Bull. Nov. Comp. Center, Math. Model. in Geoph., 6 (2000), 55–64

A numerical algorithm for simulation of two-component flows in the Earth's mantle

Z.A. Liapidevskaya, V.E. Petrenko

The equations of motion of a two-component isothermal viscous fluid for two cases are considered, when 1) velocity–pressure and 2) stream function – vortex are taken as unknown variables. Such equations can, in particular, be used for the mathematical simulation of some geodynamic processes. The algorithm of numerical solution of the two-dimensional equations is given for the following variables: a stream function, vortex, concentration. An example of the numerical calculation is presented.

1. Equations of motion of a two-component high viscous fluid in velocity–pressure variables

We consider the model of two-component medium consisting of izothermal incompressible viscous fluid of the density ρ_{01} and of a heavy component of the density ρ_{02} and of small mass concentration C. The model is applied for simulating of slow convective flows in the Earth's mantle with the characteristic scale of 1 cm/year.

The Navier-Stokes equations may be written in the form [1]:

$$\rho\frac{d\boldsymbol{V}}{dt} = -\nabla p + \mu\nabla^2\boldsymbol{V} + \rho_{01}(1+\beta C)\mathbf{g}. \tag{1}$$

Here ρ is the density of mixture, $\boldsymbol{V}$ is the mean velocity of mixture, p is the pressure, μ is viscosity, $\mathbf{g}$ is the gravity acceleration, $\beta = (\rho_{02} - \rho_{01})/\rho_{02}$ is a relative difference of density of the particles and the fluid.

The equation for concentration takes into account the falling velocity a of particles according to the Stokes law [2]:

$$\frac{\partial C}{\partial t} + \boldsymbol{V}\nabla C = a\frac{\partial C}{\partial y}. \tag{2}$$

In the Boussinesq approximation, we obtain the following equations of motion for a two-component isothermal viscous fluid:

$$\begin{aligned} &\frac{d\boldsymbol{V}}{dt} = -\frac{1}{\rho_{01}}\nabla p + \nu\nabla^2\boldsymbol{V} + (1+\beta C)\mathbf{g}, \\ &\frac{\partial C}{\partial t} + \boldsymbol{V}\nabla C = a\frac{\partial C}{\partial y}, \qquad \operatorname{div}\boldsymbol{V} = 0, \end{aligned} \tag{3}$$

where $\nu = \mu/\rho_{01}$ is the kinematic viscosity of the first liquid component. Unknown functions in (3) are the velocity vector $\boldsymbol{V}$, the concentration C, and the pressure p.

Let us consider the following reference scales of length, velocity, density, viscosity and concentration difference: d, a, ρ_{01}, ν_0, ΔC, also considering the pressure in terms of the hydrostatic equilibrium state $\nabla p_1 = \rho_{01}\mathbf{g}$. Then in dimensionless variables, equations (3) will take the form

$$\begin{aligned} &(A_c)^{-1}\frac{d\boldsymbol{V}}{dt} = -\nabla p + \nabla^2\boldsymbol{V} - \mathrm{Ra}_c C\boldsymbol{\gamma}, \\ &\frac{\partial C}{\partial t} + \boldsymbol{V}\nabla C = \frac{\partial C}{\partial y}, \qquad \operatorname{div}\boldsymbol{V} = 0, \end{aligned} \tag{4}$$

where $\boldsymbol{\gamma}$ is the unit vector along the y axis. The set of equations (4) contains two dimensionless parameters: the Rayleigh number

$$\mathrm{Ra}_c = \frac{\beta g \Delta C d^2}{\nu_0 a} \tag{5}$$

describing the convection intensity and the sedimentation number $A_c = \nu/ad$.

At the reference velocity $a \sim 1$ cm/year, the width of a stratum $d \sim 10^3$ km and the viscosity $\mu \sim 10^{21}$ P we have $A_c \sim 10^{20}$. Therefore, the inertial terms in the Navier–Stokes equation can be omitted and (4) may be written as follows

$$\begin{aligned} &-\nabla p + \nabla^2\boldsymbol{V} - \mathrm{Ra}_c C\boldsymbol{\gamma} = 0, \\ &\frac{\partial C}{\partial t} + \boldsymbol{V}\nabla C = \frac{\partial C}{\partial y}, \qquad \operatorname{div}\boldsymbol{V} = 0. \end{aligned} \tag{6}$$

