Journal of Engineering Physics and Thermophysics, Vol. 75, No. 6, 2002

CANONICAL-ELEMENT METHOD FOR MODELING HYDRODYNAMICS AND HEAT AND MASS EXCHANGE IN ARBITRARILY SHAPED REGIONS

N. I. Nikitenko,[a] **Yu. N. Kol'chik,**[b] **and N. N. Sorokovaya**[a]

UDC 532.516:536.24

A numerical method of solution of nonstationary problems of flow and heat and mass exchange of a viscous incompressible fluid in two-dimensional multiply connected regions of an arbitrary shape with curvilinear boundaries is presented; this numerical method is based on the canonical-element method, the three-layer scaling difference scheme, and the three-layer explicit difference scheme. A method of finding the vortex function at the curvilinear boundaries of the region is proposed. Results of solution of some two-dimensional problems of hydrodynamics and heat exchange for different regimes of flow are presented.

A new approach to solution of partial differential equations for arbitrarily shaped regions which has been called the canonical-element method has been proposed in [1–3]. This approach is based on approximation of the initial difference equation by a balance equation for a canonically shaped element constructed on a uniform difference grid, and it has certain advantages over the existing numerical methods (in particular, the finite-element method) used for such problems for simplicity, universality, and exactness of solution. The finite-difference method is characterized by the fact that searching for the solution of the differential equation is replaced by finding the solution of the corresponding integral equation, i.e., the variational equation or the integral identity. A number of disadvantages are inherent in the finite-element method. The algorithm of its implementation is quite complicated, has no efficient evaluation of the error of solution results, and necessitates a large consumption of computer time and a high capacity of random-access memory. In a number of cases, the solution of the integral equation indeed may not be a solution [4] of the initial differential equation. The method, as a rule, is used to solve stationary problems. Passage to solution of nonstationary problems on the basis of the finite-element method leads to a sharp increase in the volume of computations, since it is required that the global matrix of the system be formed at each time step. Furthermore, replacement of the curvilinear boundary of the region by a broken one leads to an additional error, and discretization of the region into finite elements can be automated only for regions of a relatively simple shape.

The differential equations describing nonstationary processes of hydrodynamics and heat and mass exchange in the variables stream function ψ, vortex function ω, temperature T, and volume concentration C in divergent dimensionless form appear as

$$\frac{\partial \omega}{\partial t}+\frac{\partial u\omega}{\partial x}+\frac{\partial v\omega}{\partial y}=\frac{1}{\mathrm{Re}}\left(\frac{\partial^2 \omega}{\partial x^2}+\frac{\partial^2 \omega}{\partial y^2}\right)+\frac{\mathrm{Gr}}{\mathrm{Re}^2}\left(\frac{g_y}{g}\frac{\partial T}{\partial x}-\frac{g_x}{g}\frac{\partial T}{\partial y}\right)+\frac{\mathrm{Gr}_D}{\mathrm{Re}^2}\left(\frac{g_y}{g}\frac{\partial C}{\partial x}-\frac{g_x}{g}\frac{\partial C}{\partial y}\right), \tag{1}$$

$$\frac{\partial T}{\partial t}+\frac{\partial uT}{\partial x}+\frac{\partial vT}{\partial y}=\frac{1}{\mathrm{Re\,Pr}}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right), \tag{2}$$

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}=\frac{1}{\mathrm{Re\,Sc}}\left(\frac{\partial^2 C}{\partial x^2}+\frac{\partial^2 C}{\partial y^2}\right), \tag{3}$$

[a]Institute of Technical Thermal Physics, National Academy of Sciences of Ukraine, Kiev, Ukraine; [b]Kiev National University of Civil Engineering and Architecture, Kiev, Ukraine. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 75, No. 6, pp. 74–80, November–December, 2002. Original article submitted March 18, 2002.

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

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

Although the canonical-element method can be implemented on arbitrary nonuniform grids, it is appropriate to employ regularized grids to simplify the algorithm and to ensure the possibility of automated construction of nonuniform difference grids [2]. The grids can be regularized by placing nodal points on the grids of coordinate surfaces and lines. For the particular case of a singly connected region such a grid is determined in Cartesian coordinates by the equations

$$\begin{gathered} y_m = y_{m-1} + h_{y,m-1} \,, \quad m = 1, 2, ..., M \,, \quad y_0 = y' \,, \quad y_M = y'' \,; \\ x_{im} = x_{i-1,m} + h_{x,i-1,m} \,, \quad i = 1, 2, ..., I_m \,, \quad x_{0m} = x'_m \,, \quad x_{I_m,m} = x''_m \,; \\ t_n = t_{n-1} + h_{t,n-1} \,, \quad n = 1, 2, ..., \quad h_{tn} > 0 \,, \quad t_0 = 0 \,. \end{gathered} \tag{6}$$

Here y' and x'_m are the minimum values of the coordinates respectively: y for the points of the region and x for the points of the section of the region by the coordinate straight line y_m; y'' and x'' are the maximum values of the coordinates for the same elements of the region. The simplest form of a regularized grid is a quasiuniform grid [1] for which $h_{ym} = h_y = \text{const}$, $h_{xim} = h_{xm} = \text{const}$, and $h_{tn} = \text{const}$.

