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CALCULATION OF TEMPERATURE FIELDS AND THERMAL CONDUCTIVITY IN STRUCTURIZED SYSTEMS

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We suggest a new numerical method to calculate temperature fields and thermal conductivity coefficients in structurized systems. It allows one to describe the processes of heat conduction in deformation and transformation of the structure of the system. Calculations were carried out for an organomineral system and for a system consisting of sand, water, and air.

As is known, in natural disperse systems such as soils, peat, sapropels, and their composites the processes of heat and mass transfer depend strongly on the structure of the systems themselves. Here the structure should be understood in the broad sense of the word. In this category we can also place elemental composition, mutual arrangement of components, distribution of pores in a system, and the large number of their levels.

To calculate the processes of interrelated heat and moisture transfer and transformation of a structure, we developed and continue to refine the method of dynamic structural elements [1]. It is based on the premises that a system consists of structural elements, at the center of which the whole mass and energy corresponding to these elements are concentrated. The interaction of neighboring elements is accomplished through linear connections along which exchange by heat and mass occurs. For a viscoelastic mechanical model it is assumed that under the action of viscous forces appearing on the connections due to their linear deformation and of the forces of frictional viscosity due to the difference in the velocities of neighboring elements, the displacement of the element over time takes place. And moreover, structural elements can come into contact with one another in a random fashion and change their neighbors. This approach allows one to model the transformation of the structure of a system up to the formation of cracks and cavities.

Without going into the problems of mechanical character, we will center our attention on the problems that arise with adequate modeling of the processes of heat exchange in a structurized system. Here, a very important problem is the establishment of the relationship between the characteristics of heat transfer along the connections of discrete structural elements and similar parameters of the system which are typical of a continuous medium. Let us consider the scheme of thermal interaction between elements (Fig. 1). Marked in Fig. 1a are: 1) nodes of the elements; 2) linear connections between the elements; 3) faces of a structural element; 4) vertices of a structural element. In a general case a structural element is a polygon the number of whose vertices can change from 4 to 8. These elements are located randomly over the entire body. To determine the boundaries of the structural element unequivocally, we will agree that its vertices correspond to the geometric center of the triangle formed by the nodes of contacting elements. Assuming that the heat flux q_{ik} over the connection between the elements is proportional to the temperature gradient on this connection and to the length of the face by which the elements contact, we will write

$$q_{ik} = -\lambda_{el} \frac{T_i - T_k}{l_{ik}} L_{ik} . \tag{1}$$

For geometrically regular figures, for example, for a hexagonal array, we will bring Eq. (1) to the form

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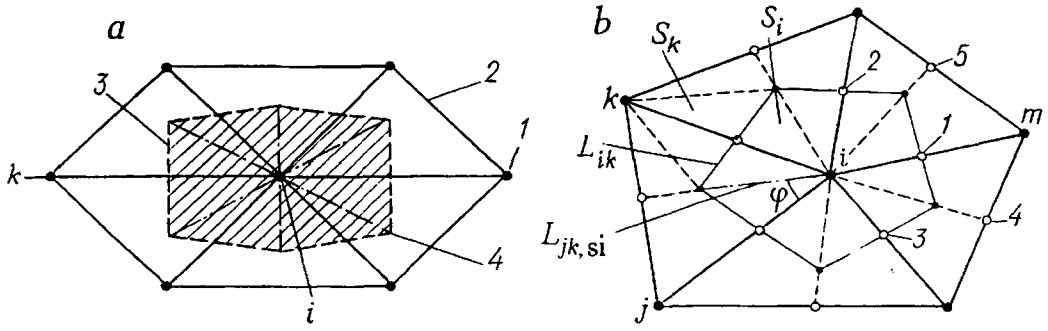

Fig. 1. Schematics of a structural element: a) general; b) with additional elements.

$$q_{ik} = -\lambda_{el}(T_i - T_k)\tan\varphi\,, \quad \varphi = \frac{\pi}{3}. \tag{2}$$

It can be verified here that λ_{el} corresponds to the thermal conductivity coefficient of a homogeneous continuous medium. Calculations of heat fluxes from formulas (1) and (2) for test problems show that these relations are general and allow one to describe the processes of heat transfer rather accurately for figures of arbitrary shape. Here φ is the averaged angle of a structural element, which is defined as $2\pi/N$. In the general case the heat flux over the connection between the elements i and k can be found from the formula

$$q_{ik} = -\lambda(T_i - T_k)\frac{2\tan\left(\frac{\pi}{N_i}\right)\tan\left(\frac{\pi}{N_k}\right)}{\tan\left(\frac{\pi}{N_i}\right) + \tan\left(\frac{\pi}{N_k}\right)}. \tag{3}$$