Consider the motion of mixture in the two-dimensional rectangular domain (x, y) with the length l and the height d. We search for a solution of (6) in the form

$$\boldsymbol{V}(x,y,t) = u, v, \qquad C = C(x,y,t), \qquad p = p(x,y,t).$$

Consider the boundaries of the domain as rigid walls with a slip condition of fluid. On the lower and the upper boundaries we set the condition of zero shift stress:

$$\tau_{xy} = \mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right).$$

In addition, on the side boundaries we set a symmetry condition. We consider the concentration of impurity as a given function with respect to time only at the upper boundary: $C(x, d, t) = C_0(t)$. The boundary conditions in the plane case become

$$\begin{aligned} &u = 0, \quad \frac{\partial v}{\partial x} = 0 \quad \text{at} \quad x = 0,\ L/d, \quad 0 \le y \le 1, \\ &v = 0, \quad \frac{\partial u}{\partial y} = 0 \quad \text{at} \quad y = 0,\ 1, \quad 0 \le x \le L/d, \\ &C = C_0(t) \quad \text{at} \quad y = 1, \quad 0 \le x \le L/d. \end{aligned} \tag{7}$$

2. Equations of motion of two-component high viscous fluid in stream function–vortex variables

If we eliminate from (6) the pressure term, and as new independent variables consider the stream function ψ:

$$u = -\frac{\partial \psi}{\partial y}, \qquad v = \frac{\partial \psi}{\partial x} \tag{8}$$

and the vortex

$$\xi = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}, \tag{9}$$

then we obtain the following set of equations describing the convection due to sedimentation in the Earth's mantle by variables (ψ, ξ):

$$\nabla^2 \xi = \mathrm{Ra_c} \frac{\partial C}{\partial x}, \tag{10}$$

$$\nabla^2 \psi = \xi, \tag{11}$$

$$\frac{\partial C}{\partial t} + \frac{\partial Cu}{\partial x} + \frac{\partial Cv}{\partial y} = \frac{\partial C}{\partial y}, \tag{12}$$

where $\nabla^2 = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2}$.

The boundary conditions for the variables (ψ, ξ) in a plane case are the following: The boundary conditions for the variables (ψ, ξ) in a plane case are the following:

$$\begin{aligned} &\psi = 0, \quad \xi = 0, \quad \text{at} \quad x = 0,\ L/d, \quad 0 \le y \le 1, \\ &\psi = 0, \quad \xi = 0, \quad \text{at} \quad y = 0,\ 1, \quad 0 \le x \le L/d, \\ &C = C_0(t), \quad \text{at} \quad y = 1, \quad 0 \le x \le L/d. \end{aligned} \tag{13}$$

At the time $t = 0$, inside the cavity the concentration distribution is given as:

$$C = C_1(x, y, 0). \tag{14}$$

3. Difference method for solution of mass transport equations

Let us describe the difference method of solution of (10)–(13) for a two-component highly viscous fluid. As it consists of the Poisson equations for a stream function ψ and a vortex ξ, and of the equation of mass transport for the concentration of mixture C, we should separately approximate each of these equations.

3.1. Difference scheme for the Poisson equation. Consider the Dirichlet problem for the Poisson equation in the rectangular domain G with the boundary Γ:

$$\begin{aligned} &\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\varphi(x, y), \qquad (x, y) \in G, \\ &u(x, y)|_\Gamma = g(x, y). \end{aligned} \tag{15}$$

The difference approximation for the Poisson equation is reduced to the solution of the system of linear algebraic equations $[(N-1)(M-1)]^2$ with a block three-diagonal matrix of coefficients:

$$\begin{cases} C_1 U_1 + B_2 U_2 = F_1, \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ A_i U_{i-1} + C_i U_i + B_i U_{i+1} = F_i, \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ A_{M-1} U_{M-2} + C_{M-1} U_{M-1} = F_{M-1}, \end{cases} \tag{16}$$

where $U_i = (u_{i,1}, u_{i,1}, \ldots, u_{i,N-1})^T$ is the solution of the system in the difference grid nodes, A_i, B_i, C_i are $(N-1)\times(N-1)$ matrices, F_i is the right-hand side of the system, $i = 1, \ldots, M-1$, $j = 1, \ldots, N-1$ are the internal grid nodes. Thus, A_i, B_i are diagonal matrices, and C_i is a three-diagonal matrix.

The distinct feature of the linear system of the algebraic equations (16) for a difference grid with a large number of nodes is that its sparse five-diagonal matrix has a high order. The ratio of the minimal eigenvalue σ_1 to the maximal eigenvalue σ_2 for the obtained five-diagonal matrix at mesh step $h = \text{const}$ looks like [4]:

$$\frac{\sigma_1}{\sigma_2} = \mathrm{tg}^2 \frac{\pi h}{2}.$$

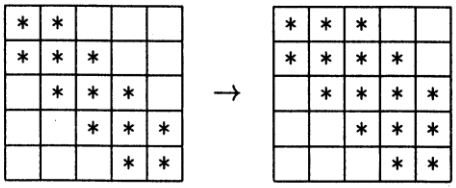
At $h \to 0$ we have

$$\frac{\sigma_1}{\sigma_2} = \frac{\pi^2 h^2}{4} + O(h^4).$$

Due to smallness of this value in the case of a large number of nodes, there is a poor conditioning of system (16). For this reason, the obvious iterative methods for solution of this system converge slowly. This fact underlines the expediency of usage of the direct methods for solution of the systems under consideration.