For a multiply connected region the regularized grid is constructed by subdividing it conventionally into a family of singly connected subregions. The boundary nodal points of each subregion lie at the external or internal boundaries of a body or are at a distance of a grid step along the coordinate straight line from the boundary nodal point belonging to the neighboring subregion.

For an arbitrary internal nodal point of the region the derivatives of the sought function which is contained in the initial differential equations are determined in terms of the derivatives along the normals to the boundary surfaces of a canonical element that is constructed in the vicinity of this nodal point using the coordinate surfaces of the orthogonal coordinate system. For the nodal point (x_{im}, y_m) of grid (6) the canonical element is a rectangle formed by the coordinate straight lines $x = x_{i+0.5,m}$, $x = x_{i-0.5,m}$, $y = y_{m+0.5}$, and $y = y_{m-0.5}$.

For an arbitrary difference grid the interrelationship between the derivatives $\partial W/\partial x$ and $\partial W/\partial y$ ($W = C$, T, u, v, ψ, ω) in the orthogonal coordinates (x, y) and the derivatives $\partial W/\partial x'$ and $\partial W/\partial y'$ in the direction of the nonorthogonal axes x' and y' making the angles (x, x') and (x, y'), respectively, with the x axis is determined by the differential equations of [2]. For the case of a regularized grid of the form (6) for which the angle (x, x') is equal to zero, we reduce these equations to a single equation:

$$\frac{\partial W}{\partial y} = -\left(\frac{\partial W}{\partial x} \operatorname{ctan}\,(x, y') - \frac{\partial W}{\partial y'} \frac{1}{\sin\,(x, y')} \right). \tag{7}$$

On the regularized difference grid, the derivative $\partial W/\partial x$ on the sides $x = x_{i+0.5,m}$ and $x = x_{i-0.5,m}$ is determined with an error of the order of h_{xim}^2 by the symmetric difference relations

$$\delta_x W_{i+0.5,m} = \frac{W_{i+1,m} - W_{im}}{h_{xim}} \,, \quad \delta_x W_{i-0.5,m} = \frac{W_{im} - W_{i-1,m}}{h_{x,i-1,m}} \,. \tag{8}$$

Equation (8)-based difference expressions of the derivatives $\partial W/\partial x$ and $\partial^2 W/\partial^2 x$ at the nodal point (x_{im}, y_m) have the form

$$\delta_x W_{im} = \alpha_x \delta_x W_{i+0.5,m} + (1 - \alpha_x)\, \delta_x W_{i-0.5,m}\ , \quad \delta_{xx} W_{im} = (\delta_x W_{i+0.5,m} - \delta_x W_{i-0.5,m}) / [(h_{xim} + h_{x,i-1,m})/2]\ , \tag{9}$$

where $\alpha_x = h_{x,i-1,m} / (h_{xim} + h_{x,i-1,m})$.

We find the derivative $\partial W / \partial y$ at the point $(x_{im}, y_{m+0.5})$ of the side $y = y_{m+0.5}$ of the canonical element by combining the difference approximations of Eq. (7) which are written for the cases where the y' axis intersects the coordinate straight line $y = y_{m+1}$ at the two neighboring nodal points $(x_{i'',m+1}, y_{m+1})$ and $(x_{i''+1,m+1}, y_{m+1})$ at the shortest distance from the coordinate straight line $x = x_{im}$. The difference expression of the derivative $\partial W / \partial y$ at the point $(x_{im}, y_{m+0.5})$ can be written, with an error of $O(h_{xim}^2 + h_{ym}^2)$, in the form [3]

$$\delta_y W_{i,m+0.5} = \frac{(W_{i'',m+1} - W_{im})\, h''_{x,m+1} + (W_{i''+1,m+1} - W_{im})\, h'_{x,m+1}}{h_{ym}\, (h'_{x,m+1} + h''_{x,m+1})} - \frac{h'_{x,m+1} h''_{x,m+1}}{2h_{ym}}\, \delta_{xx} W_{i,m}\ , \tag{10}$$

where $h'_{x,m+1} = x_{im} - x_{i'',m+1}$ and $h''_{x,m+1} = x_{i''+1,m+1} - x_{im}$.

The abscissas $x_{i'',m+1}$ and $x_{i''+1,m+1}$ of the nodal points $(x_{i'',m+1}, y_{m+1})$ and $(x_{i''+1,m+1}, y_{m+1})$ lying on the straight line $y = y_{m+1}$ at the shortest distance from the straight line $x = x_{im}$ are determined from the requirement of satisfaction of the condition

$$\left| x_{i'',m+1} - x_{im} \right| + \left| x_{i''+1,m+1} - x_{im} \right| = \min\left(\left| x_{s,m+1} - x_{im} \right| + \left| x_{s+1,m+1} - x_{im} \right| \right)\ , \quad s = 1, 2, ..., I_{m+1} - 1\ . \tag{11}$$

If one of the points $(x_{i'',m+1}, y_{m+1})$ or $(x_{i''+1,m+1}, y_{m+1})$ lies in the plane $x = x_{im}$, the formula for $\delta_y W_{i,m+0.5}$ becomes a symmetric difference relation analogous to the expression for $\delta_x W_{i+0.5,m}$. The difference approximation of the derivative $\partial W / \partial y$ at the point $(x_{im}, y_{m-0.5})$ of the side $y = y_{m-0.5}$ of the canonical element is written analogously to (10). The number of nodal points on the coordinate straight line $y = y_{m+1}$ that are employed in obtaining the difference expression of the derivative $\partial W / \partial y$ on the side of the canonical element can generally be increased to attain a higher accuracy; however, in so doing the algorithm of solution of the problem becomes substantially more complicated.

