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NUMERICAL SIMULATION OF HEAT-AND-MASS TRANSFER AND STRUCTURAL TRANSFORMATION IN DISPERSE MATERIALS

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This paper discusses a new approach to the investigation of highly deformable natural disperse systems based on the introduced notion of the physical element as a cell of the material structure. A method for calculating the heat-and-mass transfer and the structural transformation in disperse systems is described. The general principles and procedures of the technique of disperse system simulation, which is proposed to be named the method of physical elements, have been formulated.

Among the highly deformable disperse systems are grounds, peaty grounds, and peats. They have a complex and diverse composition and contain mineral and organic components, water, and water-soluble compounds. Mineral particles incorporate solid grains differing in their composition, size, and shape. These are mainly gravel, sand, and clay. The organic component is a product of the decomposition of plants. Thus, the organic peat mass [1] can be broken up into bitumen, humin, highly hydrolyzable and nonhydrolyzable substances, and cellulose. High-molecular organic and mineral compounds in the colloidal, molecular, and ionic states are classified with the water-soluble compounds [2]. Water and the compounds dissolved in it play an important role in the formation of contacts between particles and the structure of the system as a whole. Between particles capillary and intermolecular forces can exist and chemical bonds can be formed. Depending on the nature of the active forces between particles, the contacts can conditionally be subdivided into two main types: coagulation and phase contacts. The former are mainly realized by intermolecular and capillary forces and the latter — by chemical bonds. The fundamental difference between them is that coagulation contacts are completely reversible and phase contacts are irreversible with respect to mechanical actions.

In accordance with the main types of contacts, one can also distinguish two main kinds of structures: condensation-crystallization and coagulation structures. The former are formed by spatial coalescence (chemical interaction) of many fine crystals, with the mechanical properties of the material formed corresponding to the properties of the particles. Such structures impart strength and brittleness to bodies and are not restored upon destruction. Structures of the second kind result from the coagulation adhesion of solid-phase particles through thin water interlayers. The mechanical properties of such systems are determined by the character and features of the interparticle bonds and medium interlayers rather than by the properties of particles.

The diverse composition and the various types of contacts and forces acting in natural disperse systems determine the wide set of structures in them. For instance, N. A. Tsytovich [3] describes a ground from clayey deposits, which can be represented by separate sand and clay particles bounded by colloids and forming, in the aggregate, a loose rock pierced with pores. S. V. Nerpin and A. F. Chudnovskii [4] propose a model of a soil consisting of spherical particles each of which enters into the composition of particles of the same shape but of the next consecutive size on the one hand and consists of particles of a smaller size on the other. N. V. Churaev [5] presents a model of a biporous structure consisting of chaotically arranged particles with different sizes, where two characteristic mean diameters of pores — inside particles and in the space between them — are introduced. In [6], a number of structures of inhomogeneous media are described, in particular, an oil-bearing ground in which quartz, feldspar, and mica grains of arbitrary shapes and sizes are bonded by carbonate and clayey cement is presented. The grains together with the cement form a rigid framework whose pores contain a liquid (water, oil) and its vapors. In [12], the structure of a peat is described, in particular, a model of its particle is given. The peat is represented by a space grid of "laced"

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macromolecules whose cells contain intra-aggregate water freely communicating with the external solution. A. E. Afanas'ev [7] presents a model of a peat consisting of "primary" particles, associates ("primary" particle packing), aggregates (associate packing), and macroaggregates (aggregate packing).

The complex character of the structures in natural disperse systems determines the diverse and complex rheological and strength properties of such systems and the various heat- and mass-exchange processes in them [2–6, 8–10]. Without describing these processes (they can be found in the references herein), we only note that the phenomena of heat-and-mass transfer and structural transformations in natural disperse highly deformable systems are interrelated, since they result from the same physical cause — the dispersion of particles and the field of surface forces forming a certain structure of a disperse system depending on the ambient conditions [5].

