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ACCOUNT FOR LARGE DEFORMATIONS OF A MATERIAL CAUSED BY THE MOISTURE-CONTENT GRADIENT

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An uncoupled moisture-elasticity problem is solved in Lagrangian coordinates.

Introduction. Many bodies, such as building materials, foods, and soils and grounds have structures in which the dominant role is played by the coagulation bonds formed due to the linkage of solid-phase particles through the thin water interlayers. This leads to a high mobility of the skeleton particles relative to one another, even when the forces applied to the material are insignificant. Therefore, such systems, when loaded, are prone to large deformations and form changes. In particular, they may undergo structural transformations in the course of mass exchange with the environment. In so doing, the main causes of deformations of the material and its structural changes are the capillary and disjoining pressures of thin liquid layers. It is known that in such materials the volume is related to the moisture content by the relation $V = V_0(1 + \beta_v(W - W_0))$ [1] and, e.g., for metals an analogous temperature dependence takes place: $V = V_0(1 + \alpha(T - T_0))$ [2]. Consequently, an analogy between the temperature and moisture stresses exists. Thus, in thermoelasticity, the strained-stressed state of the material is definitively determined by the nonuniform temperature distribution in the body. Likewise, in the process of drying of a moist material, stresses resulting from the nonuniform moisture distribution appear in it.

The processes of heat and mass transfer followed by deformation and stresses in materials have been investigated fairly widely. In [3, 4], the stressed-strained state under intensive drying of a thin plate with various rheological zones was investigated analytically. In [5], a closed system of interrelated equations of heat-and-mass transfer and deformation of an isotropic porous body is given. In [6], the stressed-strained state of an elastoplastic body was investigated on the basis of the known one-dimensional distributions of the temperature, moisture content, and excess pressure in the thickness. In [7, 8], the given state was investigated under intensive drying of a high-concentration disperse system. The vapor front divides the material into a dry and a saturated part. For the dry part, the Hooke law is used, and the behavior of the saturated region is described by a viscoelastic model based on the micromechanics of the approach of particles with allowance for the surface forces and the viscous flow of the disperse phase. The nonisothermal drying of an anisotropic material from wood was considered in [9], where internal stresses caused by the moisture-content gradient were calculated using the concepts of elasticity theory. In [10], on the basis of the thermodynamics of irreversible processes, a general system of interrelated equations of heat-and-mass transfer and deformation for highly deformable disperse capillary colloid systems was written. The equations presented were solved numerically in Euler coordinates. A computational experiment that permitted describing the heat-and-mass transfer and the stressed-strained state of such systems was performed. In their monograph [11], Ugolev et al. presented the results of analytical and experimental studies of the stressed-strained state in wood and made calculations for timber, using the finite-element method. A mathematical model of interrelated heat and mass transfer and a viscoelastic rheological model for a composite foodstuff are given in [12]. The heat and moisture distributions, as well as the stressed-strained state of the material, were determined by the finite-element method. The results of the calculations were compared with the experimental data for three-layer foodstuffs. In [13], on the basis of the finite-element method, a numerical procedure of calculating the formation of cracks and their propagation in elastoplastic foodstuffs due to the stressed-strained state

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caused by the nonuniform moisture distribution in the cylindrical sample was developed. The moisture distribution in a material is found by solving the problem of interrelated heat and moisture transfer.

From the above-listed works, it follows that for correct description of the behavior of a material in the drying process it is necessary to study the mechanical motion of the material and, in a number of cases, its influence on the mass-transfer processes as well.

It should be noted that unlike, e.g., metals the materials under consideration feature considerable shrinkages and form changes. In so doing, there is a change in the relative position of particles, the number of contacts, the mean distances between them, and the size distribution function of pores (which also affects the heat-exchange characteristics of materials). Therefore, it is necessary to take into account the change in the form and size of the material in the drying process. This is essential both for more accurate calculations of the processes of heat-and-mass transfer and calculations of the stressed-strained state. In this connection, we turn our attention to the computational procedure in the presence of large shears of the material.