Calculations from relation (3) showed that deviation from the test values of heat fluxes for a body split up into 30 × 30 structural elements does not exceed 2%. To decrease the error of calculations, it is necessary, instead of the averaged angle φ, to use in formula (3) the specific angles φ_{ik} that correspond to the geometrical features of the connection.

Expression (3) yields satisfactory results for a single-component system. In the case of two and more components with different thermal conductivity coefficients it is necessary to somewhat modify the computational scheme. In addition to the nodes of the elements, we will introduce additional nodes at the intersection of the boundary of the structural element and linear connection. They are denoted by digits 1-5 in Fig. 1b. Each additional node is connected with two main nodes of the elements that form a linear connection and with four additional nodes. The heat flux between the node of the element and an additional node is calculated from the formula

$$q_{ik} = -\frac{1}{2}\lambda\frac{T_i - T_{ik}}{l'_{ik}}L_{ik} = -\lambda(T_i - T_{ik})\tan\varphi\,. \tag{4}$$

The heat flux between two additional nodes is given by the expression

$$q_{jksi} = -\frac{1}{2}\lambda\frac{T_{ij} - T_{ik}}{l'_{jk}}L_{jksi} = -\frac{1}{4}\lambda(T_{ij} - T_{ik})\left(\tan\varphi + \tan\left(\frac{\pi}{2} - \varphi\right)\right). \tag{5}$$

Using formulas (4) and (5), it is possible to obtain the temperature field in a system that has components with different thermal conductivity coefficients, including solid, liquid, and gas phases.

This approach can also be used to calculate the temperature field of a three-dimensional system consisting of structural elements in the form of polyhedrons. Here relations (1), (4), and (5) in their general form, just as for a two-dimensional case, remain valid. Only the area of contact over the line of connection will represent a polygon. For a hexagonal array, when one element contacts with 12 neighboring ones, the surfaces that contact

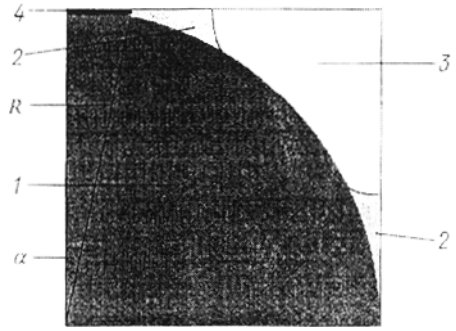

Fig. 2. Unit cell for a system consisting of sand, water, and air.

perpendicularly to the line of connections represent pentahedrons. The surfaces of side contact are triangles here. Calculations yield that the area of the main contact for a hexagonal array is equal to $S_m = 0.3469l^2$ and for the side contact it is $S_{si} = 0.13196l^2$. Test solutions showed that the error in the determination of heat fluxes is equal to about 1%. Taking into account the fact that calculation of three-dimensional systems requires a large amount of computations, a version of finding thermal conductivity in a cylindrical coordinate system has been developed for three-dimensional problems with axial symmetry. In this case, to determine heat fluxes, formulas of type (1), (4), and (5) must be supplemented with factors $\pi(r_i - r_k)$ that take into account the specifics of three-dimensional problems with axial symmetry.

To calculate nonstationary processes of heat exchange in structurized systems, along with heat fluxes it is necessary to consider the heat capacity of the structural element. This can be done by finding the area of the structural element and for two-dimensional problems by then multiplying by the density and specific heat capacity to obtain: $C_{el} = c_{sp}\rho S_{el}$. The area of the element S_{el} is calculated from the coordinates of the element and its neighbors. From Fig. 1a it is seen that S_{el} is split up into triangles. One can easily calculate the area of the triangle, knowing the coordinates of its vertices, from the formula $S_{tr} = \frac{1}{2}[(x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1)]$. The calculation of the temperature field is made with the use of an explicit scheme at each time step. The excesses of temperatures at the additional nodes are determined by using the values of temperatures at two nodes of the elements and four additional nodes at the previous step, as shown in Fig. 1b. Here the following relation is used:

$$\Delta T = \frac{\sum_j q_j}{\rho_i c_{spi} \frac{1}{2} S_i + \rho_k c_{spk} \frac{1}{2} S_k} \Delta\tau ,$$

where q_j are the heat fluxes defined by formulas (4) and (5).

