USE OF THE FINITE-ELEMENT METHOD IN PROBLEMS OF HEAT AND MASS TRANSFER IN POROUS BODIES*

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Two-dimensional isoparametric finite elements are used to solve problems of heat and mass transfer in porous bodies. A comparison of the numerical calculations with the analytic solutions of one-dimensional problems shows a very good agreement.

Using thermodynamics of irreversible processes, Lykov [1] obtained the widely accepted mathematical model of heat and mass transfer in capillary-porous bodies. The analytic solution of the corresponding system of partial differential equations is connected with considerable mathematical difficulties. Therefore, we know only a few solutions, first and foremost for one-dimensional problems – problems with boundary conditions not depending on time and with constant coefficients [2, 3].

Finite-difference methods [1, 4, 5] are widely used in engineering problems. In this paper another possible approach to numerical analysis is proposed; it is based on the finite-element method. The discretization obtained by this has considerable advantages for multidimensional problems in regions with complicated geometry or in cases with nonconstant physical properties of the materials.

The finite-element method was applied to a problem of nonstationary heat conduction for the first time in [6], while certain calculation schemes are given in [7].

Mutually connected electrical and hydrodynamic fluxes are studied in [8], and, subsequently, the finite-element method is applied to electroosmotic flows in soils in [9]. However, the boundary conditions of the problems in [8] and [9] essentially differ from those considered in the present work.

The connected problems of heat and mass exchange in the case of convective boundary conditions lead, in the case of finite elements, to systems of algebraic equations with asymmetric matrices. Since this is undesirable, in the investigation we propose such dimensionless parameters which lead to systems with symmetric matrices.

The distribution of temperature and moisture in each zone Ω^e of a moist body Ω can be described by the Lykov system [3]:

$$\rho c_q \frac{\partial t}{\partial \tau} = \lambda_q \left(\frac{\partial^2 t}{\partial x^2} + \frac{\partial^2 t}{\partial y^2} + \frac{\partial^2 t}{\partial z^2} \right) + \varepsilon r \rho c_m \frac{\partial u}{\partial \tau}, \tag{1}$$

$$\rho c_m \frac{\partial u}{\partial \tau} = \lambda_m \delta \left(\frac{\partial^2 t}{\partial x^2} + \frac{\partial^2 t}{\partial y^2} + \frac{\partial^2 t}{\partial z^2} \right) + \lambda_m \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right), \tag{2}$$

where t and u are potentials of heat and mass transfer, while the constants ρ, c_q, c_m, λ_q, λ_m, ε, and δ are taken as constant and equal to the mean values, respectively, in each zone Ω^e.

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The general boundary conditions for the system are as follows:

$$t = t_w \quad \text{on surface } \Gamma_1, \tag{3}$$

$$\lambda_q \nabla tn + j_q + \alpha_q (t - t_a) + (1-\varepsilon) r\alpha_m (u - u_a) = 0 \text{ on surface } \Gamma_2, \tag{4}$$

$$u = u_w \text{ on surface } \Gamma_3, \tag{5}$$

$$\lambda_m \nabla un + j_m + \lambda_m \delta \nabla tn + \alpha_m (u - u_a) = 0 \text{ on surface } \Gamma_4, \tag{6}$$

where t_w, u_w, t_a, u_a, j_q, j_m, α_q, and α_m are positive functions of time specified on the boundary.

Equations (1)-(6) can be written in dimensionless form as a system of mutually coupled equations of the parabolic type:

$$C_q \frac{\partial T}{\partial \theta} = L_q \left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} + \frac{\partial^2 T}{\partial Z^2} \right) + L_\varepsilon \left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} + \frac{\partial^2 U}{\partial Z^2} \right), \tag{7}$$

$$C_m \frac{\partial U}{\partial \theta} = L_\delta \left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} + \frac{\partial^2 T}{\partial Z^2} \right) + L_m \left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} + \frac{\partial^2 U}{\partial Z^2} \right), \tag{8}$$

which satisfy the boundary conditions

$$T = T_w \text{ on surface } \Gamma_1, \tag{9}$$

$$L_q \left(\frac{\partial T}{\partial X} \gamma_x + \frac{\partial T}{\partial Y} \gamma_y + \frac{\partial T}{\partial Z} \gamma_z \right) + J_q^* = 0 \text{ on surface } \Gamma_2, \tag{10}$$