3.2. Method of solution of system of linear algebraic equations with a block three-diagonal matrix of coefficients. The wide-spread methods of solution of the linear equations (16) are iterative. Thus, as the given set of equations should be solved twice (for the functions ψ and ξ), and then the process is repeated for each time step, the computer costs essentially increase.

In the given paper, the direct method of solution of the block three-diagonal system (16), based on the usage of orthogonal transformations of reflection, reducing transformation of the initial matrix of the system to the two-diagonal form [5] is used. Advantages of this method are the following: the orthogonal transformations hold the norms of vectors and, consequently, the numerical errors do not increase in calculations. The conversion of a matrix is done only once, and the calculated reflection vectors are written into the initial matrix, which takes the following form:



i.e., vectors of reflection are written into a matrix having a block four-diagonal structure. The problem consists in keeping only non-zero entries of such a matrix and their further use in the process of calculation.

This method was well reasonably tested [6, 7], and it has shown sufficient stability and reliability in operation.

3.3. Difference scheme for concentration equation. Consider the equation of concentration in the following form:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = 0 \tag{17}$$

or taking into account the equation of continuity we write it as conservation law

$$\frac{\partial C}{\partial t} + \frac{\partial Cu}{\partial x} + \frac{\partial Cv}{\partial y} = 0. \tag{18}$$

This equation is approximated according to [8].

Let us consider in the plane (x, y) a rectangular grid with the mesh sizes h_x, h_y on the appropriate coordinate axes and a cell with number $(i+1/2, j+1/2)$. Let us assume the value of the function C in the cell to be constant. The purpose is to determine the value of the function C on the $n+1$ time layer by its values on the n time layer.

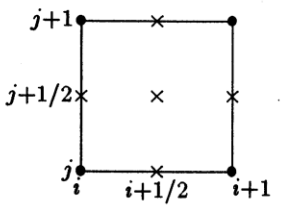


Figure 1. Gridpoints for $(i + 1/2, j + 1/2)$-th cell

To construct the difference scheme, we use the Gauss–Ostrogradskii theorem reducing the volume integral from divergence of the vector to the integral over flow through the boundary of the closed domain

$$\int_\omega \operatorname{div} \boldsymbol{a}\, d\omega = \int_\sigma \boldsymbol{n} \cdot \boldsymbol{a}\, d\sigma,$$

where ω is the volume limited by the surface σ, $\boldsymbol{n}$ is the basis vector of the external normal to the surface σ.

Integrate the equation of transport of concentration (18) for the volume ω:

$$\int_\omega \left(\frac{\partial C}{\partial t} + \frac{\partial Cu}{\partial x} + \frac{\partial Cv}{\partial y}\right) dt\, dx\, dy = \int_\sigma (C\, dx\, dy + Cu\, dt\, dy + Cv\, dt\, dx),$$

where ω corresponds to the mesh $(i + 1/2, j + 1/2)$ and the time $0, \tau$. Let us pass to the integral on the lateral boundaries. As a result, we obtain

$$(C^{n+1}_{i+1/2,j+1/2} - C^n_{i+1/2,j+1/2})h_x h_y +$$
$$\tau(Cu|^n_{i+1,j+1/2} h_y - Cu|^n_{i,j+1/2} h_y + Cv|^n_{i+1/2,j+1} h_x - Cv|^n_{i+1/2,j} h_x) = 0.$$

It follows that

$$C^{n+1}_{i+1/2,j+1/2} = C^n_{i+1/2,j+1/2} - \tau\Big[(Cu|^n_{i+1,j+1/2} - Cu|^n_{i,j+1/2})\frac{1}{h_x} +$$
$$(Cv|^n_{i+1/2,j+1} - Cv|^n_{i+1/2,j})\frac{1}{h_y}\Big] = 0. \tag{19}$$

The values u, v on the lateral boundaries of meshes are determined according to the formulas (8) using the values of the function ψ at the nodes of the grid:

$$u_{i,j+1/2} = -\frac{\psi_{i,j+1} - \psi_{i,j}}{h_y}, \qquad v_{i+1/2,j} = \frac{\psi_{i+1,j} - \psi_{i,j}}{h_x}. \tag{20}$$

