USE OF FINITE ELEMENTS IN CALCULATIONS OF THE FLOW OF NON-NEWTONIAN MEDIA*

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The finite-element method (FEM) is applied to the solution of rheodynamic problems. As an example, the flow of non-Newtonian fluids in a channel is examined.

Analytical and numerical methods are widely used for solving rheodynamic problems. Up to now, the grid method has been considered to be the most useful method for solving problems of this type.

In recent years, the finite-element method (FEM) has been increasingly applied to such problems [1-4]. With its help, it is possible to solve successfully problems of heat and mass transfer and rigid body mechanics and to calculate flows of various media. Compared to the grid method, the advantage of FEM lies in separation of the geometrically complicated regions into small elements and in the simple manner in which the boundary conditions are taken into account.

The FEM can be based on variational problems using Ritz's method or on differential equations using the method of weightedresiduals for a given physical problem [5-10]. In some cases, it is possible to use energy balance [11].

Since for many hydrodynamic problems the variational functional is not known, the method of weighted residuals (MWR) is used. Then, the two-dimensional region Ω, $x = (x_1, x_2) \in \Omega$, examined is separated into discrete parts (elements) Ω_e, $(e = 1, \ldots, m)$. Within each of them or on their edges, nodes are chosen $x^k \in \Omega_e$, at which the reference values $u^{k(e)} = u^{(e)}(x^k)$ of the unknown function $u^{(e)}(x)$, $x \in \Omega_e$, must be determined. The basic function $N^{k(e)}$ and the approximation

$$u^{(e)}(x) = N^{k(e)}(x)\, u^{k(e)} \tag{1}$$

are introduced.

The basis functions in (1) must satisfy the condition

$$N^{k(e)}(x^l) = \begin{cases} 1 & \text{for} \quad k = l, \\ 0 & \text{for} \quad k \neq l \end{cases} \tag{2}$$

for the x^i element to be compatible at the nodes.

Numerous types of elements, with the help of which a good approximation is attained to solutions of problems of various degrees of complexity, have already been realized in practice [12, 13]. The use of the FEM corresponding to the initial problem leads to a system of linear or nonlinear equations, whose matrix has a band structure and is symmetrical in certain cases.

We will limit ourselves to studying the isothermal flow of an incompressible non-Newtonian medium. The general formulation includes the following equations:

continuity

$$v_{i,i} = 0 \tag{3}$$

and motion

$$\rho \frac{dv_j}{dt} = \rho g_j + \sigma_{ij,i}. \tag{4}$$

System (3) and (4) must be supplemented by boundary and initial conditions, and, in addition, the stress tensor σ_{ij} must be specified. It characterizes the behavior of the medium and it is expressed by the rheological

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equation of state.

In a purely viscous medium, the stress is uniquely related to the strain velocity

$$\sigma_{ij}=F(D_{ij}). \tag{5}$$

The simplest Newtonian rheological equation of state has the form

$$\sigma_{ij}=-p\delta_{ij}+2\eta D_{ij}. \tag{6}$$

Here, η = const and

$$D_{ij}=\frac{1}{2}(v_{i,j}+v_{j,i}). \tag{7}$$

Substituting (7) into (4) taking into account (3) leads to the Navier–Stokes equation

$$\rho(v_{j,i}+v_i v_{j,i})=\rho g_j-p_{,j}+\eta v_{j,ii}. \tag{8}$$

Relation (6) cannot be generalized to such media as solutions, suspensions, melts, etc.

In order to describe the characteristics of flowing media of this type, nonlinear rheological equations of state are used. In choosing them, the particular properties (viscosity, elasticity, plasticity) exhibited by the medium and how well they are described by the model should be noted. In calculations, equations of state for purely viscous media, taking into account structural viscosity, dilatancy, thixotropy, and rheopexy, are most often used. They reflect the dependence of the viscosity on the strain velocity as well as on time.

Such equations, often empirical, are useful for describing simple shear flows and are based on the II invariant of the strain velocity tensor for two-dimensional and three-dimensional flows. For example, the following are used:

Ostwald–de Ville power law

$$\eta(\mathrm{II})=k_0(4\mathrm{II})^{\frac{n-1}{2}} \tag{9}$$

and the Prandtl–Eyring law

$$\eta(\mathrm{II})=A\frac{\arcsin h(\sqrt{4\mathrm{II}}/B)}{\sqrt{4\mathrm{II}}/B)}, \tag{10}$$

where $\mathrm{II}=2D_{ij}D_{ij}$.