$$U = U_w \text{ on surface } \Gamma_3, \tag{11}$$

$$L_m \left(\frac{\partial U}{\partial X} \gamma_x + \frac{\partial U}{\partial Y} \gamma_y + \frac{\partial U}{\partial Z} \gamma_z \right) + J_m^* = 0 \text{ on surface } \Gamma_4, \tag{12}$$

where J_q^* and J_m^* are given by the following expressions:

$$J_q^* = A_q (T - T_a) + A_\varepsilon (U - U_a) + J_q, \tag{13}$$

$$J_m^* = A_\delta (T - T_a) + A_m (U - U_a) + J_m. \tag{14}$$

In the expressions (7)-(14), $T = t/t_a$, $U = u/u_a$, $\theta = \tau/\tau_0$, $X = x/l$, $Y = y/l$, $Z = z/l$ are dimensionless quantities, C are generalized capacities, and L, A, and J* can be understood, respectively, as generalized coefficients of transfer and specific flows.

By means of an appropriate definition of the generalized coefficients we can always ensure fulfillment of the condition

$$L_\varepsilon = L_\delta, \tag{15}$$

thus making the system of Eqs. (7)-(8) symmetric.

With this aim, taking

$$L_\varepsilon = L_\delta = \varepsilon r \lambda_m \delta / \lambda_q, \tag{16}$$

from Eqs. (1)-(6) we have

$$C_q = \left(\frac{\rho c_q l^2}{\lambda_q \tau_0} \right) \left(\frac{t_a \delta}{u_a} \right), \quad C_m = \left(\frac{\rho c_m l_2}{\lambda_m \tau_0} \right) \left(\frac{\varepsilon r \lambda_m u_a}{\lambda_q t_a} \right),$$

$$L_q = \left(\frac{\lambda_q + \varepsilon r \lambda_m \delta}{\lambda_q} \right) \left(\frac{t_a \delta}{u_a} \right), \quad L_m = \frac{\varepsilon r \lambda_m u_a}{\lambda_q t_a},$$

$$J_q = \left(\frac{j_q l \delta}{u_a \lambda_q} \right) \left(\frac{\lambda_q + \varepsilon r \lambda_m \delta}{\lambda_q} \right), \quad J_m = \left[\left(j_m - \frac{\lambda_m \delta}{\lambda_q} j_q \right) \left(\frac{l}{\lambda_m u_a} \right) \right] \left(\frac{\varepsilon r \lambda_m u_a}{\lambda_q t_a} \right),$$

$$A_q = \left(\frac{\alpha_q l}{\lambda_q} \right) \left(\frac{\lambda_q + \varepsilon r \lambda_m \delta}{\lambda_q} \right) \left(\frac{t_a \delta}{u_a} \right), \quad A_m = \left(\frac{\alpha_m l}{\lambda_m} \right) \left[1 - \left(\frac{1-\varepsilon}{\varepsilon} \right) \left(\frac{\varepsilon r \lambda_m \delta}{\lambda_q} \right) \right] \left(\frac{\varepsilon r \lambda_m u_a}{\lambda_q t_a} \right),$$

$$A = -\left(\frac{\varepsilon r \lambda_m \delta}{\lambda_q} \right) \left(\frac{\alpha_q l}{\lambda_q} \right), \quad A = \left(\frac{1-\varepsilon}{\varepsilon} \right) \left(\frac{\alpha_m l}{\lambda_m} \right) \left(\frac{\lambda_q + \varepsilon r \lambda_m \delta}{\lambda_q} \right) \left(\frac{\varepsilon r \lambda_m \delta}{\lambda_q} \right). \tag{17}$$

The dimensionless quantities obtained by us insignificantly differ from those introduced by Lykov [3]. Such a form provides a certain amount of freedom in the description of the problem when the properties of the material depend on spatial variables.

The unknown functions T and U can be approximated for a certain θ in the entire domain of definition as follows:

$$T = \sum_{r=1}^{k} N_r(X, Y, Z)\, T_r(\theta) = NT \tag{18}$$

and

$$U = \sum_{r=1}^{k} N_r(X, Y, Z)\, U_r(\theta) = NU, \tag{19}$$

where N_r are functions that are smooth on elements and are piecewise smooth in the entire region, while T_r (or T) and U_r (or U) are parameters of the nodes [5].