The difference equations of the derivatives $\partial W / \partial y$ and $\partial^2 W / \partial^2 y$ at the nodal point (x_{im}, y_m) have the form

$$\delta_y W_{im} = \alpha_y \delta_y W_{i,m+0.5} + (1 - \alpha_y)\, \delta_y W_{i,m-0.5}\ , \quad \delta_{yy} W_{im} = \frac{\delta_y W_{i,m+0.5} - \delta_y W_{i,m-0.5}}{y_{m+0.5} - y_{m-0.5}}\ , \tag{12}$$

where $\alpha_y = h_{y,m-1} / (h_{ym} + h_{y,m-1})$.

The equations of vortex and energy transfer are solved numerically on the basis of the three-layer (three-level) scaling difference scheme of [5]. Two difference equations are made to correspond to the differential equation of transfer, and the function sought is computed in two approximations at each time step. The difference equation for the first approximation is two-layer and can approximate an incomplete transfer equation in which only the convective terms and the time derivative are preserved. For the second approximation we employ a three-layer difference equation constructed by approximating all the terms of the initial differential equation. With account for the difference expressions (9) and (12) for spatial derivatives we can write the approximations of the differential equations (1)–(3) in the form

$$\delta_t \overline{\omega}_{im} + \delta_x\, (u\omega)_{im} + \delta_y\, (v\omega)_{im} = 0\ , \tag{13}$$

$$\frac{\omega_{im}^{n+1} - \omega_{im}^{n}}{h_{tn}}\, (1 + \theta_{\omega im}^{n}) - \frac{\omega_{im}^{n} - \omega_{im}^{n-1}}{h_{t,n-1}}\, \theta_{\omega im}^{n} + \delta_x\, (u\overline{\omega})_{im} + \delta_y\, (v\overline{\omega})_{im} =$$

$$= \frac{1}{\mathrm{Re}}\, (\delta_{xx} \overline{\omega}_{im} + \delta_{yy} \overline{\omega}_{im}) + \frac{\mathrm{Gr}}{\mathrm{Re}^2} \left(\frac{g_y}{g}\, \overline{T}_{im} - \frac{g_x}{g}\, \delta_y \overline{T}_{im} \right) + \frac{\mathrm{Gr}_D}{\mathrm{Re}^2} \left(\frac{g_y}{g}\, \delta_x \overline{C}_{im} - \frac{g_x}{g}\, \delta_y \overline{C}_{im} \right), \tag{14}$$

$$\delta_t \overline{T} + \delta_x\, (uT)_{im} + \delta_y\, (vT)_{im} = 0\ , \tag{15}$$

$$\frac{T_{im}^{n+1}-T_{im}^{n}}{h_{tn}}(1+\theta_{Tim}^{n})-\frac{T_{im}^{n}-T_{im}^{n-1}}{h_{t,n-1}}\theta_{Tim}^{n}+\delta_x(u\overline{T})_{im}+\delta_y(v\overline{T})_{im}=\frac{1}{\mathrm{Re\,Pr}}(\delta_{xx}\overline{T}_{im}+\delta_{yy}\overline{T}_{im}), \tag{16}$$

$$\delta_t\overline{C}+\delta_x(uC)_{im}+\delta_y(vC)_{im}=0, \tag{17}$$

$$\frac{C_{im}^{n+1}-C_{im}^{n}}{h_{tn}}(1+\theta_{Cim}^{n})-\frac{C_{im}^{n}-C_{im}^{n-1}}{h_{t,n-1}}\theta_{Cim}^{n}+\delta_x(u\overline{C})_{im}+\delta_y(v\overline{C})_{im}=\frac{1}{\mathrm{Re\,Pr}_D}(\delta_{xx}\overline{C}_{im}+\delta_{yy}\overline{C}_{im}), \tag{18}$$

where θ_{wim}^n, θ_{Tim}^n, and θ_{Cim}^n are the weight parameters. The necessary stability conditions for the solution of the difference equations (13)–(18) are found using the method of conventional definition of certain sought functions of the system [6]. For $\theta_{\gamma im}^n = 0$, $\gamma = \omega$, T, and C, when Eqs. (14), (16), and (18) are two-layer [7], the time step h_{tn}^0 must satisfy the condition

$$h_{tn}^0 \le \min\{l_V, l_\omega, l_T, l_C\}, \tag{19}$$

where $l_V = (u_{im}^n/h_{xim} + v_{im}^n/h_{ym})^{-1}$, $l_\omega = [2(1/h_{xim}^2 + 1/h_{ym}^2)/\mathrm{Re}]^{-1}$, $l_T = [2(1/h_{xim}^2 + 1/h_{ym}^2)/(\mathrm{Re\,Pr})]^{-1}$, and $l_C = [2(1/h_{xim}^2 + 1/h_{ym}^2)/(\mathrm{Re\,Pr}_D)]^{-1}$. If $l_V > l_\gamma$, owing to the parameter $\theta_{\gamma im}^n$ one can select a larger step $h_{tn} > h_{tn}^0$ in accordance with the condition $l_V \ge h_{tn} > l_\gamma$, $\gamma = \omega$, T, and C. The parameter $\theta_{\gamma im}^n$ is found from the conditions

$$\theta_{\gamma im}^n = (h_{tn}/l_\gamma - 1)/2 \quad \text{for} \quad h_{tn}/l_\gamma > 1 \quad \text{and} \quad \theta_{\gamma im}^n = 0 \quad \text{for} \quad h_{tn}/l_\gamma \le 1\,. \tag{20}$$

ensuring the stability of the numerical solution.

