes of structure transformation were made with allowance for the influence of the hydrostatic pressure that develops in drying of flat samples on mass-transfer processes. Figures 3 and 4 present flat-sample structures with and without the possibility of cracking for identical parameters. As is seen, cracking exerts a substantial influence on the material geometry and structure. Figure 5 shows the hydrostatic-pressure

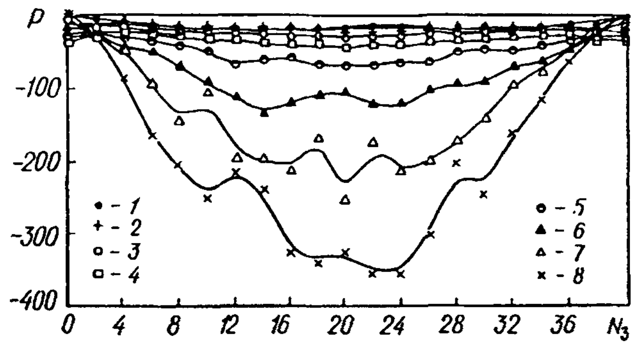


Fig. 5. Hydrostatic-pressure distribution over the sample layers: 1) on the lower surface; 2, 3, 4, 5, 6, 7) at a distance of $0.1H$, $0.2H$, $0.4H$, $0.6H$, $0.8H$, $0.9H$ from the lower surface of the sample, respectively (H is the sample height); 8) on the upper surface of the sample.

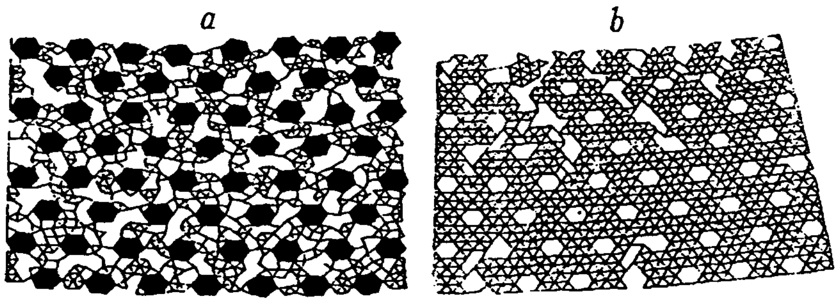


Fig. 6. Structure transformation with rigid (a) and easily deformable (b) inclusions.

distribution in sample layers at different distances from the lower boundary as a function of the zone number N_z for a sample without cracking. The number of a zone corresponds to its location a distance $N_z\Delta h$ from the left-hand edge of the body reckoned along the horizontal direction.

The reported data indicate that the hydrostatic pressure depends on both the horizontal and vertical coordinates. Moreover, the maximum absolute values of pressure are observed at the center of the upper part of the sample. Comparatively small hydrostatic pressures are typical for the lower part and lateral surfaces of the sample. The negative value of the hydrostatic pressure indicates the predominance of tensile stresses on the links between the elements. Nonuniformity of the hydrostatic-pressure in the sample exerts an influence on moisture transfer during drying. Thus, according to the hydrostatic-pressure distribution shown in Fig. 5, the additional moisture flow due to the hydrostatic-pressure gradient will be directed from the periphery and the lower part to the center of the upper part of the sample. This influences, naturally, the drying process.

In the case of fulfillment of the cracking conditions, calculations showed that no considerable hydrostatic stresses develop in the samples. Here, cracks of the open type exert an influence on the moisture-transfer processes by means of which heat and mass transfer can proceed via the vapor-air medium. The upper part of the sample becomes loose, and as in the former case sample bending is practically not observed.

We also calculated the drying processes and structure transformation of samples with a typical distribution of inhomogeneous inclusions in the form of rigid (Fig. 6a) and easily deformable (Fig. 6b) elements in them. The calculations showed that in the presence of rigid inclusions cracking is at its maximum, while in the case of easily deformable inclusions minimum cracking is observed as compared to homogeneous samples.

The possibility of introducing into the system new structural elements with characteristics corresponding to those of a pore or the medium surrounding the body makes it possible to describe more exactly the processes of external heat and mass transfer with structure transformation and cracking and to solve not only related heat and mass transfer problems but also conjugate "body–external medium" problems.

Mathematical modeling has shown that cracking and the mechanical strength of the structures obtained in the drying process are determined, along with the strength parameters of the links, by the dehydration regime, the possibility of relaxation of the stressed state owing to a change in shape, and the structural inhomogeneities of the samples.

The modeling carried out indicates the possibility in principle of using the developed approach to perform computer-aided modeling of interrelated heat and mass transfer processes with complicated structure transformations, including macrocracking and a change in the shape and dimensions of samples made of various materials.

NOTATION

q_{ik}, heat (moisture) flux on a link, W/m, kg/(m·sec); λ, thermal conductivity (moisture conductivity) of an element, W/(m·K), (kg·sec)/m^3; Θ, transfer potential, K, J/kg; Θ_{mt}, matrix potential of transfer, K, J/kg; Θ_k, Θ_i, energy (mass) transfer potentials at the corresponding nodes k and i, K, J/kg; M_i, M_k, number of neighboring points of the elements with the numbers i and k, respectively; T, temperature, K; W, moisture content, kg/kg; ΔW, change in the moisture content, kg/kg; ΔT, change in the temperature, K; T_0, initial temperature, K; W_0, initial moisture content, kg/kg; ρ_m, density, kg/m^3; c_{sp}, specific heat, J/(kg·K); S_i, element area, m^2; $\Delta\tau$, time step, sec; l_i, link length, m; Δl_i, change in the link length, m; l_0, initial link length, m; α, temperature coefficient of linear expansion, 1/K; β, linear-shrinkage coefficient; F_e, elastic tension on a link, Pa; F_v, tangential shear stress, Pa; V_i, element velocity, m/sec; V_n, neighboring-element velocity, m/sec; η, viscosity, Pa·sec; N, number of neighboring points of an element; N_z, zone number; P, hydrostatic pressure, Pa; E_{link}, elasticity modulus of a link, Pa; P_{link}, link strength, Pa; k, coefficient of load susceptibility; v, specific volume, m^3/kg; Bi, Biot mass-transfer number; Δh, pitch of the rectangular grid, m; Δr, element displacement, m. Indices: mt, matrix; m, material; sp, specific; e, elasticity; v, viscosity; n, neighboring element; link, link; z, zone; 0, initial.

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