The excess of temperature at the main nodes of an element is calculated from the values of temperatures at the additional nodes that surround the given element, with the formula

$$\Delta T = \frac{\sum_j q_j}{\rho c_{sp} S_{el}/2} \Delta\tau ,$$

where q_j is the heat flux determined from formula (4).

We will consider the structure of a specific disperse system. Let it consist of sand, water, and air. For this system we will adopt a cubic array of spherical particles of sand that have a point of contact among themselves. The pores between particles are filled with water and air. For this system we can isolate a unit cell whose thermal conductivity is equal to the thermal conductivity of the entire system. A two-dimensional representation of this system is shown in Fig. 2, where 1 indicates a quartz particle, 2 stands for water seals, 3 for an air pore, and 4 indicates the zone of contact. A three-dimensional representation of this cell can be obtained as a result of rotation about the left vertical axis. In this way we can obtain a three-dimensional problem with an axial symmetry for a system consisting of sand, water, and air. It is also necessary to take the contact zone between the particles into account. Several elements in the left upper part of the unit cell cannot have the thermal conductivity of either quartz

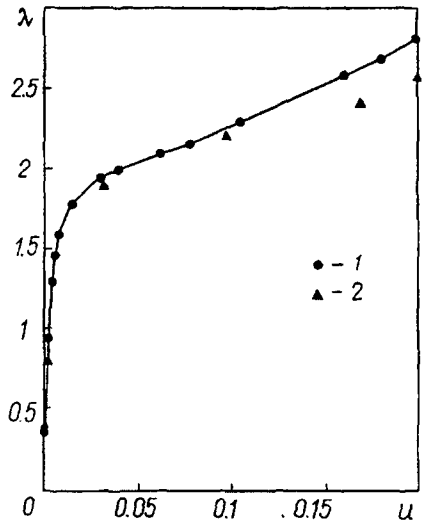

Fig. 3. Thermal conductivity coefficient of quartz sand vs moisture content: 1) numerical calculation; 2) experimental data.

or water, since the structural element has dimensions that exceed the volume occupied by either the quartz or water in the zone of contact. Therefore, from the left upper angle along the horizontal we must take several elements whose thermal conductivity must differ from that of quartz or water. Moreover, for each element there is its own angle $\alpha = \arcsin \frac{x_{el}}{R}$, where x_{el} is the horizontal coordinate of the center of the structural element, which is reckoned from the left vertical straight line. The number of these elements determines the linear dimension of the contact zone along the horizontal. The size of this zone should be such that the next element following it could be entirely in water and could determine its properties. The thermal conductivity of the contact zone is calculated from the formula $\lambda_c = \lambda_q \frac{\lambda_w(l + h)}{\lambda_w l + \lambda_q h}$, where $h = 4R \sin^2 \frac{\alpha}{2} + h_0$, $h_0 = 0.001R$.

Using the procedure proposed above, an algorithm was composed and a program was written in the language *C* to calculate the thermal conductivity of composite materials, with the following values taken for the components: $\lambda_q = 7$, $\lambda_w = 0.6$, $\lambda_a = 0.025$. The calculated dependence of the thermal conductivity of quartz sand on moisture content and the data obtained from the experiment, which are presented in Fig. 3, show their satisfactory agreement. Thus, the procedure developed allows one to calculate the thermal conductivity coefficient of inhomogeneous disperse systems with account for the specific features of their structure and the mutual arrangement of the components. As applied to the calculation of the thermal conductivity coefficient of sand systems, this procedure makes it possible to take account of the thermal conductivity coefficient of the particles of sand, moisture, and air pores, and also of the special features of the thermal contact between particles.