If it is necessary to take into account elastic or viscoelastic properties, then it is necessary to use the equation of state which is derived either from fundamental Hooke and Newton (e.g., Maxwell's model) models or directly from the mechanics of continuous media with the help of physical and functional analytic analysis (e.g., Colemann–Noll).

In what follows, the characteristics of flows are calculated with the help of the FEM only for purely viscous media. The application of the FEM to non-Newtonian or viscoelastic media is examined in [1, 3, 12-16].

In order to analyze the two-dimensional problem, the equations of motion (8) and continuity (3) and the dependent variables, velocity v_i (i = 1, 2) and pressure p, are used. The use of v_i and p instead of the stream function and vorticity or only the stream function has certain advantages: the boundary conditions are easily formulated, the pressures immediately determined, and weaker conditions are imposed on the basis functions.

The variables chosen are approximated according to Eq. (1):

$$v_i=N^k v_i^k,\ p=N^k p^k, \tag{11}$$

and, in addition, it is not necessary for the velocity and pressure basis functions to coincide. They can be chosen so that they correspond to the required quality of the approximation.

In previously published papers, it has been shown that the best results are obtained with a quadratic approximation of the velocity and linear approximation of the pressure. For purposes of simplification, the same basis functions are used for both unknowns, since higher order derivatives in the equations for both unknowns with partial integration have the same order.

Using one of the methods of weighted residuals, in particular, Galerkin's method with N^k as linearly independent weighting functions, and (11) it is possible to obtain three equations for v_i and p at each node x^k in the region of flow.

Thus, the x_j component of Eq. (8) at the K-th node after integration over the given element Ω^e has the form

$$\sum_{e=1}^{\overline{M}} \left\{ \int_{\Omega^e} \rho [N^K N^L] d\Omega^e v^L_{j,t} + \int_{\Omega^e} [N^K [\rho (v^L_i v^L_j N^L N^L_{,i} - g_j) + N^L_{,j} p^L] + \eta N^L_{,i} N^K_{,i} v^L_j] d\Omega^e - \int_{\omega^e} \eta N^K N^L_{,i} v^L_j n_i d\omega^e \right\} = 0, \quad (12)$$

and, in addition, ω^e is the boundary of the region Ω^e and is made up of all elements to which the K-th node is related.

The integral over the surface is the flow $v^{(e)}_{j,n}$ with the weighting function N^k and is calculated only when the element is a part of the boundary ω of the region Ω and the normal derivative of the velocity is specified on it. However, the integral need not be taken into account [19].

Among the possible boundaries of the region Ω, it is necessary to distinguish clearly between impermeable ω_1 and permeable ω_2 boundaries. The boundary conditions can be as follows: the values of the velocity, surface forces, and normal derivative of the velocity are specified. The choice of particular boundary conditions depends on the geometric, hydraulic, or physical aspects of the problem.

The following relation is satisfied by the equation of continuity (3):

$$\sum_{e=1}^{M} \int_{\Omega^e} N^K v_{i,i} d\Omega^e - \sum_{e=1}^{M} \int_{\Omega^e} N^K N^L_{,i} v^L_i d\Omega^e = 0. \quad (13)$$

For highly viscous non-Newtonian media, the assumption that viscous forces greatly exceed inertial forces and volume forces is valid. For this reason, in what follows, we will drop both the convective terms and the term containing the volume force.