The equation for the stream function (4) is solved by the establishment method on each time layer with the use of the three-layer explicit difference scheme [5]. On the grid differing from (6) in that the discrete variable $t_k = t_{k-1} + h_{t,k-1}$, $k = 1, 2, ..., h_{tk} > 0$, and $t_0 = 0$ is introduced instead of the real time t_n, we write the difference approximation of Eq. (4) with an error of the order of $h_{tk} + h_{xim}^2 + h_{yim}^2$ as follows:

$$\frac{\psi_{im}^{k+1}-\psi_{im}^{k}}{h_{tk}}(1+\theta_{\psi im}^{k})-\frac{\psi_{im}^{k}-\psi_{im}^{k-1}}{h_{t,k-1}}\theta_{\psi im}^{k}=\delta_{xx}\psi_{im}^{k}+\delta_{yy}\psi_{im}^{k}-\omega_{im}^{n+1}, \tag{21}$$

where $\theta_{\psi im}^k$ is the weight parameter, $\theta_{\psi im}^k \ge 0$. Upon the arbitrary selection of the steps h_{tk}, h_{xim}, and h_{ym} we determine the values of the weight parameter $\theta_{\psi im}^k$ in accordance with the stability conditions of Eq. (21):

$$\theta_{\psi im}^k = (h_{tk}/l_\psi - 1)/2 \quad \text{for} \quad h_{tk} > l_\psi \quad \text{and} \quad \theta_{\psi im}^k = 0 \quad \text{for} \quad h_{tk} \le l_\psi\,; \tag{22}$$

here, $l_\psi = [2(1/h_{xim}^2 + 1/h_{ym}^{2)}]^{-1}$. The results of the numerical experiments have shown that the consumption of computer time by establishing the solution for the stream function is minimum when the value of the parameter $\theta_{\psi im}^k$ is 2 to 2.5; this value corresponds to a five- to sixfold increase in the time step as compared to the maximum one for an ordinary two-layer explicit difference scheme. The process of establishment of the solution of (21) is considered to be completed when the condition $\sum_i \sum_m (\psi_{im}^{k+1} - \psi_{im}^k)/h_{tk} \le \Delta$, where Δ is the small positive number, is satisfied. In this case it is assumed that $\psi_{im}^{n+1} = \psi_{im}^k$. We take $\psi_{im}^k = \psi_{im}^n$ as the initial approximation corresponding to the value $k = 0$. The components of the velocity vector u_{im}^{n+1} and v_{im}^{n+1} are determined from the difference equations following from relations (5):

$$u_{im}^{n+1} = \delta_y \psi_{im}^{n+1}, \quad v_{im}^{n+1} = -\delta_x \psi_{im}^{n+1}\,. \tag{23}$$

Difference equations on whose basis one determines the values of the sought grid functions at the boundary nodal points exert quite a substantial influence not only on the stability of a numerical solution but on its exactness as well. If the value of the stream function at a certain boundary point P_0 is ψ_0, its value ψ_1 at the point P_1 at the same boundary is determined in terms of the integral over the contour of the region:

$$\psi_1 = \psi_0 + \int_{P_0}^{P_1} (udy - vdx) \ . \tag{24}$$

Since the components u and v of the velocity vector at the boundaries of the region are considered to be specified, it is not difficult to define the function ψ_{im} for the boundary nodal points. A specific feature of the search for the values of the vortex function at the boundary points is that, formally, the boundary conditions are not specified for this region. Numerous works in which one presents different means of finding the vortex function ω at the nodal points of an orthogonal difference grid that lie at the plane boundaries of the region are analyzed in sufficient detail in [7]. These means cannot be employed for regions with curvilinear boundaries.

