

## NUMERICAL METHOD OF SIMULATION OF THE HEAT AND MASS TRANSFER IN DIFFERENT FLOWS IN A CHANNEL WITH PENETRABLE WALLS

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*A mathematical model and a numerical method for calculating the dynamics of a fluid and the heat and mass transfer in it in a channel with penetrable walls are presented. Turbulent and transient flows in this channel were simulated on the basis of Navier–Stokes equations by the method of decreasing the rate of change in desired functions at certain nodes. The results of comparison of calculation and experimental data are presented.*

The study of the dynamics of the heat and mass transfer in laminar, transient, and turbulent flows of a fluid in channels with penetrable walls is of interest in a number of modern technologies involving the processes of porous cooling, drying, combustion, condensation, vaporization, sorption, and desorption. Mathematical simulation of the heat and mass transfer in a flow allows one to obtain detailed information on it, in particular to determine the local dynamic and heat-and-mass transfer characteristics of the flow.

The heat and mass transfer in a flow in a channel with penetrable walls is usually simulated on the basis of boundary-layer equations [1, 2]. In [3], a grid method was proposed for calculating the heat exchange in a laminar flow of an incompressible, one-component viscous fluid in channels with blowing on the basis of Navier–Stokes equations and an explicit difference two-layer computational scheme.

Mathematical models of the heat and mass transfer in turbulent convective flows are usually based on Reynolds' suggestion that the Navier–Stokes equations can be averaged. According to this suggestion, the instantaneous values of the velocity, pressure, density, and temperature represent sums of their average and fluctuating values. In this case, the initial Navier–Stokes equations are transformed with the use of certain additional conditions of averaging of desired functions over time, called the Reynolds postulates, into the equations for the relatively averaged desired functions. The averaged transfer equations involve terms defining the turbulent friction, heat conduction, and diffusion, appearing due to the fluctuations of the velocity, temperature, and component concentration of a flow. The averaged transfer equations are brought to the form of Navier–Stokes equations by introducing the effective coefficients of kinematic viscosity  $\nu_{ef} = \nu + \nu_t$ , heat conduction  $\lambda_{ef} = \lambda + \lambda_t$ , and diffusion  $D_{ef} = D + D_t$ , where  $\nu_t$ ,  $\lambda_t$ , and  $D_t$  are the turbulent viscosity, heat conduction, and diffusion coefficients, into them. However, the equations obtained are not closed. Determination of the interrelation between the characteristics of the averaged transfer and the fluctuating transfer is a fairly complex independent problem, the solution of which calls for a large amount of empirical data. At present, there are a large number of turbulence models that approximately define the interrelation between the coefficients  $\nu_t$ ,  $\lambda_t$ , and  $D_t$  and the averaged characteristics of a flow. Each of these models involves a number of empirical parameters determined for concrete conditions of flow and heat and mass transfer. This impairs the reliability and versatility of calculated values of the turbulent convection.

In the present work, we propose a method of simulation of the heat and mass transfer in different flows in a channel with penetrable walls with the use of Navier–Stokes equations and a three-layer explicit difference computational scheme. In calculating transient and turbulent flows, the method of decreasing the rate of change in their velocity, temperature, and volume concentration at certain nodal points of the computational region was additionally used. The essence of this method is described in [4] as applied to the problem on natural convection.

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**Mathematical Model.** As the initial system of equations for simulation of a flow in a channel and the heat and mass exchange in it, the following system of two-dimensional Navier–Stokes equations written in divergent dimensionless stream function  $\psi$ , vortex function  $\omega$ , temperature  $T$ , and mixture-component volume concentration  $C_j$  ( $j = 1, 2, \dots, j_k$ ) variables is used:

$$\frac{\partial \omega}{\partial t} + \frac{\partial u \omega}{\partial x} + \frac{\partial v \omega}{\partial y} = \frac{1}{\text{Re}} \left( \frac{\partial^2 \omega}{\partial x^2} + \frac{\partial^2 \omega}{\partial y^2} \right) + \frac{\text{Gr}}{\text{Re}^2} \left( \frac{g_y}{g} \frac{\partial T}{\partial x} - \frac{g_x}{g} \frac{\partial T}{\partial y} \right) + \sum_j \frac{\text{Gr}_{dj}}{\text{Re}^2} \left( \frac{g_y}{g} \frac{\partial C_j}{\partial x} - \frac{g_x}{g} \frac{\partial C_j}{\partial y} \right), \quad (1)$$

$$\frac{\partial T}{\partial t} + \frac{\partial u T}{\partial x} + \frac{\partial v T}{\partial y} = \frac{1}{\text{Re Pr}} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right), \quad (2)$$

$$\frac{\partial C_j}{\partial t} + \frac{\partial u C_j}{\partial x} + \frac{\partial v C_j}{\partial y} = \frac{1}{\text{Re Sc}} \left( \frac{\partial^2 C_j}{\partial x^2} + \frac{\partial^2 C_j}{\partial y^2} \right), \quad (3)$$

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} = \omega, \quad (4)$$

$$u = \frac{\partial \psi}{\partial y}, \quad v = -\frac{\partial \psi}{\partial x}, \quad \omega = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}, \quad (5)$$

where  $\text{Re} = VL/\nu$ ,  $\text{Gr} = g\beta_T L^3 \Delta T / \nu^2$ ,  $\text{Gr}_{dj} = g\beta_j L^3 \Delta C_j / \nu^2$  is the diffusion Grashof number for the  $j$ th component of a mixture,  $\text{Pr} = \nu/a$ ,  $\text{Sc} = \nu/D$ ,  $\beta_T = -(\partial\rho/\partial T)/\rho$ , and  $\beta_j = -(\partial\rho_j/\partial C_j)/\rho_j$ .