Computer analysis of the photographs of the materials under investigation has shown that the described objects have several characteristic steps of the structure. Such properties can be displayed by both systems consisting of a complicated interlacement of a fibrous framework inside of which there is a fine-dispersion medium and systems representing multilevel formations. Proceeding from the foregoing, it is natural to take into account the common properties of such systems and break down the material being investigated into particles-elements. In so doing, the degree of detail depends on the aim of the investigation. A similar approach is also used in other fields of science [11].

Mathematical description of the heat-and-mass transfer processes with a structural transformation leads to a system of interrelated nonlinear differential equations with variable coefficients [5, 12–14]. Moreover, complete description of the deformation and transformation of the structure requires that the model being used should realize cracking, displacement of elements relative to one another for large distances, and the formation of new elements in the place where a crack appears. It is impossible to solve such problems analytically; they can be solved by numerical methods. In this case, too, however, certain difficulties arise. For a particular application of numerical methods, it is necessary to carry out a theoretical analysis for stability and convergence, but for nonlinear systems such a theory is absent thus far. Therefore, to investigate the processes under consideration, the computing experimental procedure described in [11, 15–17] was chosen. Note that these works give different approaches to it; however, they do not exclude but, on the contrary, complement one another, yielding a more complete picture. Here we will not dwell on the discussion of this question but only note that this approach was used by us in solving the problems under investigation. The computing experimental procedure that has made it possible to solve a number of problems is described below.

First an element is given, and, in so doing, to form an isotropic structure, a stochastic distribution of elements in the space is used. Once the desired properties have been assigned to the element, it becomes self-contained and behaves depending on the interaction with its neighbors. Its behavior is not analyzed in advance and is not described by any equations, including differential equations (all is analogous to the behavior of molecules in molecular dynamics). Since such elements are many, we have a system of many bodies whose behavior cannot be predicted. Information on the behavior of such elements can only be obtained after calculations; therefore, the computing experiment becomes one of the methods of theoretical analysis of the behavior of systems.

Once the element is given, calculations are made and the results, on the basis of which it is refined, are analyzed; then the difference formulas are constructed again and calculations are carried out. The new cycle is repeated and this procedure is carried out until all errors are corrected and satisfactory results are obtained. This makes it possible to gain a deeper insight into many features of the problem being solved and look at it from different sides. Already at this stage the solution becomes predictable and the behavior of the system becomes clear. Thus, a numerical experiment on the investigation of the physical processes is realized.

In accordance with the foregoing, we have used methods analogous to those developed in molecular dynamics [11, 15, 18], where the paths of a large number of interacting particles are calculated. First the force acting on the particles is calculated from concrete physical conditions. This force can be their elastic collision or the two-particle force function, depending on the spacing between them; but if these are charged particles, then the force can be calculated on the basis of the Coulomb law or by solving the Poisson equation. The next step is to find, on the basis of the equation of motion, the velocities and displacements by the formulas

$$v_x^{n+1} = v_x^n + \frac{\Delta t}{m} F_{\text{total}\,x}\,, \tag{1}$$

$$v_y^{n+1} = v_y^n + \frac{\Delta t}{m} F_{\text{total}\,y} , \tag{2}$$

$$x^{n+1} = x^n + \Delta t v_x^{n+1} , \tag{3}$$

$$y^{n+1} = y^n + \Delta t v_y^{n+1} . \tag{4}$$

For our system consisting of elements an analogous procedure is used, and the forces thereby are calculated from the rheological properties of the element; then, using formulas (1)–(4), the new position of the system is calculated.

In [9], a method of particles in cells is proposed. In this method, the domain of variability of independent variables is broken up by a stationary calculation (Euler) grid and a continuous medium is given in the form of an aggregate of particles of a fixed mass (Lagrange grid) moving through the Euler grid. This approach, however, does not solve all problems either. In the mechanics of continuous media, alternative methods are also developed. For instance, in [20] a method of free points with Lagrange coordinates without a fixed coordinate grid is presented. To calculate the values of the functions, particles closely spaced at a given instant of time are used. In [21], this ideology is extended to the deformation and destruction of elastoplastic bodies.