From (12), for stationary flow, follows

$$\sum_{e=1}^{M} \int_{\Omega^e} (N^K N^L_{,j} p^L + \eta N^K_{,i} N^L_{,i} v^L_j) d\Omega^e - \int_{\omega^e} \eta N^K N^L_{,i} v^L_j n_i d\omega^e = 0. \quad (14)$$

After integrating, for each node in the two-dimensional case, we obtain three algebraic equations. Examining all nodes in the region Ω, we arrive at the system

$$\|A\| \{\delta\} = \{F\}, \quad (15)$$

and, in addition, $\{\delta\}$ is the variable node vector, defined by the relation

$$\{\delta^k\} = \begin{Bmatrix} v^k_1 \\ v^k_2 \\ p^k \end{Bmatrix}. \quad (16)$$

The matrix $\|A\|$ is not symmetrical and has a band structure. The element a^{KL}, the minor formed from the matrix, has the form

$$a^{KL} = \int_{\Omega^e} A^{KL} dx_1 dx_2, \quad (17)$$

where

$$A^{KL} = \begin{Vmatrix} \eta (N^K_{,1} N^L_{,1} + N^K_{,2} N^L_{,2}) & 0 & N^K N^L_{,1} \\ N^K N^L_{,1} & N^K N^L_{,2} & 0 \\ 0 & \eta (N^K_{,1} N^L_{,1} + N^K_{,2} N^L_{,2}) & N^K N^L_{,2} \end{Vmatrix}. \quad (18)$$

The vector on the right side of Eq. (15) has the form

$$\{F^K\} = \int_{\omega^e} \eta N^K \begin{Bmatrix} v_{1,n} \\ 0 \\ v_{2,n} \end{Bmatrix} d\omega^e. \tag{19}$$

The region of flow Ω is separated into triangular elements with nodes at the vertices. A linear polynomial, whose coefficients are expressed in terms of the coordinates of the vertices of the triangle, are used as the basis function [17] (Fig. 1):

$$N^\alpha = (a^\alpha + b^\alpha x_1 + c^\alpha x_2)/\overline{A}, \tag{20}$$

where

$$a^\alpha = x_1^\beta x_2^\gamma - x_1^\gamma x_2^\beta,\quad b^\alpha = x_2^\beta - x_2^\gamma,\quad c^\alpha = x_1^\gamma - x_1^\beta \tag{21}$$

and

$$\overline{A} = \det \begin{Vmatrix} 1 & x_1^\alpha & x_2^\alpha \\ 1 & x_1^\beta & x_2^\beta \\ 1 & x_1^\gamma & x_2^\gamma \end{Vmatrix}. \tag{22}$$

The other coefficients are obtained by cyclic permutation of the indices. The use of triangular coordinates permits carrying out the integration over the surface of the element easily [17].

The predetermined value at the nodes can be taken into account by changing the vector $\{F\}$ and the matrix $\|A\|$. For example, let the velocity v_1 at the edge node n equal ν. Then, for the vector on the right side, the following expression is valid:

$$\overline{F}_i = F_i - a_{in}\nu \quad (i = 1,\ \ldots,\ n-1,\ n+1,\ \ldots,\ M),\ \overline{F}_n = \nu. \tag{23}$$

Here M is the number of equations.

The elements of the corresponding rows and columns of the matrix are equated to zero, while the diagonal element is equated to unity [18]. The linear system of equations obtained is solved by the Gaussian elimination method.

For Newtonian media, the viscosity η is the same at all nodal points. In non-Newtonian media, the viscosity depends on the shear strain velocity tensor, i.e., it is characterized by the second invariant. For this reason, the matrix $\|A\|$ of the system is also a function of the second invariant II

$$\|A(\eta(\mathrm{II}))\|\{\delta\} = \{F\}. \tag{24}$$

In this case, the system of equations must be solved by iteration.

Starting from the approximate value II_0 for II, the Newtonian approximation can be written as follows:

$$\{\delta\}_1 = \|A(\eta(\mathrm{II}_0))\|^{-1}\{F\}. \tag{25}$$

From here, for each node, it is possible to calculate II_1 and the function $\eta(\mathrm{II}_1)$ with the help of the viscosity function given above, e.g., from expressions (9) or (10). The next approximation then has the form

$$\{\delta\}_2 = \|A(\eta(\mathrm{II}_1))\|^{-1}\{F\} \tag{26}$$

or for arbitrary order

$$\{\delta\}_{m+1} = \|A(\eta(\mathrm{II}_m))\|^{-1}\{F\}. \tag{27}$$

Iteration terminates when the following condition is satisfied:

$$\max_{i=1\ldots KNO} \frac{\|v_i^{m+1} - v_i^m\|}{\|v_i^{m+1}\|} < \varepsilon. \tag{28}$$

The solution algorithm was first checked out with the help of a simple program [20], written in the FORTRAN language for the BÉSM-6 computer. The band structure of the matrix $\|A\|$ was not taken into account and external storage was not used, permitting processing only 50 nodes (150 unknowns). The slow flow of a non-Newtonian fluid in flat, as well as asymmetric converging, channels was investigated. The physical parameters were set arbitrarily and did not characterize any particular substance.