The equations for vortex transfer (1), energy transfer (2), and component-mass transfer (3) as well as the equation for the stream function (4) were derived on the assumption that, at each instant of time  $t$ , the relative deviation of the density of a mixture  $\rho(t, x, y)$  and its kinematic viscosity  $\nu(t, x, y)$  from their average values is small for the space region considered at this instant of time. The pressure distribution in a fluid flow in a channel can be determined by solving the following Poisson equation obtained from the Navier–Stokes equations:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} - 2 \left[ \frac{\partial^2 \psi}{\partial x^2} \frac{\partial^2 \psi}{\partial y^2} - \left( \frac{\partial^2 \psi}{\partial x \partial y} \right)^2 \right] + \frac{\text{Gr}}{\text{Re}^2} \left( \frac{g_y}{g} \frac{\partial T}{\partial x} + \frac{g_x}{g} \frac{\partial T}{\partial y} \right) + \sum_j \frac{\text{Gr}_{dj}}{\text{Re}^2} \left( \frac{g_y}{g} \frac{\partial C_j}{\partial x} + \frac{g_x}{g} \frac{\partial C_j}{\partial y} \right). \quad (6)$$

Initial and boundary conditions are set for Eqs. (1)–(3) and boundary conditions are set for Eq. (4). In the general case, the distribution of the initial velocity, temperature, and volume-concentration has the form

$$W(0, x, y) = W_{\text{in}}(x, y), \quad W = u, v, T, C_j. \quad (7)$$

When it is necessary to obtain a nonstationary solution of the system of equations (1)–(5), the vortex function is determined at the instant of time  $t = 0$  and then an approximate solution of Eqs. (1) and (4) is found by the method of ascertainment at conditions (7). Hereinafter, for simplicity, the boundary conditions for the heat and mass transfer in a flow in a straight slot channel  $-X < x < X$  will be used.

For the input cross section of the channel  $y = 0$ , the following conditions are set:

$$W(t, x, 0) = W_0(t, x), \quad W = u, v, T, C_j. \quad (8)$$

In this case, the average density of the mass flow of the mixture component  $j$  through the input cross section of the channel is equal to

$$J_{j0} = \frac{1}{2X} \int_{x=-X}^X C_j(t, x, 0) v(t, x, 0) dx. \quad (9)$$

At the penetrable boundary  $x = X$ , the densities of the flows of blown-in components, the equations of their state, and the heat-exchange conditions of the first, second, and third kind are determined. The resulting normal velocity of a flow  $u(t, X, y)$  at this boundary is related to the flow rates and the volume concentrations of components by the relation

$$u(t, X, y) = \sum_j J_j'(t, X, y) / \sum_j C_j(t, X, y), \quad (10)$$

and the volume concentration  $C_j(t, X, y)$  of the component  $j$  at the boundary  $x = X$  is determined from the mass-conservation equation

$$J_j'(t, X, y) = C_j(t, X, y) u(t, X, y) - \frac{1}{\text{Re Sc}} \frac{\partial C_j}{\partial x}. \quad (11)$$

In the simplest case, it may be assumed that, at this boundary, the longitudinal velocity component is equal to zero and heat-exchange conditions of the first kind are fulfilled:

$$v(t, X, y) = 0, \quad T(t, X, y) = T'(t, y). \quad (12)$$

If the velocity, temperature, and volume-concentration fields of components are symmetric relative to the middle plane of the channel  $x = 0$ , the following conditions are fulfilled in this plane:

$$v(t, 0, y) = 0, \quad \frac{\partial u(t, 0, y)}{\partial y} = \frac{\partial T(t, 0, y)}{\partial y} = \frac{\partial C_j(t, 0, y)}{\partial y} = 0. \quad (13)$$

If the length of the channel  $Y$  is fairly large ( $Y/X \gg 1$ ) and  $y = Y$  near the boundary, the flow and the heat and mass transfer stabilize; at  $y = Y$ , the boundary conditions take the form

$$\frac{\partial W^s}{\partial x^s} \approx 0, \quad W = u, v, T, C_j, \psi, \omega; \quad s = 1, 2, \dots \quad (14)$$

To obtain a more exact solution in the process of numerical realization of the model in addition to the above-described uniqueness conditions, the following mass-balance equations are used for each component of a mixture for the period of establishment of a flow and the heat exchange in it:

$$\begin{aligned} & \int_0^Y C_j(t, 0, y) u(t, 0, y) dy - \int_0^X C_j(t, x, Y) v(t, x, Y) dx + \int_0^X C_j(t, x, 0) v(t, x, 0) dx - \\ & - \int_0^Y C_j(t, X, y) u(t, X, y) dy = 0. \end{aligned} \quad (15)$$

The first, second, third, and fourth terms in the left side of the equation define the flow rates of the component  $C_j$  through the boundaries of the region  $x = 0$ ,  $y = Y$ ,  $y = 0$ , and  $x = X$  respectively. Analogous mass and energy conservation equations can be written for the system as a whole.

If the stream function at the boundary point  $B_0$  is equal to  $\psi_0$ , its value  $\psi_1$  at the point  $B_1$  of the same boundary will be determined by integration over the contour of the region:

$$\psi_i = \psi_0 + \int_{B_0}^{B_1} (u dy - v dx). \quad (16)$$

Since the components  $u$  and  $v$  of the velocity vector at the boundaries of the region are assumed to be prescribed, it is easy to determine the function  $\psi$  at the boundary nodes.

A peculiarity of the determination of the vortex function  $\omega_b$  at the boundary nodes is the absence of boundary conditions (e.g., like the boundary conditions of the energy-transfer equation) for the vortex-transfer equation (1). In [5], various methods of determining  $\omega_b$  at a given point of a boundary surface by the values of the stream function at individual points of the normal to this surface have been analyzed. Below, we present a method of determining  $\omega_b$  at boundary surfaces, which can be not coordinate surfaces, and for the case where nonorthogonal grids are used. The following equation is used as the boundary condition of (1):

$$\omega_b = \left. \frac{\partial^2 \psi}{\partial x^2} \right|_b + \left. \frac{\partial^2 \psi}{\partial y^2} \right|_b, \quad (17)$$

which follows from (4). It is assumed that the velocity vector of the fluid at an arbitrary point of the boundary surface is known and the values of the stream function  $\psi$  at one or several inner points positioned in its neighborhood are known. Under these conditions, the right side of Eq. (17) is determined by expansion of the function  $\psi$  at the indicated inner points by Taylor's theorem. In the particular case where the normal to the boundary surface is parallel to the  $x$  axis,  $v_b = v$ ,  $u_b = u$ ,  $\psi_b = \psi(x, y) = \psi_0$ , and  $\psi(x + \Delta x_1, y) = \psi_1$ , the function  $\omega_b$  can be determined with an error of the order of  $\Delta x_1$  in the following way. According to the first of conditions (5),  $\left. \frac{\partial^2 \psi}{\partial y^2} \right|_b = \left. \frac{\partial u}{\partial y} \right|_b$ . The derivative  $\left. \frac{\partial^2 \psi}{\partial x^2} \right|_b$  is determined from the expansion of the function  $\psi(x + \Delta x_1, y)$  by Taylor's theorem in terms of powers of  $\Delta x_1$ . Retaining the first three terms in the series and taking into account the second of conditions (5), we find that  $\left. \frac{\partial^2 \psi}{\partial x^2} \right|_b = 2(\psi_1 - \psi_0 + v_b \Delta x_1) / \Delta x_1^2 + O(\Delta x_1)$  and obtain the following expression for  $\omega_b$  with an error of the order of  $O(\Delta x_1)$ :

$$\omega_b = \frac{2(\psi_1 - \psi_0 + v_b)}{\Delta x_1^2} + \left. \frac{\partial u}{\partial y} \right|_b. \quad (18)$$