Thus, in order to construct a numerical method suitable for natural highly deformable disperse systems, it is necessary to make use of the experience in other fields of sciences, generalize the obtained results, and correctly apply them to the materials being investigated, taking into account their specific features. From [11] it follows that it is expedient to break up the disperse system into particles with such a degree of detail which is required by the problem under consideration. We also make use of the basic principles proposed in [20–23]: breaking up of the system into elements (cells); imparting all the necessary properties to them; giving certain bonds between them, and using the ideology of a free neighborhood of particles. The point of the latter principle is that the bonds between the particles are not rigid and can meanwhile change their neighbors, which makes it possible to avoid a strong deformation of the grid and calculate large deformations of the system (i.e., if between the particles there are linear bonds, then it is necessary to realize the procedure of their rupture or replacement). For a more complete description of the hydrodynamic properties it is necessary to introduce the notion of the element area [22, 23] through which interactions between particles are also realized. As in the works under consideration, we relate all information about the state of the physical system to elements. We also relate to them information about all neighbors of an element. In addition to the above-mentioned properties the system should exhibit the properties used in the molecular dynamics [11, 15, 18]. One advantage of these properties is the formulation of the problem without explicit use of differential equations and numerical calculations of the behavior of the gas with a minimal theoretical analysis of its behavior prior to calculations (method of direct numerical modeling of a physical phenomenon).

We now describe the element that should be used in modeling disperse systems (see Fig. 1a). It incorporates: nodes in the form of geometric points at which all linear bonds of the element converge; linear bonds — lines interconnecting the nodes; boundary — a surface limiting the element's volume (in the two-dimensional case, this is a line limiting its area); vertices — points of intersection of boundaries; angles between linear bonds; volume (in the two-dimensional case, this is the area); and nodes of its neighbors. The consideration of an isolated (solitary) element has no meaning. Therefore, to obtain a more complete picture, it is necessary to explain the notion of neighboring element. An element is a neighbor of a given element if there is a bond and, accordingly, a common boundary between them. When this bond is lost, they are no longer neighbors. The basic diagram of element discretization is given in Fig. 1b. Since a given element describes not only the structural features of the system but its physical, mechanical, and heat-and-mass exchange properties as well, it can be called a physical element.

The physical element also permits modeling bar systems, solid bodies, complex rheological materials, and liquids. This corresponds to the real scatter of the properties of disperse systems — from colloidal solutions to solid materials (for example, concrete). In this case, it should be remembered that to model a particular material, it is not necessary to use all properties of the element. For instance, in modeling elastic materials, it may be enough to use

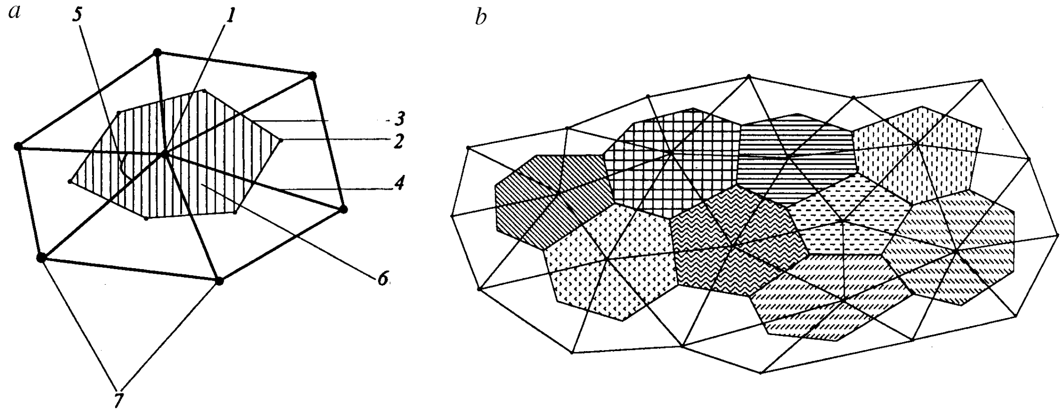

Fig. 1. (a) Scheme of the element [1) node; 2) vertex; 3) boundary; 4) bond between nodes; 5) angle between nodes; 6) element area; 7) nodes of neighboring elements); (b) schematic diagram of element discretization.