The numerical results for the flow of a non-Newtonian medium in a flat channel, as shown in Fig. 2, with equidistant positions of the elements, independent of their number, determine the exact analytical solution. Deviations appear for nonequidistant positioning of the elements, which can be explained by the different geometrical dimensions of the triangular element, as well as by the linear approximation of the velocity within it.

The non-Newtonian behavior of the medium is conveyed more or less well according to the choice of rheological parameters, as well as to the number and positioning of triangular elements. Thus, it is evident from Fig. 2 that in spite of the fact that the rheological parameters and pressure gradients with different numbers of elements are the same, deviations are observed (in the example being examined, of the order of ~8%). These deviations increase with an increase in pressure gradient as well as with the non-Newtonian nature of the medium. This behavior can be explained by the linear approximation of the velocity and by the discontinuity of the velocity gradient between elements observed in this case.

It may be stated that as the number of elements increases and the given pressure gradient decreases, as well as the volume flow rate, we can expect large nonlinearity in using the iteration method chosen. However, further analytic and numerical studies are necessary to evaluate the relations completely.

Figure 2 illustrates the choice of the number of iteration steps in order to attain an accuracy ε of the order of 10^{-4}, as well as the necessary computational time for a single iteration step.

The results, obtained for the flow of non-Newtonian media in an asymmetric converging channel, show that the use of a simple program permits obtaining the correct qualitative predictions for the change in flow rate with given pressure gradient. It is as yet impossible to compare the numerical results obtained with a closed-form analytic solution.

It is evident from Fig. 3 that in spite of an identical fixed pressure gradient and equality of the channel outlet and inlet height ratios h/H, appreciably different flow rates are attained due to the different form of the converging channel. In the examples presented, in going over from the geometry in Fig. 3a to that of Fig. 3c, the flow rate increases by 30% and by 20% with a transition from 3b to 3c.

The pressure distribution at the walls of the converging channel agrees qualitatively with the values computed. Therefore, geometries with pressure decreasing monotonically with length (Fig. 3c) are preferable from the point of view of the best characteristics of the flow rate (head). The nonlinearity in the pressure change at the channel inlet with height h is related to the development of flow up to the establishment of completely stabilized velocity fields.

In order to estimate the influence of the positioning of the elements on the numerical results, the geometry in Fig. 3b was separated into elements, which, in contrast to Fig. 3a, were positioned similarly to the outer geometry of the channel. Then, for Newtonian fluids, a deviation in the flow rate up to 18% was obtained. The results turned out to be more accurate in locations where the region is subdivided more exactly, i.e., at the channel inlet (Fig. 3b) and at the channel outlet (Fig. 4).

For a non-Newtonian flow, the magnitude of the deviation was up to 8%. Eight iterations were required to attain the limiting fixed accuracy ε for the geometry in Fig. 3b, while seven iterations were required for geometry in Fig. 4. Six seconds were used for each step of the iteration.

Thus, we can conclude that the program used permits obtaining only qualitative estimates of the flow characteristics. The limiting accuracy cannot be attained in this case due to the small number of nodes chosen. For this reason, it is not possible to separate accurately the region of the flow into elements and, therefore, increase the accuracy of the calculation.

In developing improved programs, the symmetry properties (integration over an element in the region in Eq. (12)) or the band nature of the matrix for the system or the band structure of the unsymmetrical matrix $\|A\|$ (the basic assumption for taking into account convective terms in Eq. (8) using iteration, Picard's iteration) is used or Hood's frontal method is used to solve the problem [21]. Depending on the type of program, the number of unknowns increases by a factor of 3-6 using a single magnetic core storage device in BÉSM-6 and by a factor of 10-15 in using all the external storage devices.