To determine  $\omega_b$  more exactly with an error of the order of  $O(\Delta x^2)$ , it will suffice to additionally determine the value of the stream function  $\psi(x + \Delta x_2, y) = \psi_2$  for one more point of the normal. Then, retaining the first four terms in the expansions of the functions  $\psi(x + \Delta x_1, y)$  and  $\psi(x + \Delta x_2, y)$  and combining these expansions, we obtain

$$\omega_b = 2 \frac{\varphi^3 \psi_1 - \psi_2 - (\varphi^3 - 1) \psi_0 + (\varphi^2 - 1) \varphi v_b \Delta x_1}{\varphi^2 (\varphi - 1) \Delta x_1} + \left. \frac{\partial u}{\partial y} \right|_b, \quad \varphi = \frac{\Delta x_1}{\Delta x_2}. \quad (19)$$

When the boundary surface is not parallel to the coordinate plane or a nonorthogonal difference grid is used, it is necessary that the inner nodes, which are positioned in the neighborhood of a given boundary point, lie on the normal to the boundary surface. In this case, the value of  $\omega_b$  is determined in the following order. A Cartesian coordinate system with origin at the boundary nodal point  $P_0$  is constructed. One of the coordinate axes is directed along the inner normal  $\eta$  to the boundary surface at the point  $P_0$  and the other axis is directed along the tangent  $\tau$ . A number  $S$  of nodal points  $P_s$  with coordinates  $\eta_s, \tau_s$  ( $s = 1, 2, \dots, S$ ) are selected in the neighborhood of  $P_0$ . The coordinates of these points are related to their coordinates  $x$  and  $y$  in the initial coordinate system by the relation

$$\eta_s = [x(P_s) - x(P_0)] \cos(\eta, x) + [y(P_s) - y(P_0)] \sin(\eta, x),$$

$$\tau_s = -[x(P_s) - x(P_0)] \sin(\eta, x) + [y(P_s) - y(P_0)] \cos(\eta, x).$$

For each of the points  $P_s$ , the stream function  $\psi_s$  is expressed in terms of the function  $\psi$  and its derivatives with respect to the coordinates  $\eta$  and  $\tau$  at the point  $P_0$  by taking a Taylor series expansion of  $\psi_s$  with a finite number of terms. If the velocity vector  $\mathbf{V}$  at the boundaries of the region is prescribed, its projections  $V_\eta$  and  $V_\tau$  at the point  $P_0$  and their derivatives with respect to the tangent  $\tau$  should be assumed to be known. This allows one to express, using the relations  $\partial\psi/\partial\eta = V_\tau$ ,  $\partial\psi/\partial\tau = -V_\eta$ , and  $\partial^2\psi/\partial\tau^2 = -\partial V_\eta/\partial\tau$  similar to relations (5), some of the derivatives of the function  $\psi$  at the point  $P_0$  that are involved in the above-indicated expansions in terms of the velocity components  $V_\eta$  and  $V_\tau$ . Then, varying the rearranged expansions, we will find an expression for the derivative  $\partial^2\psi/\partial\eta^2|_{P_0}$  and then the value of  $\omega_b = \omega_{P_0}$  from the equation  $\omega_{P_0} = \partial^2\psi/\partial\eta^2|_{P_0} + \partial^2\psi/\partial\tau^2|_{P_0}$ . To determine  $\omega_b$  with an error of the order of  $O(\Delta\eta_1 + \Delta\tau_1)$ , it will suffice to determine the value of  $\psi(\eta + \Delta\eta_1, \tau + \Delta\tau_1) = \psi_1$  at a single point with coordinates  $\eta + \Delta\eta_1$  and  $\tau + \Delta\tau_1$ . From the Taylor series expansion of the function  $\psi_1$  in powers of  $\Delta\eta_1$  and  $\Delta\tau_1$ , in which only the terms containing the derivatives of the function  $\psi$  with respect to the coordinates  $\eta$  and  $\tau$  of order of not higher than the second one are involved, we obtain, after corresponding rearrangements, an expression defining  $\partial^2\psi/\partial\eta^2|_{P_0}$  as a function of  $\psi_0$ ,  $\psi_1$ ,  $V_\eta$ , and  $V_\tau$ . On substitution of the quantities  $\partial^2\psi/\partial\eta^2|_{P_0}$  and  $\partial^2\psi/\partial\tau^2|_{P_0}$  into the equation for the stream function, we find

$$\omega_{P_0} = \frac{2}{\Delta\eta_1^2} \left[ \psi_1 - \psi_0 + \Delta\eta_1 V_\tau \Big|_{P_0} - \Delta\tau_1 V_\eta \Big|_{P_0} - \frac{1}{2} (\Delta\eta_1^2 + \Delta\tau_1^2) \frac{\partial V_\eta}{\partial\tau} \Big|_{P_0} + \Delta\eta_1 \Delta\tau_1 \frac{\partial V_\tau}{\partial\tau} \Big|_{P_0} \right]. \quad (20)$$

For the case of an immovable, impenetrable wall, where  $V_\eta|_b = V_\tau|_b = 0$ , the expression obtained is transformed into the known Thom formula [5].