nodes and linear bonds, whereas for a Newton liquid, instead of bonds, areas are brought to the forefront. We also note that a certain property of the system can be modeled by different methods. The elasticity of the whole body is given, for example, by the elasticity of bonds determined by their elongation or compression; by the change in the angle between bonds from a certain initial (or mean) value; by the compression or extension of the element volume [24–26]:

$$F = E \frac{\Delta l}{l} S \,, \tag{5}$$

$$F = E \left(1 - \frac{\alpha_0}{\alpha} \right) S \,, \tag{6}$$

$$F = (P_{\text{e}} - P_{\text{neigh}}) \, S \,, \tag{7}$$

$$P = E_{\text{v}} \frac{V_0 - V}{V} \,. \tag{8}$$

Viscosity can be modeled by means of the relative motion of the nodes of the neighboring elements [24–26]:

$$F = -\,\eta \frac{v_{\text{e}} - v_{\text{neigh}}}{l} S \,. \tag{9}$$

We write the formula for the force determined by the deformation of the linear bond between elements i and k; in the cylindrical system of coordinates [24, 27]:

$$F = \frac{\pi}{2} E \, (l_{ik} - l_{0ik}) \left(\tan\frac{\pi}{N_i} + \tan\frac{\pi}{N_k} \right) (R_i + R_k) \,. \tag{10}$$

In the same system of coordinates the force associated with the deformation of the circle of rotation will act:

$$F = 2\pi E \frac{R - R_0}{R_0} S_{\text{e}} \,. \tag{11}$$

The method under consideration makes it possible to take into account the volume forces caused by the gravitational or electromagnetic interaction as well. The introduction of such forces acting on the element causes no complications and is not limited by anything.

Plasticity can be given in terms of both bonds and volumes. Some of the methods of its realization can be found in [24, 27]. Below we give the formulas for calculating plastic deformations in terms of bonds:

$$P_{\mathrm{m}} = -\frac{1}{N} E \sum_{i=1}^{N} \frac{\Delta l_i}{l_i} , \tag{12}$$

$$\Delta l_0 = kf \left(\frac{P_{\mathrm{m}}}{E} l + \Delta l \right), \tag{13}$$

$$\Delta l_{0\mathrm{s}} = -\frac{\sum_i \Delta l_{0i} \, l_{0i}}{\sum_i l_{0i}^2} \, l_0 , \tag{14}$$

$$\Delta l_{0\mathrm{f}} = \Delta l_0 + \Delta l_{0\mathrm{s}} . \tag{15}$$

Moreover, a bond can represent not only a perfect elastic or a perfect viscous body, but it can also be a complex rheological body determined by a combination of three simple bodies. As to the rheological properties, the same can also be said about the element volume.

One source of deformations and stresses in the material under heat-and-mass transfer is the gradient temperature and moisture-content fields. In this case, the calculations of the linear and volume deformations depending on the temperature were carried out by the formulas

$$\Delta l_{ij} = l_{ij} - l_0^3 \sqrt{1 + \beta \left(\frac{T_i + T_j}{2} - T_0 \right)} , \tag{16}$$

$$\Delta V = V - V_0 \, (1 + \beta \, (T - T_0)) . \tag{17}$$

Analogous dependences were also used for the moisture content.