With the aim of obtaining difference expressions that determine the values of the vortex function at the nodal points of a nonuniform grid for an arbitrarily shaped region, we propose the following method. A Cartesian coordinate system with the origin at the boundary nodal point P_0 in question is constructed. One coordinate is directed along the internal normal n to the boundary surface at the point P_0, while the other is directed along the tangent τ. In the vicinity of P_0, we select a certain number J of nodal points P_j with the coordinates n_j, τ_j (j = 1, 2, ..., J) that are related to the coordinates x and y of the initial coordinate system by the relations $n_j = [x(P_j) - x(P_0)] \cos (n, x) + [y(P_j) - y(P_0)] \sin (n, x)$ and $\tau_j = -[x(P_j) - x(P_0)] \sin (n, x) + [y(P_j) - y(P_0)] \cos (n, x)$. For each of the points P_j, j = 1, 2, ..., J, the stream function ψ_j is expressed in terms of the values of the function ψ and its derivatives with respect to the coordinates n, τ at the point P_0 by expanding in a Taylor series in which a certain finite number of terms is retained. If the velocity vector V at the boundaries of the region is specified, for the point P_0 its projections V_n and V_τ onto the n and τ axes and their derivatives along the tangent τ should be considered to be the known quantities. This enables us, using the relations $\partial\psi/\partial n = V_\tau$, $\partial\psi/\partial\tau = -V_n$, $\partial^2\psi/\partial\tau^2 = -\partial V_n/\partial\tau$, and $\partial^2\psi/\partial n^2 = \omega + \partial V_n/\partial\tau$ which are analogous to (5), to express part of the derivatives (involved in the expansions) of the function ψ at the point P_0 in terms of the velocity components V_n and V_τ. Next, as a result of variation of the transformed expansions, we find the difference equation to compute the vortex function ω_0 at the point P_0 in terms of the values ψ_j, j = 0, 1, ..., J. The order of the error of determining the value of ω_0 is a unity lower than the order of the higher derivatives retained in the expansions of the quantities ψ_j. Let it be necessary to define the function ω_0 with an error of first order $O(n_j + \tau_j)$. Then the truncated Taylor series for the stream function ψ_j can be represented as follows:

$$\psi_j = \psi_0 + n_j \frac{\partial\psi}{\partial n} + \tau_j \frac{\partial\psi}{\partial\tau} + \frac{n_j^2}{2}\frac{\partial^2\psi}{\partial n^2} + \frac{\tau_j^2}{2}\frac{\partial^2\psi}{\partial\tau^2} + n_j\tau_j \frac{\partial^2\psi}{\partial n\partial\tau} + O\,(n_j^3 + \tau_j^3) \approx$$

$$\approx \psi_0 + n_j V_\tau - \tau_j V_n + \frac{n_j^2}{2}\left(\omega_0 + \frac{\partial V_n}{\partial\tau}\right) - \frac{\tau_j^2}{2}\frac{\partial V_n}{\partial\tau} + n_j\tau_j \frac{\partial^2\psi}{\partial n\partial\tau} \, . \tag{25}$$

This expression contains two unknown quantities: ω_0 and $\partial^2\psi/\partial n\partial\tau$. In this connection, we should set J = 2. We multiply the expressions of the form (25) written for the points P_1 and P_2 by the multipliers α_1 and α_2, respectively, to be determined and then add them together. The values of α_1 and α_2 are found from the condition that for unknown ω_0 and $\partial^2\psi/\partial n\partial\tau$ the multipliers must be equal to 1 and 0, respectively, in the expression obtained upon the addition. As a result we obtain

$$\alpha_1 = 2\left[n_1^2\left(1 - \frac{\tau_1 n_2}{\tau_2 n_1}\right)\right]^{-1} , \quad \alpha_2 = 2\left[n_2^2\left(1 - \frac{n_1\tau_2}{n_2\tau_1}\right)\right]^{-1} , \tag{26}$$

$$\omega_0 = 2\,\frac{\alpha_1(\psi_1 - \psi_0) + \alpha_2(\psi_2 - \psi_0) - A}{\alpha_1 n_1^2 + \alpha_2 n_2^2}\,, \tag{27}$$

$$A = V_\tau\,(\alpha_1 n_1 + \alpha_2 n_2) - V_n\,(\alpha_1\tau_1 + \alpha_2\tau_2) + \frac{1}{2}\frac{\partial V_n}{\partial \tau}\,[\alpha_1\,(n_1^2 - \tau_1^2) + \alpha_2\,(n_2^2 - \tau_2^2)]\,. \tag{28}$$

The numerical experiments demonstrate the reliability and efficiency of the above method of finding the vortex function at curvilinear boundaries. For a fixed impermeable wall, $V_n = V_\tau = \partial V_n / \partial \tau = A = 0$. If $\tau_1 = 0$, i.e., the point P_1 lies on the normal to the wall, then $\alpha_1 = 2/n_1^2$, $\alpha_2 = 0$, and $\omega_0 = 2(\psi_1 - \psi_0)/n_1^2$. The last difference expression for the boundary value of the vortex function was obtained in 1928 by Thom and it has been widely used up to the present for problems of incompressible fluid flow in simply shaped regions on orthogonal grids [7].

The temperature and the volume concentration at the boundary nodal points with the conditions of heat and mass exchange of the first kind are considered to be specified. With boundary conditions of the second and third kinds the derivative $\partial W/\partial n$ involved in these conditions is replaced by the sum

$$\frac{\partial W}{\partial n} = \frac{\partial W}{\partial x}\cos(x, n) + \frac{\partial W}{\partial y}\sin(x, n)\,. \tag{29}$$

The derivatives $\partial W/\partial x$ and $\partial W/\partial y$ are approximated by difference expressions analogous to (8) and (10).