To determine  $\omega_{P_0}$  with an error of the order of  $O(\Delta\eta^2 + \Delta\tau^2)$ , it is necessary to retain, in the expansion of the function  $\psi$ , the terms containing the derivatives of the function  $\psi$  with respect to the coordinates  $\eta$  and  $\tau$  of order of not higher than the third one. This expansion contains three unknown functions:  $\partial^2\psi/\partial\eta^2|_{P_0}$ ,  $\partial^3\psi/\partial\eta^3|_{P_0}$ , and  $\partial^3\psi/(\partial\eta^2\partial\tau)|_{P_0}$ ; therefore, in the neighborhood of the point  $P_0$ , three inner points should be selected. By combining the expansions of the stream functions at these points we determine  $\partial^2\psi/\partial\eta^2|_{P_0}$  and then  $\omega_{P_0}$ :

$$\omega_{P_0} = \sum_{s=1}^3 b_s \left[ (\psi_s - \psi_0) + \Delta\eta_s V_\tau - \Delta\tau_s V_\eta - \frac{\Delta\tau_s^2}{2} \frac{\partial V_\eta}{\partial\tau} + \Delta\eta_s \Delta\tau_s \frac{\partial V_\tau}{\partial\tau} - \frac{\Delta\tau_s^3}{6} \frac{\partial^2 V_\eta}{\partial\tau^2} + \frac{\Delta\eta_s}{2} \Delta\tau_s^2 \frac{\partial^2 V_\tau}{\partial\tau^2} \right],$$

where

$$b_1 = 1/[(a_{11} - a_{13}a_{31}/a_{33}) + (a_{12} - a_{13}a_{32}/a_{33}) (a_{21} - a_{23}a_{31}/a_{33})/(a_{32} - a_{23}a_{32}/a_{33})];$$

$$b_2 = -b_1 (a_{21} - a_{23}a_{31}/a_{33})/(a_{22} - a_{23}a_{32}/a_{33}); \quad b_3 = -b_1 a_{31}/a_{33} - b_2 a_{32}/a_{33};$$

$$a_{1s} = \Delta\eta_s^2/2; \quad a_{2s} = \Delta\eta_s^3/6; \quad a_{3s} = \Delta\eta_s^2 \Delta\tau_s/2; \quad s = 1, 2, 3.$$

**Numerical Method of Calculating the Heat and Mass Transfer in a Channel.** The system of equations (1)–(5) can be solved by numerical methods. The equations for vortex transfer (1), energy transfer (2), and mass transfer (3), containing convective terms, are solved on the basis of a three-layer difference computational scheme [6]. In

this scheme, to each differential transfer equation correspond two difference equations, and a function determined in each time layer is calculated in two approximations. The difference equations for determining the desired function in the first approximation approximate an incomplete transfer equation containing only convective terms and a time derivative. The difference equations for the desired function in the second approximation are constructed by approximation of all terms of the initial differential transfer equation. On the grid

$$\begin{aligned} x_i &= x_{i-1} + h_{x,i-1}, \quad i = 1, 2, \dots, I, \quad x_0 = x', \quad x_I = x''; \\ y_m &= y_{m-1} + h_{y,m-1}, \quad m = 1, 2, \dots, M, \quad y_0 = y', \quad y_M = y''; \\ t_n &= t_{n-1} + l_n, \quad n = 1, 2, \dots, \quad l_n > 0, \quad t_0 = 0 \end{aligned} \quad (21)$$

the difference equations serving to determine the approximate values of  $W_{im}^n$  of the functions  $W(t_n, x_i, y_m)$ , where  $W = \omega, T, \text{ or } C_j$ , and approximating Eqs. (1)–(3) with an error  $O(l_n + h_{xi}^2 + h_{ym}^2)$  have the form

$$\delta_i \bar{\omega} + \delta_x (u\bar{\omega}) + \delta_y (v\bar{\omega}) = 0, \quad (22)$$

$$\begin{aligned} & \frac{\omega_{im}^{n+1} - \omega}{l_n} (1 + \theta_\omega) - \frac{\omega - \omega_{im}^{n-1}}{l_{n-1}} \theta_\omega + \delta_x (u\bar{\omega}) + \delta_y (v\bar{\omega}) = \\ & = \frac{1}{\text{Re}} (\delta_{xx} \bar{\omega} + \delta_{yy} \bar{\omega}) + \frac{\text{Gr}}{\text{Re}^2} (g_y \delta_x \bar{T} - g_x \delta_y \bar{T}) + \sum_j \frac{\text{Gr}_{dj}}{\text{Re}^2} \left( \frac{g_y}{g} \delta_x \bar{C}_j + \frac{g_x}{g} \delta_y \bar{C}_j \right), \end{aligned} \quad (23)$$

$$\delta_i \bar{T} + \delta_x (u\bar{T}) + \delta_y (v\bar{T}) = 0, \quad (24)$$

$$\frac{T_{im}^{n+1} - T}{l_n} (1 + \theta_T) - \frac{T - T_{im}^{n-1}}{l_{n-1}} \theta_T + \delta_x (u\bar{T}) + \delta_y (v\bar{T}) = \frac{1}{\text{Re Pr}} (\delta_{xx} \bar{T} + \delta_{yy} \bar{T}), \quad (25)$$

$$\delta_i \bar{C}_j + \delta_x (u\bar{C}_j) + \delta_y (v\bar{C}_j) = 0, \quad (26)$$

$$\frac{C_{jim}^{n+1} - C}{l_n} (1 + \theta_j) - \frac{C_j - C_{jim}^{n-1}}{l_{n-1}} \theta_j + \delta_x (u\bar{C}_j) + \delta_y (v\bar{C}_j) = \frac{1}{\text{Re Sc}} (\delta_{xx} \bar{C}_j + \delta_{yy} \bar{C}_j). \quad (27)$$

In the difference equations (22)–(27), the grid functions  $W_{im}^n$  and  $\bar{W}_{im}^{n+1}$  ( $W = u, v, T, C_j, \Psi, \text{ or } \omega$ ) at the nodal point  $(x_i, y_m, t_n)$  are written without indices for simplicity, i.e.,  $W = W_{im}^n, \bar{W} = \bar{W}_{im}^n$ ;  $\theta$  is a weighting factor that makes it possible to eliminate the restriction imposed on the time step by the diffusion terms in Eqs. (1)–(3) ( $\theta \geq 0$ );

$$\delta_i \bar{W} = \frac{\bar{W}_{im}^{n+1} - W_{im}^n}{l_n}; \quad \delta_x W = \frac{W_{i+1,m}^n - W_{i-1,m}^n}{x_{i+1} - x_{i-1}}; \quad \delta_{xx} W = \left[ \frac{W_{i+1,m}^n - W_{im}^n}{x_{i+1} - x_i} - \frac{W_{im}^n - W_{i-1,m}^n}{x_i - x_{i-1}} \right] / (x_{i+1} - x_{i-1}).$$