The most suitable approach to the calculation of the transfer processes is the control-volume approach. It permits formulating difference equations without explicit writing of differential equations in second-order partial derivatives describing the transfer processes. The essence of this approach is that the law of energy conservation in the control volume surrounding the point under consideration is fulfilled. For our case, it is the element itself. The heat flow thereby is given in the form [24]

$$q = -\lambda_{\mathrm{bond}} \frac{T_i - T_j}{l} S . \tag{18}$$

It should be noted, however, that this is not the only method for calculating the heat flow. For instance, depending on a particular problem, the quantity S can be calculated in different ways. For example, for a bond that can be given in the form of a cylindrical bar it is the cross-section area (for the plane case — the cylinder diameter). In a number of cases, S can be given as the mean value of the contact area between the elements. Another example of the calculation of this quantity is given in [24, 28]. Then the expression for the flow will take on the form

$$q = \lambda_{\mathrm{bond}} \, (T_i - T_k) \frac{2 \tan\left(\frac{\pi}{N_i}\right) \tan\left(\frac{\pi}{N_k}\right)}{\tan\left(\frac{\pi}{N_i}\right) + \tan\left(\frac{\pi}{N_k}\right)} L . \tag{19}$$

However, (19) is only good for regular polygons in which the angles between the element bonds are equal. The greater the deviation of a polygon from the regular one, the larger the error.

The temperature increment is calculated by the formula

$$\Delta T = \frac{\sum\limits_i q_i}{\rho c V} \Delta t \, . \tag{20}$$

It should be noted that the distinguishing feature of the method under consideration is the possibility of calculating the temperature and moisture fields in the material with allowance for its transformations due to deformations and cracking.

Using the method being developed, it is possible to model the heat conduction of a system consisting of several randomly distributed components. The computing experiments performed yielded results that are in agreement with the percolation theory [6]. However, there are discrepancies between the calculated and experimental values of the heat-conductivity coefficients. To obtain a fair agreement with experiment, we had to introduce additional nodes and an elementary cell of the material analogously to [6]. Works [24, 28] present the computational procedure and the results of the determination of the heat conduction of inhomogeneous structured systems, taking into account the structural features of a composite material. However, the element with additional nodes cannot be used to investigate the processes of heat- and mass-transfer with cracking or with large displacements (where the procedure of replacement of bonds is realized) because of the fact that when the bond between the elements is removed, then the additional node, too, will disappear.

Other methods for calculating the displacements of elements were also realized. One of them is based on the fact that the processes of mechanical motion leading to a deformation of the material proceed much faster than the transfer processes, i.e., it may be considered that at each time step the element goes to the state of mechanical equilibrium where the total force acting on it is equal to zero. Then $\Delta \mathbf{r} = \alpha \mathbf{F}$. The quantity α is chosen so that the fastest transition to equilibrium takes place and is determined by the trial-and-error procedure. These variants were realized in [24–26, 29].

In [24, 27, 30], the following method was developed. On the basis of the analysis of the behavior of a system consisting of physical elements, it has been established that the total force acting on the element tends to displace it to a position where the force value will approach zero. The method using this fact in detail and the algorithms are given in the above-mentioned works. However, having saved some time, we lose stability. In a number of cases, the element node tends to "jump out" of the limits of the polygon composed of adjacent elements, after which the system loses stability and the program executes an emergency halt. To exclude such situations, it is necessary to take additional measures complicating the algorithm, which is lengthy enough as it is, and increasing the computer time. We would like to note that this method is not indisputable, since any body moves in the direction of action of the force, which, in so doing, should not necessarily decrease. For instance, the gravity remains constant independent of the motion of the body. Moreover, this method is complicated in terms of algorithmization, programming, and modification.

As noted above, one important advantage of the proposed method is the possibility of modeling material deformations and structural transformations. The basic principles on which the modeling is based are as follows:

(a) possibility of displacement of element nodes (modeling of deformations);

(b) removal of bonds between them (realization of cracking in the material);

(c) replacement of bonds between them (possibility of displacing elements for long distances from one another);

(d) creation and removal of new elements (modeling of the filling of cracks with another medium upon their formation and displacement of this medium when they close).