We obtained by the Galerkin method described in [8] a system of equations relative to k values of T_r and k values of U_r. For the point r the integrals, on the region Ω, of the product of the weighting function N_r with the expressions obtained by substituting (18) and (19) into Eqs. (7) and (8) are zero:

$$\int_{\Omega} N_r \left[L_q \left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} + \frac{\partial^2 T}{\partial Z^2} \right) + L_\varepsilon \left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} + \frac{\partial^2 U}{\partial Z^2} \right) - C_q \frac{\partial T}{\partial \theta} \right] d\Omega = 0, \tag{20}$$

$$\int_{\Omega} N_r \left[L_\delta \left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2} + \frac{\partial^2 T}{\partial Z^2} \right) + L_m \left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2} + \frac{\partial^2 U}{\partial Z^2} \right) - C_m \frac{\partial U}{\partial \theta} \right] d\Omega = 0. \tag{21}$$

Equations (20) and (21) are transformed according to Green's expressions and in matrix form are

$$L\Phi + C\dot{\Phi} + J = 0, \tag{22}$$

where L and C are symmetric 2k × 2k matrices

$$L = \begin{vmatrix} L_q & L_\varepsilon \\ L_\delta & L_m \end{vmatrix}, \quad C = \begin{vmatrix} C_q & 0 \\ 0 & C_m \end{vmatrix}, \tag{23}$$

while Φ and J are vectors with 2k components,

$$\Phi = [T, U]^T, \quad J = [J_q, J_m]^T. \tag{24}$$

The dot in (22) denotes differentiation with respect to time.

We present the values of the matrix elements:

$$(L_{rs})_q = \Sigma \int_{\Omega^e} L_q \left(\frac{\partial N_r}{\partial X} \cdot \frac{\partial N_s}{\partial X} + \frac{\partial N_r}{\partial Y} \cdot \frac{\partial N_s}{\partial Y} + \frac{\partial N_r}{\partial Z} \cdot \frac{\partial N_s}{\partial Z} \right) d\Omega, \tag{25}$$

$$(C_{rs})_q = \Sigma \int_{\Omega^e} C_q N_r N_s d\Omega, \tag{26}$$

$$(J_r)_q = \Sigma \int_{\Gamma^e} \left(J_q^* + J_m^* \frac{L_\varepsilon}{L_m} \right) N_r d\Gamma, \tag{27}$$

$$(J_r)_m = \Sigma \int_{\Gamma^e} \left(J_m^* + J_q^* \frac{L_\delta}{L_q} \right) N_r d\Gamma. \tag{28}$$

The elements $(L_{rs})_\varepsilon$, $(L_{rs})_\delta$, and $(L_{rs})_m$ of the matrices L_ε, L_δ, and L_m are obtained from (25) by the respective substitution of the index q by ε, δ, and m, while the elements $(C_{rs})_m$ of the matrix C_m are obtained from (26) by substitution of the index q by m.

In the expressions Ω^e during summation we take into account the contribution of each element; Ω^e is the region of each element, while Γ^e refers only to elements having an outer boundary on which the conditions (9)-(12) are specified.

It should be noted that Eqs. (22) are not linear, since the generalized flows J_g^* and J_m^* do not depend on the values of the potentials at the boundary nodes. We note that this nonlinearity is slight, since it appears only in the vector J.

To solve the problem given by Eqs. (22), discrete with respect to space, we use a difference scheme that is three-layered with respect to time:

$$L^\theta(\Phi^{\theta+\Delta\theta} + \Phi^\theta + \Phi^{\theta-\Delta\theta})/3 + C^\theta(\Phi^{\theta+\Delta\theta} - \Phi^{\theta-\Delta\theta})/(2\Delta\theta) + J^\theta = 0. \quad (29)$$

After certain algebraic transformations we obtain the following expression for successive computation:

$$\Phi^{\theta+\Delta\theta} = -[L^\theta/3 + C^\theta/(2\Delta\theta)]^{-1}[L^\theta\Phi^\theta/3 + L^\theta\Phi^{\theta-\Delta\theta}/3 - C^\theta\Phi^{\theta-\Delta\theta}/(2\theta) + J^\theta]. \quad (30)$$

Since only the central values of the matrices L, C, and J take part in the expressions (29) and (30), at the point r we can avoid iterations for finding Φ in each layer, but in the calculation of the matrices L and C in the given case this fact yields no special advantages.