The conditions necessary for obtaining a stable solution of Eqs. (22)–(27) are found by the method of conditional prescription of some desired functions of the system [1]. In the case where  $\theta_{jim}^n = 0, \gamma = \omega, T, \text{ or } C$ , and Eqs. (23), (25), and (27) are two-layer, the time step  $l_n^0$  is selected starting from the following numerical-solution stability condition:

$$l_n^0 \leq \min \{l_V, l_\omega, l_T, l_C\}, \quad (28)$$

where

$$l_V = \left( u_{im}^n / h_{xi} + v_{im}^n / h_{ym} \right)^{-1}; \quad l_\omega = \left[ 2 \left( 1/h_{xi}^2 + 1/h_{ym}^2 \right) \text{Re} \right]^{-1}; \quad l_T = \left[ 2 \left( 1/h_{xi}^2 + 1/h_{ym}^2 \right) \text{Re Pr} \right]^{-1};$$

$$l_C = \left[ 2 \left( 1/h_{xi}^2 + 1/h_{ym}^2 \right) \text{Re Sc} \right]^{-1}.$$

If  $l_V > l_\gamma$ , owing to the parameter  $\theta_{\gamma im}^n$ , a larger step  $l_n > l_n^0$  can be selected in accordance with the relation  $l_V \geq l_n > l_\gamma$  ( $\gamma = \omega, T, \text{ or } U$ ). In this case, the parameter  $\theta_{\gamma im}^n$  is determined from the conditions providing the obtaining of a stable solution of Eqs. (22)–(27):

$$\theta_{\gamma im}^n = (l_n / l_\gamma - 1) / 2, \quad l_n / l_\gamma > 1;$$

$$\theta_{\gamma im}^n = 0, \quad l_n / l_\gamma \leq 1. \quad (29)$$

The equation for the stream function (4) is solved in each time layer  $n$  by the method of ascertainment with the use of an explicit three-layer difference scheme [6]. Difference approximation of Eq. (4), performed with an error of  $l_k + h_{xi}^2 + h_{ym}^2$  on a grid, differing from (21) by the fact that the discrete variable  $t_k = t_{k-1} + l_k$  ( $k = 1, 2, \dots, l_k > 0, t_0 = 0$ ) is used in it instead of the actual time  $t_n$ , has the form

$$\frac{\Psi_{im}^{k+1} - \Psi_{im}^k}{l_k} \left( 1 + \theta_{\Psi im}^k \right) - \frac{\Psi_{im}^k - \Psi_{im}^{k-1}}{l_{k-1}} \theta_{\Psi im}^k = \delta_{xx} \Psi_{im}^k + \delta_{yy} \Psi_{im}^k - \omega_{im}^{n+1}, \quad (30)$$

where  $\theta_{\Psi im}^k$  is the weight factor ( $\theta_{\Psi im}^k \geq 0$ ). After the steps  $l_k, h_{xi}$ , and  $h_{ym}$  are selected arbitrarily, the values of the weight factor  $\theta_{\Psi im}^k$  are determined in accordance with the conditions providing the stability of Eq. (15):

$$\theta_{\Psi im}^k = (l_k / l_\Psi - 1) / 2, \quad l_k > l_\Psi;$$

$$\theta_{\Psi im}^k = 0, \quad l_k \leq l_\Psi, \quad (31)$$

in this case,  $l_\Psi = [2(1/h_{xi}^2 + 1/h_{ym}^2)]^{-1}$ . The results of numerical experiments indicate that a minimum time is necessary for determining the stream function on a computer when  $\theta_{\Psi im}^k = 2-2.5$ . To this value corresponds a five- or six-fold increase in the time step as compared to the maximum step used in the usual explicit two-layer difference scheme. The process of solving Eq. (15) is considered as completed when the condition  $\sum_i \sum_m (\Psi_{im}^{k+1} - \Psi_{im}^k) l_k \leq \Delta$ , where  $\Delta$  is

a small positive number, is fulfilled. In this case, it is assumed that  $\Psi_{im}^{n+1} = \Psi_{im}^k$ . It should be noted that, since the last-named term on the right side of Eq. (30) is changed for one time step by a value of the order of  $l_k$ , a small number of iterations is necessary for solving Eq. (30). As the initial approximation corresponding to  $k = 0$ , the approximation  $\Psi_{im}^k = \Psi_{im}^n$  is used.

The velocity-vector components  $u_{im}^{n+1}$  and  $v_{im}^{n+1}$  are determined by the difference equations following from relations (5):

$$u_{im}^{n+1} = \delta_y \Psi_{im}^{n+1}, \quad v_{im}^{n+1} = -\delta_x \Psi_{im}^{n+1}. \quad (32)$$

Numerical solution of the problem on a flow in a channel and the heat and mass transfer in it is carried out in the following order. In a time layer  $n = 0$ , the values of the desired grid functions  $u$ ,  $v$ ,  $T$ ,  $C_j$ ,  $\Psi$ , and  $\omega$  are determined by conditions (7) and relations (5). If the functions  $u_{in}$ ,  $v_{in}$ ,  $\Psi_{in}$ , and  $\omega_{in}$  are equal to zero at the instant of time  $t = 0$ , and  $T_{in}$  and  $C_{jin}$  are constants,

$$u_{im}^0 = v_{im}^0 = \Psi_{im}^0 = \omega_{im}^0 = 0, \quad T_{im}^0 = T_{in}, \quad C_{jim}^0 = C_{jin}. \quad (33)$$

Let us assume that the grid functions for the time layers 1, 2, ...,  $n$  are known and it is necessary to determine their values for the layer  $n$ . At first, the preliminary values of the functions  $\bar{\Psi}_{im}^{n+1}$ ,  $\bar{T}_{im}^{n+1}$ , and  $\bar{C}_{jim}^{n+1}$  at the inner nodal points  $i = 1, 2, \dots, I-1$ ,  $m = 1, 2, \dots, M-1$  are determined from Eqs. (22), (24), and (26); in this case,  $x_0 = 0$ ,  $x_I = X$ ,  $y_0 = 0$ , and  $y_M = Y$ . It is assumed that, at the boundary nodal points,

$$\bar{\Psi}_{im}^{n+1} = \Psi_{im}^n, \quad \bar{T}_{im}^{n+1} = T_{im}^n, \quad \bar{C}_{jim}^{n+1} = C_{jim}^n. \quad (34)$$