Using the method developed, calculations of the thermal conductivity of organomineral systems, which correspond to the cubic array of mineral particles, were carried out. It was assumed that a moist organogen component was located in the contact zones of mineral particles. The system considered consisted of quartz, moist peat, and a vapor-air phase. Due to the fact that the thermal conductivity coefficients of organogen and water components have closely coinciding values (0.47 and 0.6 W/(m·K), respectively) [2, 3] and that moisture is located mainly within the peat aggregates, the peat–water system is considered as a single component whose thermal conductivity can be calculated by the method of interpenetrating components [4]. Taking account of what has been said above, the structural model of an organomineral system is presented as a three-component system with interphase surfaces. The scheme of a unit cell of such a system is presented in Fig. 4, where 1 denotes a quartz particle, 2 moist peat, and 3 a vapor-air phase. This unit cell presupposes axial symmetry about the axis parallel to the heat flux. The thermal conductivity coefficients of the components and the vapor-air phase took the following values: $\lambda_q = 7$, $\lambda_{m.p} = 0.55$, $\lambda_{v.a} = 0.07$. The latter value was selected, taking account of heat exchange due to evaporation and condensation of vapor in the pores. In calculations the relationship between the mineral, organogen

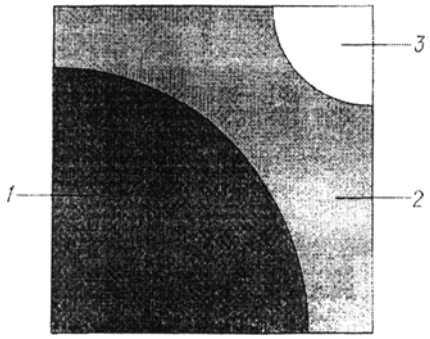

Fig. 4. Unit cell for a system consisting of quartz, moist peat, and air.

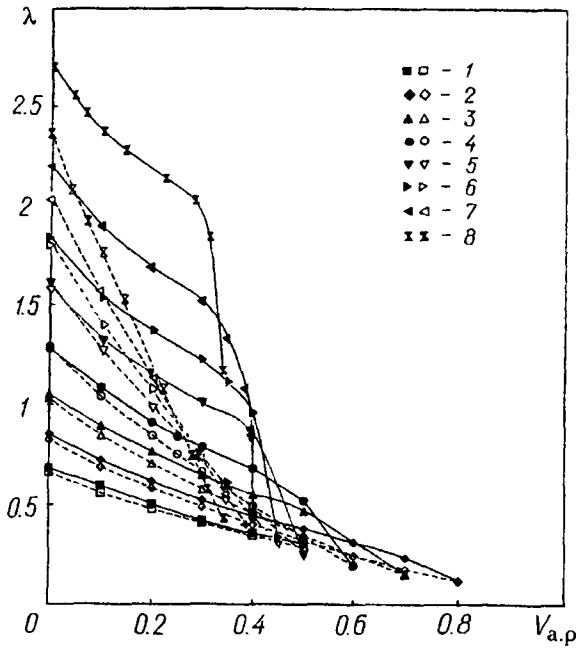

Fig. 5. Thermal conductivity coefficient of organomineral systems vs the volume fraction of air pores $V_{a.p}$ with a different volumetric portion of sand component V_s: 1) $V_s = 0.1$, 2) 0.2, 3) 0.3, 4) 0.4, 5) 0.5, 6) 0.55, 7) 0.6, 8) 0.66.

components, and pore space filled with a vapor-air phase was varied. Concurrently we made calculations of the thermal conductivity of the indicated systems by the analytical methods used to determine the thermal conductivity coefficients of inhomogeneous systems [4]. In these calculations, first we determined the thermal conductivity of a mixture of the organogen component with the vapor-air phase by the method of interpenetrating components and then the thermal conductivity of the entire system, where the mineral component was considered to be an isolated inclusion. Data on the thermal conductivity coefficients of organogen systems obtained by means of the method developed (solid lines) and similar data obtained by analytical methods (dashed lines) are presented in Fig. 5. Each curve corresponds to a certain relative volume of the mineral component and represents the thermal conductivity coefficient as a function of the relative volume of a vapor-air phase. It is assumed that the remaining part of the relative volume is filled with the moist organogen component.

Comparison of the data given indicates that in the absence of a free porous space, up to the volumetric fraction of the mineral component, equal to 0.55, good correspondence is observed between the values of the thermal conductivity coefficients found by the different methods. On increase in the volume fraction of the mineral component up to 0.6 and more, certain differences are observed in the calculated data obtained by different methods. It may attain 11% and is explained by the effect of the contact zone on the thermal conductivity coefficient at large values of the relative volumetric mineral component, corresponding to direct contact of mineral particles.