To solve the problem it is yet necessary to know the values of the vector in the first two layers. Since we assume that we have stationary conditions, necessary values can easily be specified.

The given method is fairly general and applicable for arbitrary discretization of multidimensional finite-element problems. However, in our investigations we use a two-dimensional model to establish the suitability of the method for solving concrete problems.

The program realizing the algorithm just described is written in FORTRAN IV similarly to the programs found in [7].

The isoparametric elements are used for regions of various shape and they enable us to "catch" a quadratic variation of the potentials along the edges of an element, and a parabolic form of a boundary. Each element is bound with eight degrees of freedom (nodes in one element) × 2 (values of the potentials at the node). The integrals (25)-(28) are computed approximately. The complete theory of these operations can be found in [7].

Thus, the matrices L and C for each element are calculated and are recorded onto a magnetic tape. The program for the solution, based on the elimination method of Gauss, is transformed on the magnetic tape for L^e and C^e; it forms the matrices L and C and solves the system of algebraic equations for the unknown values of the potentials.

When the matrices L and C do not depend on time, we can economize the computations in each layer of the inverse matrix:

$$[L/3 + C/(2\Delta\theta)]^{-1},$$

which, according to the expression (30), is multiplied by the variable vector

$$[L\Phi^\theta/3 + L\Phi^{\theta-\Delta\theta}/3 - C\Phi^{\theta-\Delta\theta}/(2\Delta\theta) + J^\theta].$$

The final results are the potentials of heat and mass transfer T and U at each layer for each time interval. If so desired, they can be recorded on the magnetic tape and later used for the analysis of the stresses caused by temperature and moisture gradients.

In the debugging of the program the results were compared with the analytic solutions from [3] for a single one-dimensional problem. In the first example a problem is solved, concerning the variation of the temperature and mass in a plate, when the surface X = 0 is isolated, while on the surface X = 1 convective boundary conditions are specified. The initial conditions are taken as constant ($T_i = 0$, $U_i = 0$), as are the potentials of transfer of the surrounding medium ($T_a = 1, U_a = 1$). The analytic solution was calculated by means of the first five eigenvalues for the case Ly = 0.3, $\varepsilon = 0.5$, Ko = 1.2, Pn = 0.5, $Bi_q = 1.0$, $Bi_m = 10.0$, and $\theta = 0.5, 1, 2, 4$. In the second example the same problem is considered, but with boundary conditions of the first kind on the boundary X = 1, obtained, if we assume $Bi_q = Bi_m = 1000$.

We solved by the finite-element method a two-dimensional problem that essentially differs from a one-dimensional problem, since the upper and lower boundaries of the rectangle under consideration were specified as nonconductive. Even for the relatively coarse division of the region into five parabolic elements and in two examples the deviation of the numerical solution from the analytical solution is less than 1%.

In this approach, there can be an arbitrary law governing the interaction of the molecules with the surface. We restrict the present analysis to the most common approximation, according to which some of the molecules are reflected in a specular manner, while the rest are reflected in a diffuse manner:

$$f_i^+(x=0,\ v_{ix},\ v_{iy},\ v_{iz}) = (1-q_i) f_i^-(x=0,\ -v_{ix},\ v_{iy},\ v_{iz}) + q_i f_{iM}. \quad (3)$$

Here q_i is the accommodation coefficient of component i, and f_{iM} is the distribution function of the reflected molecules, which is equal to the Maxwell distribution; i.e.,

$$f_{iM} = n_i \left(\frac{m_i}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m_i \vec{v}_i^2}{2kT}\right) \quad (i=1,\ 2).$$

Below we use superscript minus and plus signs to denote the distribution functions of the incident and reflected molecules, respectively.

Obviously, the wall affects the velocity distribution of the molecules over only a finite range, so that far from the wall the distribution function converts into the Chapman–Enskog volume distribution [3]. Also, using conditions (1) and (3), we can write the distribution function for component i, that is, f_i, in the following manner:

$$f_i = f_i^0 \left\{1 + \frac{m_i}{kT} v_{iy} u_{i0} + \frac{m_i}{kT} v_{iy} \left(\frac{du}{dx}\right)_\infty x - B_i \left(\frac{m_i}{2kT}\right)^{1/2} c_{ix}c_{iy} \left(\frac{du}{dx}\right)_\infty + \Phi_i(\vec{c}_i,\ x)\right\} \quad (i=1,\ 2), \quad (4)$$

$$f_i^0 = n_i \left(\frac{m_i}{2\pi kT}\right)^{3/2} \exp\left(-\frac{m_i \vec{v}_i^2}{2kT}\right);\quad \vec{c}_i = \left(\frac{m_i}{2kT}\right)^{1/2} \vec{v}_i,$$

where B_i are coefficients independent of $\vec{c}_i$. Equations for B_i are given in [3].