Mathematical Formulation of the Problem for Deformable Media and Methods of Its Solution. The above-mentioned literature sources consider various aspects of the processes of heat and mass transfer and the stresses and strains in the material associated with them. However, in these works little consideration is given to the calculation errors associated with the deformations. For calculations, the Euler approach is used, which leads to the use of Euler coordinates. Such an approach is only applicable for small deformations of the material, and at large shrinkages it is approximate. As is known, using such an approach, one has to separate the elementary region of the space and study the characteristics of the particles passing through it. For exact solution of the problems being investigated, one has to use the Lagrangian representation, which leads to the use of Lagrangian coordinates. In such an approach, the laws of change in the quantities characterizing a given individual particle of a solid medium are investigated. Therefore, it is necessary to introduce a concomitant coordinate system associated with a moving particle of the solid medium. If, at the initial instant of time, it is chosen to be rectangular, then at the subsequent instant it will be curved, i.e., the concomitant coordinate system forms a mobile deformable curvilinear system. Note that, as in the hydrodynamics, the Euler coordinates are "natural"; for the problems considered by us, the Lagrangian coordinates are "natural" and, therefore, we will use them hereinafter.

Let us take a material with an elementary rheological behavior obeying Hooke's law. Suppose that the mass transfer occurs under isothermal conditions. We also restrict ourselves to the simplest uncoupled moisture-stressed problem in which the influence of the mechanical motion on the mass transfer is neglected. Moreover, we take into account that the process of mechanical relaxation is much faster than the mass-transfer relaxation, and, therefore, at each instant of time during drying the body can be thought to be in mechanical equilibrium. This permits us consider the static problem of moisture elasticity. For simplicity, we assume that the problem is two-dimensional, and for certainty we take the stressed state to be plane. Finally, we assume that the physical properties of the material are independent of its moisture.

We give the system of equations describing the problem stated in Lagrangian coordinates:

$$\frac{\partial W}{\partial t} = a_{\mathrm{w}} \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^k} \left(g^{kl} \sqrt{g} \frac{\partial W}{\partial x^k} \right), \tag{1}$$

$$\frac{1}{2\,(1+\nu)} g^{jk} (u_{i;k})_{;j} + \frac{1}{2\,(1-\nu)} \frac{\partial}{\partial x^i} (u^k_{;k}) - \frac{1}{1-\nu} \beta \frac{\partial W}{\partial x^i} = 0 \,, \tag{2}$$

$$u^k_{;k} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^k} (g^{kl} \sqrt{g}\, u_l) \,, \tag{3}$$

$$(u_{i;k})_{;j} = \frac{\partial^2 u_i}{\partial x^j \partial x^k} - \frac{\partial u_l}{\partial x^j} \Gamma^l_{ik} - u_l \frac{\partial \Gamma^l_{ik}}{\partial x^j} - \frac{\partial u_m}{\partial x^k} \Gamma^m_{ij} + u_l \Gamma^l_{mk} \Gamma^m_{ij} - \frac{\partial u_i}{\partial x^m} \Gamma^m_{kj} + u_l \Gamma^l_{im} \Gamma^m_{kj} \,, \tag{4}$$

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x^i} - u_k\Gamma_{ji}^k + \frac{\partial u_i}{\partial x^j} - u_l\Gamma_{ij}^l\right), \tag{5}$$

$$g_{ij} = 2\varepsilon_{ij} + g_{0ij}\,, \tag{6}$$

$$g^{ij}g_{jk} = \delta_k^i\,, \tag{7}$$

$$g = \det g_{ik}\,, \tag{8}$$

$$\Gamma_{ik}^l = \frac{1}{2}\,g^{ml}\left(\frac{\partial g_{im}}{\partial x^k} + \frac{\partial g_{km}}{\partial x^i} - \frac{\partial g_{ik}}{\partial x^m}\right). \tag{9}$$

Here the semicolon denotes the covariant derivative.

We choose a rectangular body, and at the initial instant of time we relate to the material the Cartesian orthogonal system of coordinates. We assume the following boundary conditions: at the upper boundary the mass exchange with the environment occurs by the Newton "law"

$$a_{\mathrm{w}}n^i\,\frac{1}{\sqrt{g_{ii}}}\,\frac{\partial W}{\partial x^i} = \alpha_{\mathrm{w}}\,(W_{\mathrm{eq}} - W)\,; \tag{10}$$

the other three boundaries are impenetrable. The absence of external mass and surface forces is also assumed, and, therefore, the material deforms only as a result of the nonuniform distribution of the moisture content.