The analysis of the results shows that in the presence of a vapor-air phase for systems with a relative volume of mineral component V_s not exceeding 0.3, satisfactory agreement of the data compared is observed. But at larger values of V_s the observed difference between them increases with increase in the relative volume of the vapor-air phase $V_{v.a}$. An especially large discrepancy is observed for systems containing a mineral component in an amount corresponding to the values $V_s > 0.5$ and $V_{v.a} > 0.2$.

Thus, the analysis carried out shows that calculation of the thermal conductivity coefficients of inhomogeneous structurized systems must be made with account for their structural features.

In conclusion it should be noted that the method developed allows one to obtain an adequate description of the processes of heat conduction in the processes of deformation and transformation of structure in natural disperse systems. This method directly takes account of the displacements of structural elements relative to one another and also of the changes in the structure and inhomogeneities of a disperse system, which makes it possible to adequately calculate convective and conductive heat exchange in the processes of deformation and transformation of the structure of disperse systems. This approach makes it possible to obtain a similar description also of the processes of the diffusion of moisture and water-soluble compounds. This allows one, when solving problems of interrelated transfer of heat, moisture, and water-soluble compounds, accompanied by the deformation and transformation of structure, to construct appropriately a computational scheme with a variable nodal connectedness. The method given can be used also for finding coefficients of heat conduction, diffusion of moisture, and diffusion of water-soluble compounds of inhomogeneous structured systems.

NOTATION

q_{ik}, heat flux along the connection between the elements i and k, W; q_{iksi}, heat flux between additional nodes on the connections i, k and i, j, W; q_j, heat fluxes, W; T_i, temperature of the element i, K; T_k, temperature of the neighboring element k, K; T_{ik}, temperature at the additional node over the connection between the elements i and k, K; T_{ij}, temperature at the additional node over the connection between the elements i and j, K; ΔT, increase in temperature, K; l_{ik}, length of the connection between the elements i and k, m; L_{ik}, length of the face of contact between the elements i and k, m; l'_{ik}, length of the connection between the main and additional nodes, m; l'_{jk}, distance between additional nodes over the connections i, k and i, j, m; L_{jksi}, length of the line of the side contact, m; l, length of the connection between the main elements, m; r_i, r_k, radial coordinates of the nodes of the elements i and k, m; x_i, y_i, coordinates of the vertices of a triangle, m; R, radius of a quartz particle, m; α, angle reckoned from the vertical axis, rad; h, thickness of a water interlayer, m; h_0, thickness of a water interlayer at $\alpha = 0$, m; S_{el}, area of an element, m^2; S_{tr}, area of a triangle, m^2; S_m, area of the main contact, m^2; S_{si}, area of a side contact, m^2; S_i, one of the areas of a triangle into which the element i is split, m^2; S_k, one of the areas of a triangle into which the element k is split, m^2; λ_{el}, thermal conductivity coefficient of a structural element, W/(m·K); λ, thermal conductivity coefficient of a homogeneous continuous medium, W/(m·K); q_q, thermal conductivity coefficient of a quartz particle, W/(m·K); λ_w, thermal conductivity coefficient of water, W/(m·K); λ_c, thermal conductivity coefficient of the contact zone, W/(m·K); $\lambda_{m.p}$, thermal conductivity coefficient of moist peat, W/(m·K); λ_a, thermal conductivity coefficient of air, W/(m·K); $\lambda_{v.a}$, thermal conductivity coefficient of a vapor-air phase, W/(m·K); C_{el}, heat capacity of an element, J/K; c_{sp}, specific heat, J/(kg·K); c_{spi}, c_{spk}, specific heats of the elements i and k, J/(kg·K); ρ, density, kg/m^3; ρ_i, ρ_k, densities of the elements i and k, kg/m^3; φ, angle between the connection and the line of a side contact, rad; φ_{ik}, angle corresponding to the geometric parameters of the connection, rad; V_s, volume fraction of the sand component; $V_{a.p}$, volume fraction of the air pores; u, moisture content, kg/kg; N, number of vertices of an element; N_i, number of vertices of the element i; N_k, number of vertices of the element k; $\Delta\tau$, step in time, sec. Subscripts: si, side; el, element; m, main; q, quartz; w, water; c, contact; m.p, moist peat; v.a, vapor-air; sp, specific; s, sand; a.p, air pores; tr, triangle; a, air.

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