Then the finite values of the grid functions  $\Psi_{im}^{n+1}$ ,  $T_{im}^{n+1}$ , and  $C_{jim}^{n+1}$  at the inner nodal points are determined from Eqs. (23), (25), and (27). The functions  $u_{0m}^{n+1}$ ,  $v_{0m}^{n+1}$ ,  $T_{0m}^{n+1}$ , and  $C_{j0m}^{n+1}$  at the nodal points of the cross section ( $m = 0$ ) of the channel are determined using (8) and (26):

$$W_{i0}^{n+1} = W_0(t_{n+1}, x_i), \quad W = v, T, C_j; \quad u_{0m}^{n+1} = 0; \quad \Psi_{i+1,0}^{n+1} = \Psi_{i,0}^{n+1} - \left( v_{i+1,0}^{n+1} + v_{i,0}^{n+1} \right) h_{xi}/2. \quad (35)$$

The grid functions at the nodes on the penetrable wall ( $i = I$ ) are determined by difference approximations of Eqs. (10)–(12) and (16):

$$v_{I,m}^{n+1} = 0; \quad u_{I,m}^{n+1} = \sum_j G_{j,m}^{n+1} / \sum_j C_{j,I,m}^n, \quad C_{j,I,m}^{n+1} = \left( C_{j,I-1,m}^{n+1} + G_{j,m}^{n+1} h_{xI} \operatorname{Re Sc} \right) \left( 1 + u_{I,m}^{n+1} h_{xI} \operatorname{Re Sc} \right),$$

$$T_{I,m}^{n+1} = T_m^{n+1}, \quad \Psi_{I,m+1}^{n+1} = \Psi_{I,m}^{n+1} + \left( u_{I,m+1}^{n+1} + u_{I,m}^{n+1} \right) h_{ym}/2, \quad m = 1, 2, \dots, M. \quad (36)$$

According to (13), at the nodes lying in the symmetry plane of the channel ( $i = 0$ ),

$$W_{0,m}^{n+1} = W_{1,m}^{n+1}, \quad W = v, T, C_j; \quad u_{0,m}^{n+1} = \omega_{0,m}^{n+1} = 0. \quad (37)$$

The grid functions at the nodes of the output cross section ( $m = M$ ) are determined from conditions (14) at  $s = 1$  and from (16):

$$W_{i,M}^{n+1} = W_{i,M-1}^{n+1}, \quad W = u, v, T, C_j; \quad \Psi_{i+1,M}^{n+1} = \Psi_{i,M}^{n+1} - \left( v_{i+1,M}^{n+1} + v_{i,M}^{n+1} \right) h_{xi}/2, \quad i = 1, 2, \dots, I-1. \quad (38)$$

The accuracy of solution of the problem on the basis of the mass-balance equation (15) can be increased in the following way. The values of the longitudinal velocities  $v$  obtained from (38) are considered as their first approximation  $\bar{v}_{i,M}^{n+1}$ ,  $i = 1, 2, \dots, I$ . They are used for determining (e.g., by the formula of trapezoids) an approximate rate of a fluid flow  $G_M$  through the cross section  $m = M$ . The flow rate through this cross section is determined accurately from Eq. (15). The finite values of the velocities  $v_{i,M}^{n+1}$  are calculated as

$$v_{i,M}^{n+1} = \bar{v}_{i,M}^{n+1} \frac{G_M}{G_M}. \quad (39)$$

The value of  $\Psi_{i,M}^{n+1}$  is calculated by the last-named equation of system (38).

Determination of the desired functions in the layer  $n+1$  is completed by calculation of the vortex function  $\omega$  at the boundary nodes from the relations obtained by approximation of equations (14) and (18):



$$\begin{aligned}
\omega_{i,0}^{n+1} &= -\left(v_{i+1,0}^{n+1} - v_{i-1,0}^{n+1}\right) / (h_{i-1} + h_i) + 2\left(\psi_{i,1}^{n+1} - \psi_{i,0}^{n+1} - u_{i,0}^{n+1} h_{y0}\right) / h_{y0}^2, \\
\omega_{i,M}^{n+1} &= 2\omega_{i,M-1}^{n+1} - \omega_{i,m-2}^{n+1}, \quad \omega_{0,m}^{n+1} = 0, \\
\omega_{I,m}^{n+1} &= -\left(u_{I,m+1}^{n+1} - v_{I,m-1}^{n+1}\right) / (h_{y,m-1} + h_{y,m}) + 2\left(\psi_{I-1,m}^{n+1} - \psi_{I,m}^{n+1} - u_{I,m}^{n+1} h_{I-1}\right) / h_{I-1}^2.
\end{aligned} \tag{40}$$

For the problems on natural convection in regions with impenetrable walls, a simpler computational algorithm can be used, since, in this case,  $u = v = \psi = 0$  at the boundary nodal points.

Numerical experiments have shown that, in the initial period, after the transient phases, the solution becomes nonstationary beginning with any value of the Reynolds number  $Re = Re'$ . When the numerical solution was not smoothed, it became unstable when  $Re$  further increased and exceeded the limiting value  $Re^* > Re'$ . The latter shows that the rate and other characteristics of the process tend to infinity. If a three-dimensional difference grid with a fairly large number of nodes is used, the value of  $Re^*$  is determined by the critical Reynolds number at which the flow and the heat and mass transfer in it become turbulent.

The study of turbulent convective flows is usually based on Reynolds' suggestion that the Navier–Stokes equations can be averaged. In accordance with this suggestion, the instantaneous values of the velocity, pressure, density, and temperature of a flow represent sums of their average and fluctuating values. In this case, the initial Navier–Stokes equations for desired functions are transformed, with the use of additional conditions called the Reynolds postulates, into equations for the averaged values of these functions. In the latter, the expressions for the stress tensor involve terms dependent on the fluctuating components of the velocity, pressure, density, and temperature. These equations are not closed. To close them, it is necessary to determine the interrelation between the characteristics of the averaged transfer and the fluctuating transfer. Usually, instead of the true values of the coefficients of kinematic viscosity  $\nu$ , heat conduction  $\lambda$ , and diffusion  $D$ , their effective values  $\nu_{ef} = \nu + \nu_t$ ,  $\lambda_{ef} = \lambda + \lambda_t$ , and  $D_{ef} = D + D_t$  are substituted into the flow and heat-and-mass transfer equations; in this case,  $\nu_t \geq 0$ ,  $\lambda_t \geq 0$ , and  $D_t \geq 0$  and determination of these quantities calls for a large amount of empirical data. This impairs the reliability and versatility of the calculated values of the data on a turbulent convection.