Consider the technique for calculating the sought quantities realizing the Lagrangian representation. We assume that at the initial instant of time the body is undeformed, the tensor g_{0ij} is unit, and the Christoffel symbols are equal to zero. Proceeding from this information and the boundary conditions, calculate the field of moisture contents at the new time step by formula (1). On the basis of Eqs. (2)–(4), find the deformation of the material, having calculated the displacements u_i and the new locations of the nodes. Then, using formula (5), determine the deformation tensor. Finally, using (6)–(9), find the metric tensor and the Christoffel symbols for the new state. We take the thus-determined state as the initial state for the next cycle of calculations. Note that at each time step the deformations should be small due to the small change in the moisture content at each point in the time interval Δt.

In the subsequent cycles, the metric tensor g_{ij} is no longer unit but reflects the deformed state of the coordinate system connected with the body. For approximation of differential equations, one usually employs the finite-difference method, and the computational mesh thereby coincides with the coordinate grid (i.e., with the coordinate lines). A shift of the material particles relative to one another will cause its deformation, which will lead to a decrease in the calculation accuracy, and under a strong deformation the calculation will be completely impossible. One way to improve the situation is to transform the calculation mesh into an orthogonal one at each time step. However, additional operations will lead to a decrease in the accuracy and a faster accumulation of errors. Moreover, in this case the mesh nodes will no longer coincide with the body boundaries, as a result of which an additional decrease in the calculation accuracy will occur.

The integral methods, in particular, the finite-element method, do not suffer from such disadvantages. The finite-element method permits one to use elements of various forms and sizes and to model processes in bodies of arbitrary form. The realization of the finite-element method is based on the variational principle. As applied to the given problem, it is necessary to minimize the strain energy density. Let us make use of the rectangular Cartesian system of coordinates. We formulate the variational principle as follows [14]:

$$\delta\int_V \frac{1}{2}\left(\sigma_{ij}\varepsilon_{ij} - \sigma_{ij}\varepsilon_{0ij}\right)dV = 0\,, \tag{11}$$

here ε_{0ij} is the initial deformation caused by the shrinkage of the material.

A similar result is obtained by using the expression for the free energy density F, which at a constant temperature will be of the form

$$F = \mu\varepsilon_{ij}\varepsilon_{ij} + (\lambda/2)\,\varepsilon_{kk}^2 - (3\lambda + 2\mu)\,\beta\varepsilon_{kk}\,(W - W_0) + F_c\,, \tag{12}$$

where F_c is a constant independent of ε_{ij}. Then the derivative with respect to ε_{ij} gives the stress tensor

$$\frac{\partial F}{\partial \varepsilon_{ij}} = \sigma_{ij} = 2\mu\varepsilon_{ij} + [\lambda\varepsilon_{kk} - (3\lambda + 2\mu)\,\beta\,(W - W_0)]\,\delta_{ij}\,, \tag{13}$$

and the variation

$$\delta\int_V \left(\mu\varepsilon_{ij}\varepsilon_{ij} + (\lambda/2)\,\varepsilon_{kk}^2 - (3\lambda + 2\mu)\,\beta\varepsilon_{kk}\,(W - W_0) + F_c\right)dV = 0 \tag{14}$$

leads to the equation of motion of the medium analogous to that obtained from formula (11).

For the mass-transfer equation, the variational formulation is of the usual form [15]:

$$\delta\left\{\int_V\left[a_w\left(\frac{\partial W}{\partial x}\right)^2 + a_w\left(\frac{\partial W}{\partial y}\right)^2 - 2W\frac{\partial W}{\partial t}\right]dV + \int_S \alpha_w\,(W - W_{eq})^2\,dS\right\} = 0\,. \tag{15}$$

Let us construct the calculation procedure in Lagrangian coordinates. Refine the expression for ε_{0ij} in Eq. (11). To this end, we represent the initial deformation ε_{0ij} formed at a point in the time interval Δt at the last step k as the difference of two quantities:

$$\varepsilon_{0ij} = \varepsilon_{0ij}^{(1)} - \varepsilon_{0ij}^{(2)}\,. \tag{16}$$