In (4), we have

$$\Phi_i = \begin{cases} \Phi_i^+(\vec{c}_i,\ x), & c_{ix} < 0 \\ \Phi_i^-(\vec{c}_i,\ x), & c_{ix} > 0 \end{cases} \quad (i=1,\ 2).$$

We seek the correction $\Phi_i^\pm(\vec{c}_i,\ x)$ as an expansion in Sonin polynomials in the corresponding velocity space:

$$\Phi_i^\pm(\vec{c}_i,\ x) = a_{0i}^\pm(x)\, c_{iy} + a_{1i}^\pm(x)\, c_{ix}c_{iy} \quad (i=1,\ 2).$$

The function $\Phi_i(\vec{c},\ x)$ is given by

$$\Phi_i(\vec{c}_i,\ x) = \frac{1}{2}(a_{0i}^+ + a_{0i}^-)\, c_{iy} + \frac{1}{2}(a_{0i}^+ - a_{0i}^-)\, c_{iy} \operatorname{sign} c_{ix} +$$

$$+ \frac{1}{2}(a_{1i}^+ + a_{1i}^-) c_{ix}c_{iy} + \frac{1}{2}(a_{1i}^+ - a_{1i}^-)\, c_{ix}c_{iy} \operatorname{sign} c_{ix} \quad (i=1,\ 2),$$

where

$$\operatorname{sign} c_{ix} = \begin{cases} 1, & c_{ix} > 0, \\ -1, & c_{ix} < 0. \end{cases}$$

For the average velocity of the molecules of component i we easily find

$$u_i = u_{i0} + \left(\frac{du}{dx}\right)_\infty x + \frac{1}{4}(a_{0i}^+ + a_{0i}^-) + \frac{a_{1i}^+ - a_{1i}^-}{4\sqrt{\pi}} \quad (i=1,\ 2). \quad (6)$$

Assuming

$$\frac{\rho(u_1 - u_2)}{\rho_1 u_1 + \rho_2 u_2} \ll 1, \quad (7)$$

we substitute (4)–(6) into system (2). Then multiplying the corresponding equations successively by

$$c_{iy}(1 \pm \operatorname{sign} c_{ix})\, e^{-\vec{c}_i^2} d\vec{c}_i;\quad c_{ix}c_{iy}(1 \pm \operatorname{sign} c_{ix})\, e^{-\vec{c}_i^2} d\vec{c}_i \quad (i=1,\ 2)$$

The universality of the finite-element method allows it to be used in practice, especially when we have to deal with complex regions and variable physical characteristics.

NOTATION

$Bi_q = \alpha_q l/\lambda_q$, $Bi_m = \alpha_m l/\lambda_m$	are the heat and mass exchange criteria of Biot;
c_q, c_m	are the specific heat and mass of the body;
$Ko = c_m r(u_i - u_a)/c_q(t_a - t_i)$	is the Kossovich criterion; specific fluxes of heat and mass per characteristic dimension of the body;
$Ly = (\lambda_m/\rho c_m)/(\lambda_q/\rho c_q)$	is the Lykov criterion;
n	is the outer normal of the surface of the body;
$Pn = (t_a - t_i)/(u_i - u_a)$	is the Postov criterion;
r	is the specific heat of phase conversion;
t	is the temperature;
u	is the potential of mass transfer;
x, y, z	are the spatial coordinates;
α_q, α_m	are the coefficients of heat and mass exchange;
γ_x, γ_y, γ_z	are the direction coefficients of the outer normal of the surface of the body;
Γ	is the surface of the body;
ε, δ	are the coefficient of thermal gradient, criterion of phase transition;
λ_q, λ_m	are the coefficients of thermal and mass conductivity;
Ω	is the region occupied by the body;
ρ	is the density of the moist body;
τ	is the time.

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