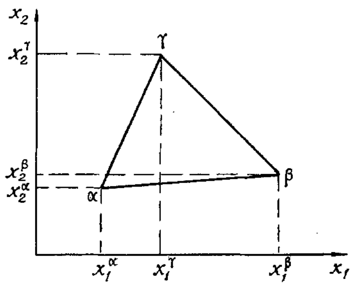

Fig. 1. Triangular element with three nodes.

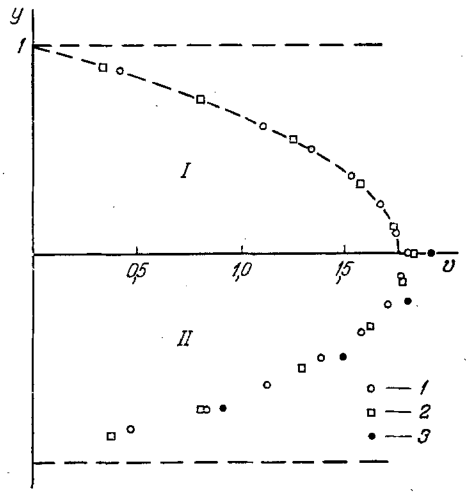

Fig. 2. Velocity distribution in a flat channel: I) Newtonian medium; II) non-Newtonian medium; 1) 34 nodes, 32 elements, 5 iterations, time for a single iteration is 3.8 sec; 2) 26, 24, 6, and 3, respectively; 3) 18, 16, 4, and 2, respectively ($\eta_0 = 5$ N • sec • cm^{-2}, $\eta_1 = 50$ N • sec • cm^{-2}, n = 0.5; $p_{,x} = 0.009$ N • cm^{-3}).

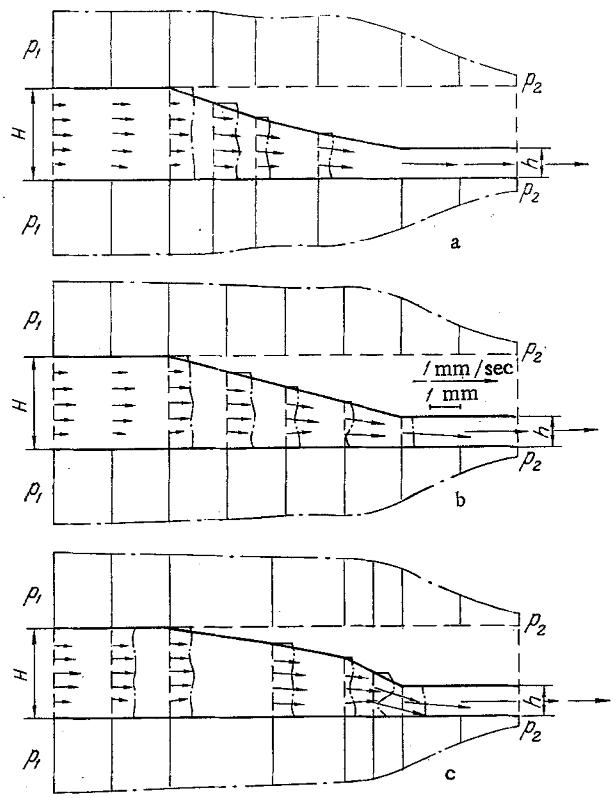

Fig. 3. Velocity and pressure fields in a non-Newtonian medium with an asymmetric converging channel: a, b, and c) eight iterations.

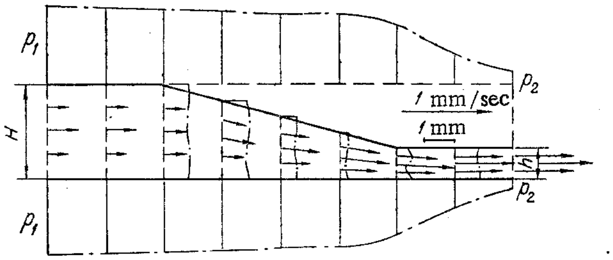

Fig. 4. Velocity and pressure distribution in a non-Newtonian medium with the asymmetric converging channel geometry of Fig. 3c with a different distribution of elements (7 iterations): $\eta_0 = 5\ N \cdot sec \cdot cm^{-2}$; $\eta_1 = 50\ N \cdot sec \cdot cm^{-2}$; n = 0.5; H = 0.3 cm; h = 0.1 cm; L = 1.6 cm; $p_1 = 0.0.01\ N \cdot cm^2$; $p_2 = 0.001\ N \cdot cm^{-2}$; the rheological parameter varies as $\eta = \eta_0 - \eta_1 |\sqrt{II}/2|^{(n-1)}$.