Here $\varepsilon_{0ij}^{(1)} = \beta_l(W - W_0)\delta_{ij}$ is the deformation caused by the difference of the moisture contents; W_0 is the moisture content at the initial instant of time t_0 (initial moisture content of the material); W is the current moisture content; and $\varepsilon_{0ij}^{(2)}$ is the deformation caused by the shift of the nodal points from the initial instant of time t_0 to t_{k-1}. Consequently, we can write $\varepsilon_{0ij}^{(2)} = f(u_0)$, where $u_0 = \sum_{i=1}^{k-1} u_i$. Then, choosing the time step Δt small enough so that the shifts determined by the moisture gradient can be considered to be small, we find, by formula (15), the W distribution and then, by formula (11), the shifts of the nodal points corresponding to equilibrium for the new distribution of moisture. On the basis of the shifts obtained, we calculate the new values of the coordinates of the element nodes, which yields a new equilibrium deformed state of the material. Determine the u_0 values for each node. Taking the obtained state of the material as the initial one, we complete the cycle.

To calculate the shifts, it is necessary to know the expression for the strain tensor due to displacements, which in the Cartesian rectangular coordinate system will have the form

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} + \frac{\partial u_l}{\partial x_i}\frac{\partial u_l}{\partial x_j}\right) \tag{17}$$

or

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right). \tag{18}$$

Formula (17) is used to calculate large deformations and (18) — small ones. Because each time the equilibrium problem with changing moisture content distribution in the body at a small time step is solved, at each point the change in the moisture content is small and, consequently, the deformations of the material at them will also be small. Therefore, Eq. (18) can be used with a good accuracy. Note that (2)–(5) are also written taking into account the smallness of deformations.

The procedure of numerical calculation by the finite-element method used by us is based on the procedure proposed in [14, 15]. Therefore, we shall only describe the features of the method being developed.

Let us break up the body under investigation into elements and take them as two-dimensional simplex-elements. This permits us to use, in solving the problem, the linear interpolation polynomials. Then the components of the vector of displacements through their nodal values $\{U\}$ will be written as

$$\{u\} = [N]\,\{U\} . \tag{19}$$

The deformation vector $\{\varepsilon\}$ is related to the nodal displacements $\{U\}$ by the expression

$$\{\varepsilon\} = [B]\,\{U\} . \tag{20}$$

Substituting expression (19), (20) into (11) and using Hooke's law, we differentiate with respect to $\{U\}$ and then integrate with respect to V and S to obtain finally a system of algebraic equations of the form

$$[K]\,\{U\} = \{f\} - [K]\,\{U_0\} . \tag{21}$$

In expression (21), the second term on the right takes into account the features of the solution of the problem under consideration by the Lagrangian method. Note that the stiffness matrix $[K]$ and the load column vector $\{f\}$ are calculated by means of the matrix $[B^e]$ of the element and the element area S^e by the formulas

$$[K] = \sum_{e=1}^{N} [K^e] ,$$

$$\{f\} = \sum_{e=1}^{N} \{f^e\} ,$$

$$[K^e] = [B^e]^{\grave{o}}\,[D^e]\,[B^e]\,S^e h ,$$

$$\{f^e\} = [B^e]^{\grave{o}}\,[D^e]\,\left\{\varepsilon_0^{(1)e}\right\} S^e h .$$

Note that both $[B^e]$ and S^e depend on the coordinates of the element nodes. Therefore, neither $[K]$ nor $\{f\}$ remain constant and are calculated at each time step. Recalculation of the stiffness matrix and the load column vector is also performed in determining the moisture field.

It should be emphasized that, proceeding from the results of [14], the proposed method can also be generalized to nonlinear physical problems.