A different method was proposed in [4] for numerically solving problems on natural convection at large  $Re$  numbers ( $Re > Re^*$ ). It involves solution of Navier–Stokes equations and the procedure of decreasing the rates of change in the desired functions  $\omega$ ,  $T$ , and  $C$  at certain nodal points at which these rates exceed the physically permitted values providing a stable solution. The necessity of decreasing the indicated rates is explained by the following facts. The factors responsible for the instability arising in the process of numerical solution of the Navier–Stokes equations share a number of traits with the factors responsible for the instability of an actual process at fairly large Peclet and Reynolds numbers. However, when a numerical instability arises, the value, e.g., of the velocity of a fluid tends to infinity, while all physical parameters of any actual flow and the heat and mass transfer in it (velocity, temperature, concentration of components) as well as their time derivatives remain limited (e.g., the velocity of a flow cannot reach the velocity of light). This discrepancy in the character of development of the indicated instabilities can be remedied by imposing the following restrictions on the time derivatives of the functions  $\omega$ ,  $T$ ,  $C$ , and  $\psi$  at any nodal points at which these velocities exceed the values allowed by the stability conditions:

$$\frac{\partial W}{\partial t} = A_W \frac{\partial W}{\partial t} \Big/ \left| \frac{\partial W}{\partial t} \right|, \quad \text{if} \quad \left| \frac{\partial W}{\partial t} \right| > A_W, \quad W = \omega, \psi, T, C. \tag{41}$$

Here,  $A_W$  is a positive quantity that can be selected starting from the requirement that the number of nodal points  $B_W$ , at which the velocity  $\partial W / \partial t$  in a time layer at the instant a solution is found is corrected according to (41), be minimum.

The procedure of decreasing the above-indicated rates can be considered as the removal of an excess energy from some points of the region considered. This energy is converted into the energy of turbulent fluctuations that do not appear in the process of numerical solution because their amplitude is smaller than the scale of a difference grid.

TABLE 1. Values of  $b_\omega$  Determined in Relation to the Reynolds Number  $Re$  and the Minimum Relative Pitch  $\bar{h}_{\min} = \min(h_i)/X$

Re	$\bar{h}_{\min} \cdot 10^3$		
	0.567	0.2835	0.14175
$1 \cdot 10^4$	0.0024	0.0008	0
$5 \cdot 10^4$	0.0332	0.0184	0.0021
$1 \cdot 10^5$	0.3917	0.0824	0.0042
$5 \cdot 10^5$	0.5153	0.0119	0.0049
$1 \cdot 10^6$	0.772	0.5086	0.0084
$2 \cdot 10^6$	0.8956	0.6723	0.5210
$1 \cdot 10^7$	0.9680	0.9421	0.9242

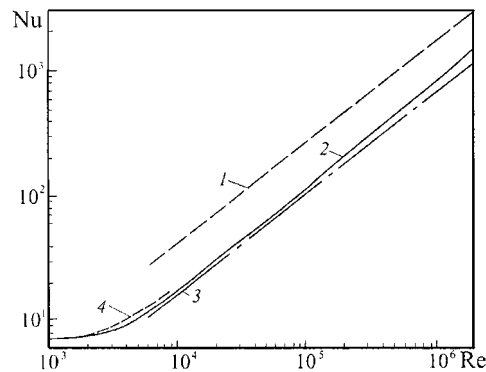


Fig. 1. Dependence of the Nusselt number  $Nu$  on the Reynolds number  $Re$  at  $Pr = 1$  for channels with impenetrable walls: 1) calculation by formula (42) for a round tube; 2) results of numerical solution for a plane slot channel; 3) calculation by formula (43) for a ring channel; 4) calculation by formula (44) for a slot channel.

Thus, it may be inferred that the procedure of decreasing the rates of change in the functions  $\omega$ ,  $\psi$ ,  $T$ , and  $C$  makes it possible to exclude small-scale turbulent fluctuations from consideration.

**Results of Numerical Simulation.** Numerical experiments have shown that  $A_W$  depends weakly on the number of nodes of a three-dimensional grid  $B = I \cdot M$  and the  $Re$  number. This enables the quantity  $A_W$  to be invariable in a wide range of Reynolds numbers. When the  $Re$  number increases, all things being equal,  $B_W$  increases and the condition  $B_\omega > B_T > B_C$  is fulfilled in practically all cases. In the case of a turbulent transfer, the relative number  $b_W = B_W/B$  of nodes at which the velocity of a flow is corrected initially increases fairly rapidly and then, when it reaches a maximum, decreases monotonically and stabilizes at a later time. It is seen from Table 1 that the value of  $b_\omega$  at which the solution is stable decreases monotonically with decrease in the pitches of a difference grid. As these pitches decrease, smaller and smaller vortices are taken into account in numerically solving Eqs. (1)–(5); this allows the conclusion that, in the case where a fairly fine grid is used, the method of decreasing the rate of change in desired fluctuations makes it possible to solve the Navier–Stokes equations for a turbulent flow and the heat and mass transfer in it with a high degree of accuracy.

On the basis of the numerical method described, we solved the problem on the dynamics of a vapor–gas mixture flowing in a plane slot channel  $-X < x < X$  and the heat and mass transfer in it and the problem on blowing of vapor through penetrable walls at Reynolds numbers changing within a wide range. It was assumed that the uniqueness conditions are symmetrical relative to the middle plane of a slot. A difference grid uniform along the  $y$  axis of the channel and bunching consecutively in the transverse direction near its walls was used. The size of the pitch at each stage remains unchanged in the direction to the wall of the channel, the pitch at each subsequent stage being two

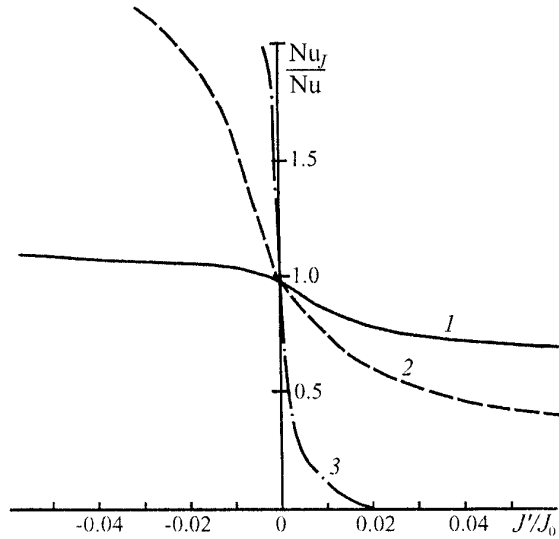


Fig. 2. Dependence of the relative Nusselt number  $Nu_j/Nu$  on the relative density of a mass flow  $J'/J_0$  through a penetrable wall at different Reynolds numbers:  $Re = 10^3$  (1),  $10^4$  (2), and  $10^5$  (3).

times smaller than the pitch at the previous stage. This makes it possible to perform approximation relative to the pitches of the three-dimensional difference grid with a second-order error for all nodal points.