At the same time, for calculations involving non-Newtonian media, it is necessary to use higher-order elements (triangular element with six nodes) in order to satisfy the requirement of continuity of the first derivative between elements. With the help of a local generalization of four triangular elements to a rectangular element, after eliminating internal angular variables, the number of unknowns can be decreased without loss of accuracy.

It should be emphasized that in this work only some of the possibilities of using the method of finite elements in hydrodynamics have been discussed. Future work, apparently, must extend the finite element method of viscoelastic media.

NOTATION

$\|A\|$, matrix of the system; $\bar{A}$, surface; A and B, material characteristics; D_{ij} strain velocity tensor; e, an element; $\{F\}$, right-side vector; H, height of the inlet section; h, height of the outlet section; k_0, consistency factor; M, number of elements relating to a single node; m, maximum number of elements; N, basis function; n, index of the flow; p, pressure; t, time; u, function; u^j, reference value of the function; v_k, velocity vector; $x \equiv x_1, x_2$, Cartesian coordinates; x^j, coordinates of the nodal point; $\{\delta\}$, variable vector of a node; δ_{ij}, Kronecker's symbol; η and η_0, viscosities; ρ, density; σ_{ij}, stress tensor; II, second invariant of the strain velocity; KNO, maximum number of nodes.

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TEMPERATURE FLUCTUATIONS IN A DISPERSE MEDIUM

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Large-scale temperature fluctuations in a thermally nonuniform disperse medium are analyzed by the methods of the thermodynamics of irreversible processes. Calculated results are compared with experimental data.

By participating in motions of various scales, particles of a thermally nonuniform disperse medium can "transport temperature" as an inert scalar admixture. Consequently, in certain regions of the system local large scale temperature fluctuations will arise with intensities appreciably greater than the level of equilibrium thermal agitation. Convective heat transfer between particles and the continuous medium must affect the dissipation of these fluctuations. The damping of large-scale fluctuations can be analyzed within the framework of the thermodynamics of irreversible processes (TIP), the thermodynamic theory of which was developed in [1] and discussed in detail in [2]. The theory was applied to hydrodynamic fluctuations in [3, 4].

The correlation function of temperature fluctuations T' can be written in the form

$$\varphi(t) = \varphi(t-t') = \langle T'(0)\,T'(t)\rangle = \langle T'(t)\,\overline{T'(t)}\rangle = \lim \frac{1}{\tilde{T}}\int_0^{\tilde{T}} T'(t)\,T'(t')\,dt',\quad \tilde{T}\to\infty, \tag{1}$$

where $<\ldots>$ denotes probability averaging of all possible values of T' at times t and t'. $\overline{T'}$ is the average value of T' for t > 0 under the condition that this quantity had a given value T' at t = 0. Thus $\varphi(t)$ takes account of the previous history of the system from $t = -\infty$ to t = 0.

We consider the damping of temperature fluctuations T' of a continuous medium and T_1' of particles by TIP methods [1, 2, 5]. The phenomenological equation for them can be written in the form [2]

$$\dot{\mathbf{x}} = -\mathbf{M}\mathbf{x},\quad \mathbf{x} = \begin{pmatrix} T' \\ T_1' \end{pmatrix}. \tag{2}$$

The matrix **M** is evaluated in [6]:

$$\mathbf{M} = \begin{pmatrix} \alpha_0 C^{-1} & -\alpha_0 C^{-1} \\ -\alpha_0 C_1^{-1} & \alpha_0 C_1^{-1} \end{pmatrix},\qquad \alpha_0 C^{-1} = \frac{6\alpha(1-\varepsilon)}{d\rho c\varepsilon},\qquad \alpha_0 C_1^{-1} = \frac{6\alpha}{d\rho_1 c_1}, \tag{3}$$

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