A software system to model the heat exchange and hydrodynamics of an incompressible fluid in two-dimensional regions of an arbitrary shape has been created on the basis of the numerical method developed. The geometry of the region can be specified analytically or by the table of coordinates of a certain number of boundary points on whose basis one determined the coordinates of the boundary nodal points and the direction cosines of the external normals at these points by interpolation according to a special subprogram. Prior to computing the sought grid functions according to special subprograms, one also constructs coordinate sets for all the internal nodal points of the region, the weight parameters of the difference schemes, and the ordinal numbers i'' and i' of the grid points employed for finding the derivatives $\delta_y W_{i,m+0.5}$ and $\delta_y W_{i,m-0.5}$.

A substantial advantage of the calculation method that is based on the difference equations (8)–(28) is that a change in the configuration of the region leads just to re-specifying the coordinate sets for its boundary points. Some two-dimensional problems of natural convection have been solved on the basis of the constructed software system in singly connected and doubly connected formulations.

The results of calculating the fields of temperature and stream function for the stationary gravitational convection of air in a region of a rectangular cross section when the relative temperatures of the left-hand and right-hand region walls are equal to, respectively, 0 and 1 and the upper and lower walls are heat-insulated (for Grashof numbers of $1.25\cdot 10^4$ and 10^5) virtually do not differ from the data given in [8] in graphical form and obtained by the difference method. The problem of flow and heat exchange has been solved for a doubly connected region in the case where its external and internal boundaries are cylindrical surfaces whose directrices are a rectangle and a circle respectively. Such problems frequently arise in evaluating the heat loss in transportation of a hot liquid or a vapor in heat-supply systems.

In practical calculations of the thermal interaction between bodies separated by a liquid or gas layer, it is usually required that the heat flux from one body to the other be determined. In this connection, in generalizing experimental data, the complex process of stationary heat transfer through a liquid layer is replaced by the equivalent process of heat conduction [9]. The heat flux q_0 from one body to the other on condition that the liquid velocity in the layer separating them is equal to zero is determined analytically, numerically, or experimentally and it can usually be represented in the form $q_0 = \lambda(T_{b1} - T_{b2})\,f$, where f is the function of the geometric parameters of the system and T_{b1} and T_{b2} are the temperatures at the boundaries of the first and second bodies. For the case of the heat exchange between coaxial cylindrical surfaces with directrices in the form of a square with a side a and of a circle of radius R [10], we have the function $f = 2\pi/1n\,[1.08a/(2R)]$. The equivalent coefficient of thermal conductivity λ_{eq} is determined from the condition $q = \lambda_{eq}(T_{b1} - T_{b2})\,f$ in terms of the heat flux q (found experimentally or numerically) in the

TABLE 1. Fraction of Nodal Points at Which the Rate of Growth of the Vortex Function is Constrained as a Function of the Number of Nodal Points and the Rayleigh Number

Number of points $(I+1)(M+1)$	$\mathrm{Ra} = 10^7$	$\mathrm{Ra} = 10^8$	$\mathrm{Ra} = 10^9$	$\mathrm{Ra} = 10^{10}$
50×51	0.0061	0.0717	0.7855	0.8729
100×101	0	0.0055	0.4077	0.5866
150×151	0	0.0019	0.0352	0.1563
200×201	0	0.00079	0.0225	0.0472

presence of convection. The ratio $\varepsilon_{\text{conv}} = \lambda_{\text{eq}}/\lambda$ characterizes the influence of convection on the transfer of heat through the liquid layer and is a function of the Rayleigh number Ra = Gr Pr.

As the numerical experiments have shown, for a certain Rayleigh number $\mathrm{Ra} = \mathrm{Ra}^*$ corresponding to the transient regime of flow, the flow becomes nonstationary after the transient phases of the initial period. Unless the procedure of smoothing of a numerical solution is used, further increase in Ra leads to the violation of its stability. This is due to the extension of the range of variation of the function sought and involves the increase in the rate of change of these functions with time.

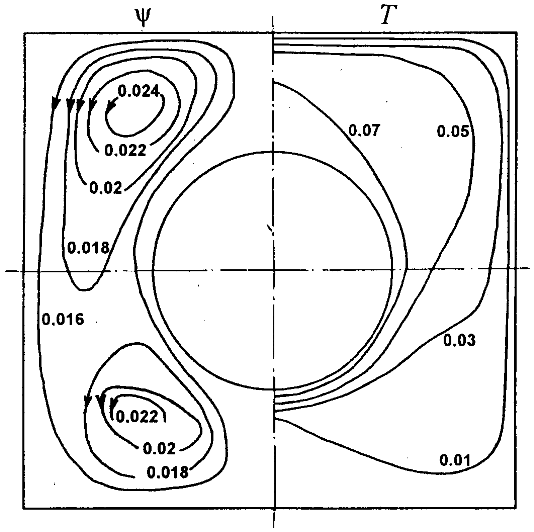
In all actual processes of flow and heat and mass exchange, the parameters of the flow (velocity, temperature, concentration of the components, and others) remain constrained as do their time derivatives. In mathematical modeling, to ensure this condition for the true values of the coefficients of kinematic viscosity ν, thermal conductivity λ, and diffusion D, one substitutes their effective values $\nu_{\text{ef}} = \nu + \nu_{\text{t}}$, $\lambda_{\text{ef}} = \lambda + \lambda_{\text{t}}$, and $D_{\text{ef}} = D + D_{\text{t}}$ into the equations of flow and heat and mass exchange; in this case $\nu_{\text{t}} \geq 0$, $\lambda_{\text{t}} \geq 0$, and $D_{\text{t}} \geq 0$. According to Eqs. (1)–(3), such a substitution leads to a decrease in all the absolute values (moduli) of the rate of change of the functions ω, T, and C in all the internal points of the region.