Results and Discussion. Figure 1 presents the results of calculation of the deformation of a material (using the example of wood) in the drying process by the method described above. The bodies considered in the problems have a vertical symmetry axis passing through their center. For the solution of the mechanical part of the problem to be unique (the absence of motion of the body as a whole is necessary), the position of the material on the symmetry axis, when $u_i(0, y) = 0$, is fixed. Figure 1 shows the deformed states of the material at different instants of time. In the initial state, the moisture content of the material $W_0 = 1$ kg/kg, and for the environment the equilibrium value of the moisture content is given: $W_{\mathrm{eq}} = 0$ kg/kg. According to [1, 9, 11, 16], the characteristic moisture conductivity coefficient for wood is $a_{\mathrm{w}} = 3{\cdot}10^{-9}$ m^2/sec, the mass-transfer coefficient $\alpha_{\mathrm{w}} = 3{\cdot}10^{-6}$ m/sec, the elastic modulus $E = 3{\cdot}10^7$ Pa, and the Poisson coefficient $\nu = 0.5$. The linear shrinkage factor of the material $\beta = 0.5$. Note that for wood

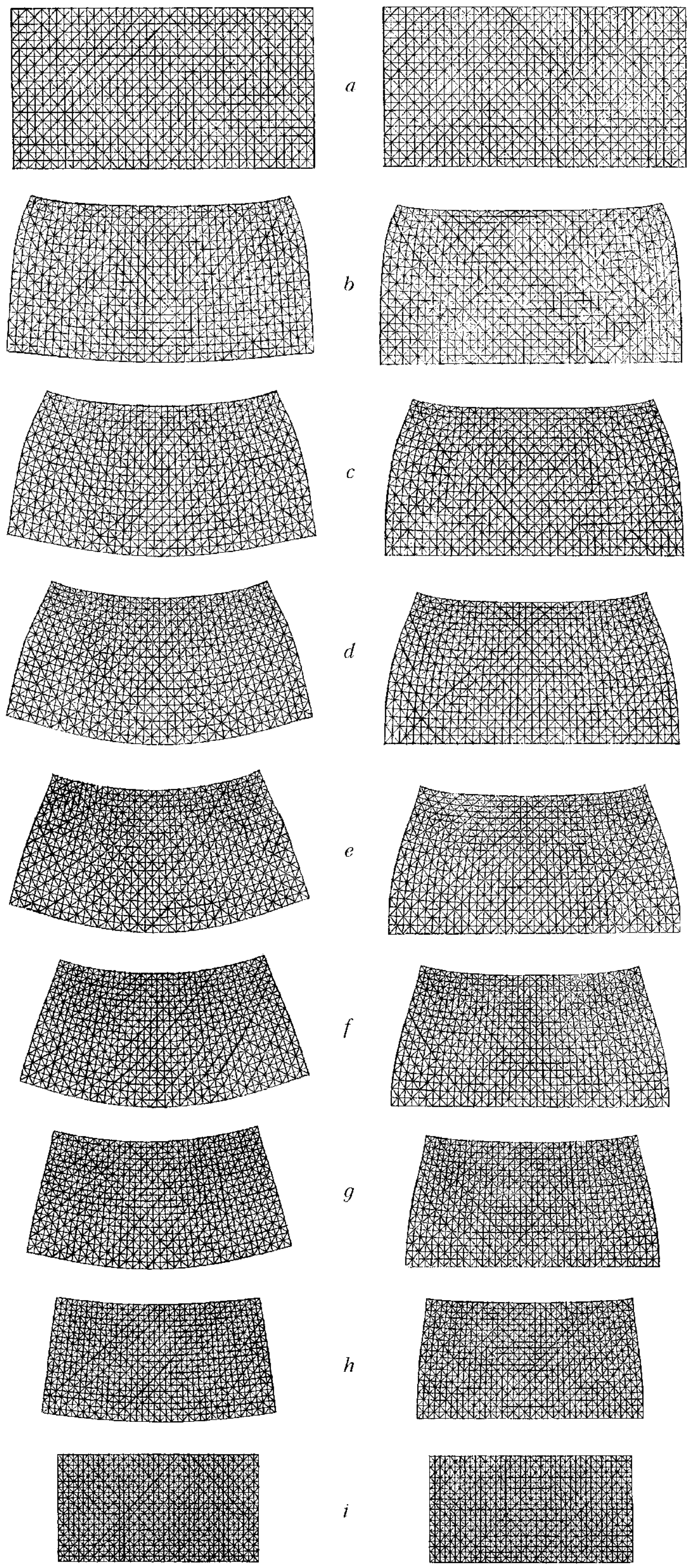

Fig. 1. Deformation of a material with a free lower boundary (on the left) and with a limited possibility of lower boundary displacement (on the right) in the drying process at different instants of time: a) t = 0; b) 1; c) 4; d) 8; e) 14; f) 25; g) 45; h) 80; i) 230 h.