For comparison purposes, Fig. 1 shows the dependences of  $Nu$  on  $Re$  at  $Pr = 1$  for channels with impenetrable walls, constructed on the basis of numerical solution, by the empirical equation [2] for a round tube

$$Nu = 0.021Re^{0.8} Pr^{0.43}, \quad (42)$$

by the empirical equation [2] for a ring channel

$$Nu = 0.017Re^{0.8} Pr^{0.4} (d_2/d_1)^{0.18} \quad \text{at } d_{eq} = d_2 - d_1 \quad \text{and } d_2/d_1 \rightarrow 1, \quad (43)$$

by the approximate analytical solution for a slot channel with impenetrable walls at a definite parabolic velocity profile [7]

$$\begin{aligned} Nu &= 1.85 (Pe d_{eq}/Y_k)^{1/3}, \quad Pe d_{eq}/L > 70; \\ Nu &= 7.50, \quad Pe d_{eq}/L < 70, \end{aligned} \quad (44)$$

where  $Pe = RePr$  and  $d_{eq} = 4X$  is the equivalent diameter of the slot. It is seen from the figure that the dependences presented agree satisfactorily. The results of numerical simulation presented in Fig. 2 show how the relative Nusselt number  $Nu_j/Nu$  changes (where  $Nu_j$  is the Nusselt number at  $J' = \sum_j J'_j \neq 0$  and  $Nu$  is the Nusselt number at  $J' = 0$ )

depending on the relative density of the mass flow  $J'/J_0$  through a penetrable wall. It is seen that an increase in the density of the blown vapor leads to a decrease in the  $Nu_j$  number and an increase in the density of the exhausted gas leads to an increase in this number.

## CONCLUSIONS

1. The mathematical model and the numerical method developed allow one to calculate the dynamics of a fluid flowing in a channel with penetrable walls and the heat and mass transfer in it at different regimes of flow in this channel.

2. Comparison of results of numerical and physical experiments shows that the procedure of decreasing the rate of change in the vortex function, stream function, temperature, and component concentration of a flow in the indicated channel makes it possible to satisfactorily define the heat and mass transfer in it in the case of transient and turbulent regimes of flow on the basis of Navier–Stokes equations.

## NOTATION

$a$ , thermal diffusivity;  $b_W$ , fraction of nodes at which the rates of time change in desired functions is decreased;  $C$ , volume concentration of a mixture component;  $d$ , diameter;  $D$ , diffusion coefficient;  $g_x$  and  $g_y$ , projections of the acceleration  $g$  produced by mass forces on the axes  $x$  and  $y$ ;  $G$ , flow rate of a fluid;  $Gr$ , Grashof number;  $Gr_d$ , diffusion Grashof number;  $h_x$  and  $h_y$ , size of the pitches along the spatial coordinates  $x$  and  $y$  of a difference grid;  $I$ , number of pitches along the  $x$  axis of the difference grid;  $M$ , number of pitches along the  $y$  axis of the difference grid;  $J$ , density of a mass flow;  $l$ , size of a pitch of the difference grid with respect to time  $t$ ;  $L$ , length scale;  $P$ , pressure;  $Pr$ , Prandtl number;  $Re$ , Reynolds number;  $Sc$ , Schmidt number;  $t$ , time;  $T$ , temperature;  $u$  and  $v$ , projections of the velocity vector on the  $x$  and  $y$  axes;  $V$ , velocity scale;  $V_\eta$  and  $V_\tau$ , projections of the velocity vector on the  $\eta$  and  $\tau$  axes;  $x$ ,  $y$ , Cartesian coordinates;  $X$ , half-width of a slot channel;  $Y$ , length of a channel;  $\beta_T$ , coefficient of volumetric thermal expansion;  $\beta_j$ , coefficient of volumetric expansion as a result of a change in the volume concentration of the  $j$ th component;  $\eta$  and  $\tau$ , normal and tangent to the boundary surface;  $\theta$ , weighting factor of the difference equation;  $\lambda$ , heat conduction;  $\nu$ , kinematic viscosity coefficient;  $\rho$ , density;  $\psi$ , stream function;  $\omega$ , vortex function. Subscripts: b, boundary points; in, initial values of functions; t, turbulence; eq, equivalent quantity; ef, effective parameter;  $i$ ,  $m$ , and  $n$ , ordinal numbers of pitches of the difference grid along the coordinates  $x$ ,  $y$ , and  $t$ ;  $j$ , ordinal number of a mixture component;  $k$ , ordinal number of iterations; d, diffusion.

## REFERENCES

1. N. I. Nikitenko, *The Theory of Heat and Mass Transfer* [in Russian], Naukova Dumka, Kiev (1983).
2. A. I. Leont'ev (Ed.), *The Theory of Heat and Mass Exchange* [in Russian], Izd. MGTU im. N. E. Baumana, Moscow (1997).
3. N. I. Nikitenko, Grid method of calculating a flow of a viscous incompressible fluid and the heat exchange in it, *Inzh.-Fiz. Zh.*, **50**, No. 3, 476–482 (1986).
4. N. I. Nikitenko, Yu. N. Kol'chik, and Yu. N. Sorokovaya, Canonical-element method for simulation of hydrodynamics and heat and mass exchange in arbitrarily shaped regions, *Inzh.-Fiz. Zh.*, **75**, No. 6, 74–80 (2002).
5. P. J. Roache, *Computational Fluid Dynamics* [Russian translation], Mir, Moscow (1980).
6. N. I. Nikitenko, *Conjugate and Inverse Problems on Heat and Mass Transfer* [in Russian], Naukova Dumka, Kiev (1988).
7. V. P. Isachenko, V. A. Osipova, and A. S. Sukomel, *Heat Transfer* [in Russian], Énergoizdat, Moscow (1981).