To ensure the stability of numerical solution of the problems of flow and heat and mass exchange for large Ra and Re numbers ($\mathrm{Ra} > \mathrm{Ra}^*$) we propose a means of imposing constraints on the rates of change of the functions sought (ω, T, C) with time at certain nodal points of the region at which these rates exceed values allowable under stability conditions. The constraint of the form

$$\frac{\partial W}{\partial t} = A_W \frac{\partial W}{\partial t} \Big/ \left| \frac{\partial W}{\partial t} \right| \quad \text{for} \quad \left| \frac{\partial W}{\partial t} \right| > A_W , \tag{30}$$

where $A_W > 0$ and $W = \omega$, T, and C, enables us to ensure the stability of the solution for any values of the Ra number. The numerical experiments have shown that for $A_T = T_{\max} - T_{\min}$, where $T_{\max}$ and $T_{\min}$ are the maximum and minimum values of the temperature at the boundaries of the region, the constrained growth in the grid function T_{im}^n is ensured for any values of the Ra number; upon the transient phases of the initial period it becomes unnecessary to impose constraint (30) on the function T for the above problems, i.e., a constraint of the form (30) imposed on T has no effect on the final result of the solution. This also holds for the function C. The quantity A_ω must also increase as the number Ra increases. A rather high reliability of the solution was ensured by selecting the quantity A_ω for the time layer $n+1$ according to the expression $A_\omega = A_{\omega 0}\tilde{\omega}^n$, where $\tilde{\omega}^n$ is the average value of the modulus of the grid function ω_{im}^n on the time layer t_n.

The degree of influence of constraint (30) on solution results is characterized by the quantity ξ defined as the ratio of the number of nodal points at which constraint on the rate of growth of the vortex function is imposed to the total number of difference-grid nodes, i.e., $(I+1)(M+1)$. For a given Ra number the dependence of the quantity ξ at the moment of establishment of solution on the parameter A_ω represents a concave curve; its curvature is relatively small at the point of minimum of ξ. This circumstance enables us to select a constant A_ω in a rather wide range of Rayleigh numbers. If the steps of the difference grid are not too coarse, it is unnecessary to constrain the rate of growth of the functions ω, T, and C for $\mathrm{Ra} \leq 10^7$. Table 1 gives results of calculating the quantity ξ at the moment of stabilization of the solution for the case of a coaxial arrangement of cylindrical surfaces with directrices in the form of a square and a circle for $R/a = 0.25$ and $A_{\omega 0} = 2$. It is clear from the table that when the Rayleigh numbers are



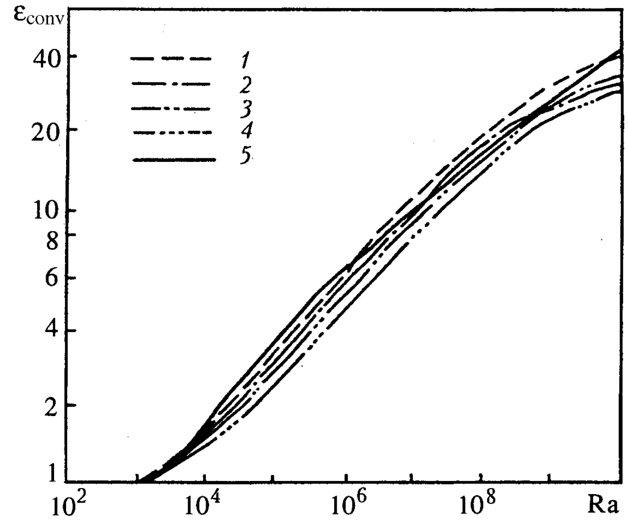


Fig. 1. Isolines of the stream function and isotherms of thermal gravitational convection of the fluid between two coaxial cylindrical surfaces with directrices in the form of a square and a circle.

Fig. 2. Dependences of the relative value of the equivalent coefficient of thermal conductivity ε_{conv} on the Rayleigh number constructed from the results of calculation of the free convection of the fluid in the region of a rectangular cross section (curve 1, $Y/X = 2$) and the region confined by cylindrical surfaces with closed directrices in the form of a square ($Y/X = 1$) and a circle of radius $R = X/4$ with the relative coordinates of the central point $\bar{x}_{cent} = x_{cent}/X$, $\bar{y}_{cent} = y_{cent}/Y$ [curve 2) $\bar{x}_{cent} = 0.5$, $\bar{y}_{cent} = 0.5$; curve 3) 0.4, 0.5; and curve 4) 0.5, 0.4] and from the experimental data (curve 5).

high the quantity ξ decreases monotonically at the moment of establishment of the solution as the total number of nodal points increases and increases with increase in the Ra number.