When large displacements of nodes take place, the elements are distorted and take on an irregular form. Initially, the closely spaced nodes recede from one another and approach other nodes which were previously located at long distances. It is logical to replace an extended bond by a short bond between approached elements. Keeping moving, the element will all the time recede from some elements and approach other ones. Sequential replacement of bonds between elements makes it possible to move them from one another for long distances. The further development

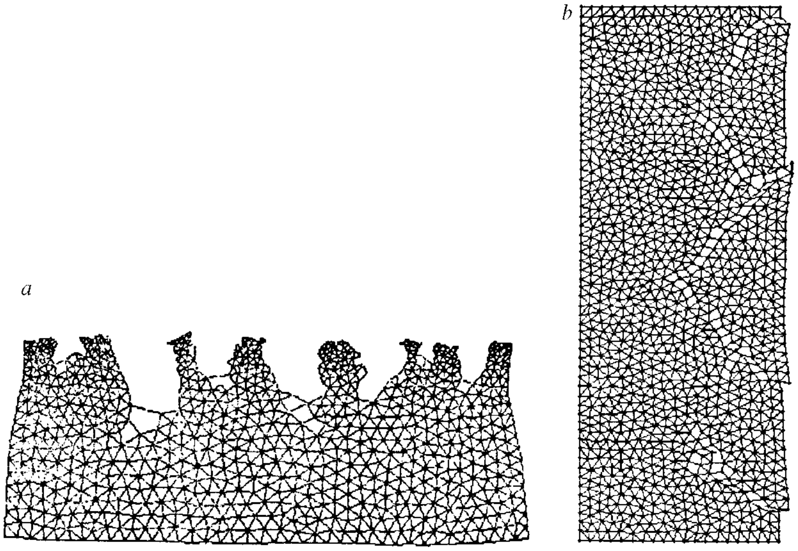

Fig. 2. Typical pattern of destruction of: a) viscoelastic sample in drying at Bi = 100 and $P_{\text{bond}}/E = 0.2$; b) elastic sample under triaxial compression at E = 1000 kPa, E_v = 100 kPa, and $P_{\text{bond}}/E = 0.3$.

of the method has shown that replacement of bonds between elements should be carried out depending not only on the location of the latter, but also on the value of the stresses on the bonds, their number, the value of the angle between them, etc.

The appearance of large stresses in the material caused by the moisture-content and temperature gradients can lead to the formation of cracks. Modeling of this process is based on the removal of bonds between elements. The condition for the rupture of the bond between them is a stress exceeding its strength. A simple analysis reveals that the maximum value of the strength for the rectangular sample in the numerical model will develop in the center. However, experience shows that cracking in natural materials is random in nature. Taking into account its stochasticity, we give the ultimate strength as a random variable distributed by the uniform law. Figure 2 a shows a typical pattern of destruction.

When the bonds are removed, the heat-and-mass exchange and mechanical interactions between elements at the point of rupture disappear. The cracks formed are filled with another medium; in a particular case, this can be air. For a more correct account of the heat-and-mass exchange, at the site of arising cracks, elements with the properties of the environment, which are first realized with the formation at the site of the broken bond of a new bond corresponding to the environment, are formed. As the crack grows further, a tetragonal element arises at the site of the new bond. As the crack grows, new elements can be formed on each of its bonds. Thus, the crack is gradually filled. At the end of the drying process, where the moisture-content gradients in the body decrease, closing of the crack is possible; therefore, the procedure of annihilation of the environmental elements has been realized. To this end, their size is checked: if it is smaller than a certain value, then the element is brought into a tetragonal form by replacing its bonds with other elements. As the crack further decreases, it is removed and only one bond with the properties of the material being investigated remains. In this manner, all elements are removed until the crack is completely closed.

An important point of the method under consideration is the setting up of a correspondence between the parameters of discrete physical elements and the analogous parameters of the whole body taken as a continuous medium. This procedure is needed for two reasons: it makes it possible to test the numerical scheme being developed and also to calculate the parameters of the material as a continuous medium by the known parameters of the physical elements.