(whose characteristic parameters were used in the calculations) this factor was set much higher for better visual demonstration of the deformation process.

The calculation shows that in a body able to deform freely stresses having lower absolute values than in a sample in which the lower boundary cannot move in the vertical direction develop. This can be explained by the fact that free deformation partially removes the unassumed shrinkage caused by the moisture gradient. Consequently, the ability to change form in response to the arising stresses leads to their partial removal. From Fig. 1, it is also seen that an initially rectangular body at the end of drying, when the moisture content in the sample equalizes and assumes a finite value, regains its initial form. Such a result is due to the fact that the calculations have been performed for a material whose behavior under deformation obeys Hooke's law. As is seen from [17, 18] however, the very presence of cracking leads to a deviation of the final state of the sample from the rectangular shape. It is known that real bodies exhibit plastic properties, which also causes a deviation of the final state of the material from the rectangular shape and causes the appearance of residual stresses. Therefore, an elastic model of the material is a rather rough approximation.

Analysis of the calculated data reveals two mutually opposite trends. On the one hand, the ability of the material to deform freely in the drying process permits drying without large stresses in it and, consequently, without cracking, which provides the possibility of obtaining a material with a strong structure. As mentioned above, however, some materials, in particular, wood, also exhibit plastic properties. Therefore, it is obvious that at the end of drying they will not take the initial shape, which will lead to their warping and deformation.

On the other hand, depriving the body of some degrees of freedom, i.e., not letting it deform in the drying process, we prevent warping of the material. In so doing, however, large stresses leading to cracking and thus to an impairment of its strength appear in it.

Conclusions. The consistency of the results obtained with the known physical notions about the behavior of materials in the drying process and its features depending on concrete conditions permits stating that, on the basis of the finite-element method, a workable method for solving problems in Lagrangian coordinates taking into account large deformations of the material has been proposed. The use of this approach permits one to avoid additional assumptions simplifying the problem [1, 3–13, 16], which decrease the adequacy of the mathematical model to the real physical process or lead to approximate and bounded solutions.

NOTATION

a_w, moisture-conductivity (diffusion) coefficient, m^2/sec; $[B]$, gradient matrix; $[D]$, matrix of material characteristics; E, elastic modulus, Pa; F, free energy density, J/m^3; $\{f\}$, global load column vector; g, metric tensor determinant; g^{ij} and g_{ij}, contravariant and covariant metric tensor components; h, material thickness, m; $[K]$, global stiffness matrix; N, number of elements; $[N]$, shape function matrix; S, area, m^2; h^i, cosines of angles between the unit vector of the normal to the surface and the coordinate lines; T, temperature, K; t, time, sec; Δt, time step, sec; $\{U\}$, nodal displacement vector; u^i and u_i, contravariant and covariant components of the displacement vector, m; $\{u\}$, displacement vector; V, volume, m^3; W, moisture content, kg/kg; W_{eq}, equilibrium moisture content, kg/kg; x^i, contravariant components of the radius vector, m; x, y, coordinates; α, coefficient of volumetric thermal expansion, 1/K; α_w, mass-transfer coefficient, m/sec; ν, Poisson coefficient; β, linear shrinkage factor; β_v, volume shrinkage factor; Γ^l_{ik}, Christoffel symbols; δ^i_j, unit tensor (Kronecker symbol); ε_{ij}, covariant components of the deformation tensor; $\{\varepsilon\}$, deformation vector; λ, μ, Lamé coefficients, Pa; σ_{ij}, covariant components of the stress tensor, Pa. Subscripts: 0, initial; v, volume; i, j, l, k, m, tensor components; e, element number; tr, transposed; eq, equilibrium; w, moisture; c, constant.

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