Figure 1 gives results of calculating the fields of the stream function and the temperature at the moment of establishment of the gravitational convection of a fluid between two coaxial cylindrical surfaces with directrices in the form of a square with a side a and a circle of radius $a/4$ and relative temperatures of 0 to 1 respectively for the Grashof number Gr = 10^5. As is seen in the figure, four vortices are formed in the flow region for this Grashof number; two vortices in the right-hand part of the region rotate clockwise and the other two vortices in the left-hand part rotate counterclockwise.

Figure 2 shows the dependence of the relative value of the equivalent coefficient of thermal conductivity ε_{conv} on the Rayleigh number in convective heat exchange in a closed region of a rectangular cross section ($0 < x < X$ and $0 < y < Y$) and a region confined by cylindrical surfaces with closed directrices in the form of a rectangle ($X \times Y$) and a circle of radius $R = X/4$. The calculation results are in agreement with the dependence (shown in the same figure) that generalizes experimental data [9] for vertical and horizontal plane slots and annular and spherical layers filled with gas or dropping liquid.

The results of the numerical experiments demonstrate the efficiency of the method proposed and the possibilities of constructing an integrated software system to model the heat exchange and hydrodynamics of an incompressible fluid in arbitrarily shaped multiply connected systems.

NOTATION

a, size of the side of the square; C, volume concentration of the components; D, diffusion coefficient; D_t, turbulent component of the diffusion coefficient; f, function of the geometric parameters of the system; g_x and g_y, projections of the vector of acceleration with a modulus g produced by the external mass force onto the x and y axes; Gr

$= g\beta L_0^3 \Delta T/\nu$, Grashof number; h_x, h_y, and h_t, steps of the difference grid along the x, y, and t axes; L_0, determining value of the dimension of the region; n, normal to the boundary surface; $\mathrm{Pr} = \nu/a$, Prandtl number; q, heat flux; q_0, heat flux from one body to another in the absence of convection; R, radius of the circle; Pr_D, diffusion Prandtl number; $\mathrm{Ra} = \mathrm{Gr}\,\mathrm{Pr}$, Rayleigh number; $\mathrm{Re} = V_0 L_0/\nu$, Reynolds number; $\mathrm{Sc} = \nu/D$, Schmidt number; t, time; T, temperature; u and v, projections of the velocity vector onto the x and y axes; V_0, determining value of the velocity (for the case of free motion it is equal to 1); V_n and V_τ, projections of the velocity vector onto the normal n and the tangent τ to the boundary surface; W, sought function of the equations of hydrodynamics and heat and mass transfer; x, y, Cartesian coordinates; $\delta_x W$, $\delta_y W$, and $\delta_t W$, difference derivatives of first order with respect to the coordinates x, y, and t; $\delta_{xx} W$ and $\delta_{yy} W$, difference derivatives of second order with respect to the coordinates x, y; $\beta = -(\partial\rho/\partial T)/\rho$, temperature coefficient of volumetric expansion; $\beta_C = -(\partial\rho/\partial C)/\rho$, diffusion coefficient of volumetric expansion; $\varepsilon_{\mathrm{conv}} = \lambda_{\mathrm{eq}}/\lambda$, relative value of the equivalent coefficient of thermal conductivity; θ, weight parameter of the difference equation; λ, thermal-conductivity coefficient; λ_{t}, turbulent component of the thermal-conductivity coefficient; λ_{eq}, equivalent thermal-conductivity coefficient; ν, coefficient of kinematic viscosity; ν_{t}, turbulent component of kinematic viscosity; ξ, fraction of nodal points at which constraint on the rate of growth of the vortex function is imposed; ρ, density of the medium; τ, tangent to the boundary surface; ψ, stream function; ω, vortex function. Subscripts: b, boundary of the region; conv, convection; eq, equivalent; ef, effective; t, turbulent; max and min, maximum and minimum values; cent, central; i, m, and n, ordinal numbers of difference-grid steps for the x, y, and t axes; k, ordinal number of iteration; 0, boundary values.

REFERENCES

1. N. I. Nikitenko, Yu. N. Kol'chik, and N. N. Nikitenko, *Inzh.-Fiz. Zh.*, **61**, No. 5, 851–857 (1991).
2. N. I. Nikitenko, *Dopovidi Nats. Akad. Nauk Ukraini* [in Ukrainian], No. 2, 55–58 (1995).
3. N. I. Nikitenko and Yu. N. Kol'chik, *Inzh.-Fiz. Zh.*, **72**, No. 5, 837–843 (1999).
4. N. S. Bakhvalov, N. P. Zhidkov, and G. M. Kobel'kov, *Numerical Methods* [in Russian], Moscow (1987).
5. N. I. Nikitenko, *Conjugate and Inverse Problems of Heat and Mass Transfer* [in Russian], Kiev (1988).
6. N. I. Nikitenko, *Heat- and Mass-Transfer Theory* [in Russian], Kiev (1983).
7. P. J. Roache, *Computational Fluid Dynamics* [Russian translation], Moscow (1980).
8. V. M. Paskonov, V. I. Polezhaev, and L. A. Chudov, *Numerical Modeling of Heat- and Mass-Transfer Processes* [in Russian], Moscow (1984).
9. V. P. Isachenko, V. A. Osipova, and A. S. Sukomel, *Heat Transfer* [in Russian], Moscow (1975).
10. S. S. Kutateladze, *Principles of Heat-Transfer Theory* [in Russian], Moscow–Leningrad (1962).