The general technique of comparing the characteristics of the whole body and its elements is as follows. A homogeneous material of a simple form, for which, in giving the boundary conditions, one can analytically calculate its parameters, is taken. Then it is split into elements with properties analogous to the body under consideration and test calculations of the parameters of the material consisting of elements are carried out. If the results obtained agree, then the numerical scheme is considered to be adjusted. Now, giving to the elements the properties reflecting the internal characteristics of the body, we determine the parameters of the latter as a whole. We can thus calculate the characteristics of materials with inhomogeneous properties and of composite and structured materials. This technique and calculations are described in more detail in [24]. An example of the calculation of heat-conductivity coefficients in structured systems is described in [24, 28]. A method for calculating the parameters of a viscous medium is given in [24, 30], where the problems of material motion between two coaxial cylinders and free convection of a viscous system in a closed volume have been solved. Works [24, 27] consider the compression modulus of elasticity, the elastic modulus, and the Poisson coefficient of elastic and elastoplastic samples calculated by the rheological parameters of the physical elements.

To analyze the calculation data, the obtained information is usually given in the form of tables and curves. In describing a fluid flow or large deformations, it is convenient to present the results in the form of figures. In particular, this simplifies their analysis at large relative shifts; therefore, visualization was carried out, which permitted observing the dynamics of material deformation under the action of the moisture-content gradient, the formation of cracks in the material, and their filling with new elements. Visual observations of the temporal progress of deformations and cracking have made it possible to reveal the basic laws of this process up to the destruction of the material upon its dehydration. They have also made it possible to describe the picture of destruction of elastic and elastoplastic samples under a load (Fig. 2b).

On the basis of the proposed method, a program package has been developed to solve the following problems:

1) structural transformation in drying highly deformable disperse systems (modeling and visualization of the deformation and transformation of the structure, including the cracking and destruction of the material);

2) calculation of the temperature and moisture fields in a system with regard for the deformation and cracking in it;

3) numerical simulation of the deformation-stressed state and destruction of elastic and elastoplastic materials of cylindrical form;

4) modeling of the mechanical motion of disperse systems in a wide range of changes in their rheological properties, including regions with viscoelastic, viscoelastoplastic, and pure viscous properties of the material;

5) calculation of the heat conductivity of composite materials.

NOTATION

v, particle velocity, m/sec; m, particle mass, kg; Δt, time step, sec; F, force acting on the element, N; x and y, coordinates along the X and Y axes, m; q, heat flow, W; λ_{bond}, heat conductivity of the bond, W/(m·K); l, bond length, m; Δl, value of the bond deformation, m; S, area of the contact face between elements, m^2; α_0, angle corresponding to the regular shape of the polygon, rad; α, real angle, rad; P, pressure in the element, Pa; V, element volume, m^3; η, viscosity, Pa·sec; T, temperature, K; L, characteristic size of the bond perpendicular to the plane of the two-dimensional element, m; R, radius to the element center, m; S_{e}, element area, m^2; R_0, radius of the element center in complete absence of moisture in the body, m; N, number of bonds in the element; kf, coefficient determining the rate of plastic deformations and being of importance in the range from 0 to 1; Δl_0, change in the initial value of the element bond length with respect to the mean value of the pressure P_{c}, m; $\Delta l_{0\text{s}}$, change in the initial value of the bond length determined by the condition of conservation of the initial area of the element, m; $\Delta l_{0\text{f}}$, change in the finite value of the initial bond length, m; β, temperature expansion coefficient, 1/K; ρ, element density, kg/m^3; c, element heat capacity, J/(kg·K); $\Delta \mathbf{r}$, displacement vector, m; P_{bond}, bond strength, Pa; E, elastic modulus of the bond, Pa; Bi, mass-exchange criterion of Biot; E_{v}, volume modulus of element elasticity, Pa. Subscripts: x and y, spatial component along the X and Y axis, respectively; n, temporal layer number; e, element; neigh, neighboring element; i, j, and k, element numbers; m, mean; s, area; f, finite; v, volume; 0, initial; bond, bond; total, total.

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