The values of the function C on the lateral boundaries are determined by the velocity sign, as equation (17) is of the hyperbolic type, and the equations for characteristics have the following form:

$$\frac{dx}{dt} = u, \qquad \frac{dy}{dt} = v. \tag{21}$$

Thus, we have

$$C_{i,j+1/2} = \begin{cases} C_{i,j}, & u_{i,j+1/2} \geq 0, \\ C_{i,j+1}, & u_{i,j+1/2} < 0, \end{cases} \qquad C_{i+1/2,j} = \begin{cases} C_{i,j}, & v_{i+1/2,j} \geq 0, \\ C_{i+1,j}, & v_{i+1/2,j} < 0. \end{cases}$$

Let us consider the problem of choosing the time step. Going from the step n to the step $n+1$ we chose the interval τ so that perturbations from the nodes of the difference grid could not be outside the given mesh. According to (21), this means that in the plane case, τ should be given from the relation

$$\tau \leq \frac{h_{\min}}{\max(|u_{i,j+1/2}|, |v_{i+1/2,j}|)}, \tag{22}$$

where $h_{\min}$ is the minimum step of the spatial grid on i, j.

3.4. Algorithm of solution of the boundary value problem for (10)–(13). The boundary value problem (10)–(13) with initial conditions (14) is solved by time steps. Thus, the values of the functions ξ, ψ are calculated at the nodes of the difference grid (i, j). Concentration C is calculated at the centers of cells $(i+1/2, j+1/2)$, the horizontal component of the velocity u is calculated on the lateral boundaries, and the vertical component v is calculated on the upper and the lower boundaries of the mesh.

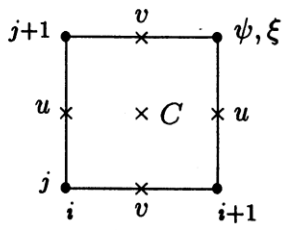


Figure 2

The algorithm of calculation has the following stages:

1. Definition of concentrations $C_{i+1/2,j+1/2}$ at an initial time $t_n = 0$ $(n = 0)$ by relations (14).
2. Calculation of a vortex $\xi_{i,j}$ $(i = 1, 2, \ldots, M-1,\ j = 1, 2, \ldots, N-1)$ using the difference approximation of the form (16) applied to the vortex equation (10).
3. Calculation of the stream function $\psi_{i,j}$ $(i = 1, 2, \ldots, M-1,\ j = 1, 2, \ldots, N-1)$ using the difference approximation of the form (16) for the stream function equation (11).

4. Calculation of the velocity components $u_{i,j+1/2}$ $(i = 0, 1, \ldots, M,\ j = 0, 1, \ldots, N-1)$ and $v_{i+1/2,j}$ $(i = 0, 1, \ldots, M-1,\ j = 0, 1, \ldots, N)$ using the difference approximations (20).

   Using the calculated values of velocity, the time step τ_n is defined according to (22) and the transition to the next time layer $t_{n+1} = t_n + \tau_n$ is carried out.

5. Calculation of the concentration $C_{i+1/2,j+1/2}$ at the next time step with the help of the difference approximation (19) for the equation of concentration transport.

6. Transition to the next step. The process lasts until t_{n+1} reaches the given maximal value T.

4. Numerical calculations

The above described method was applied for the numerical solution of some two-dimensional problems on concentration instability in the upper mantle of the Earth. As an example, we consider the problem of plume evolution.

The medium is considered as a stratum of light substance located under a stratum of a heavier one. Due to perturbations at the interface between the upper heavy fluid and the underlying light fluid, the Rayleigh–Taylor instability develops [9]. The initial configuration of layers in the rectangular domain at $t = 0$ is shown in Figure 3.

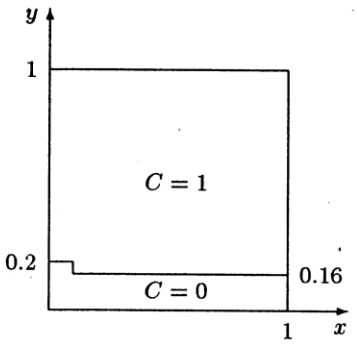


Figure 3. The initial configuration of flows at $t = 0$

The interface divides the heavy $(C = 1)$ and the light $(C = 0)$ fluids with the densities $\rho_2 = 3.315$ g/sm^3 and $\rho_1 = 3.3$ g/sm^3, the viscosity μ of fluids is equal to 10^{22} P, the width and the height of the domain being set equal to 700 km. The remaining parameters are selected so that the Rayleigh number $\mathrm{Ra}_c = 218$.

The calculations were carried out on a regular rectangular 100×100 grid.

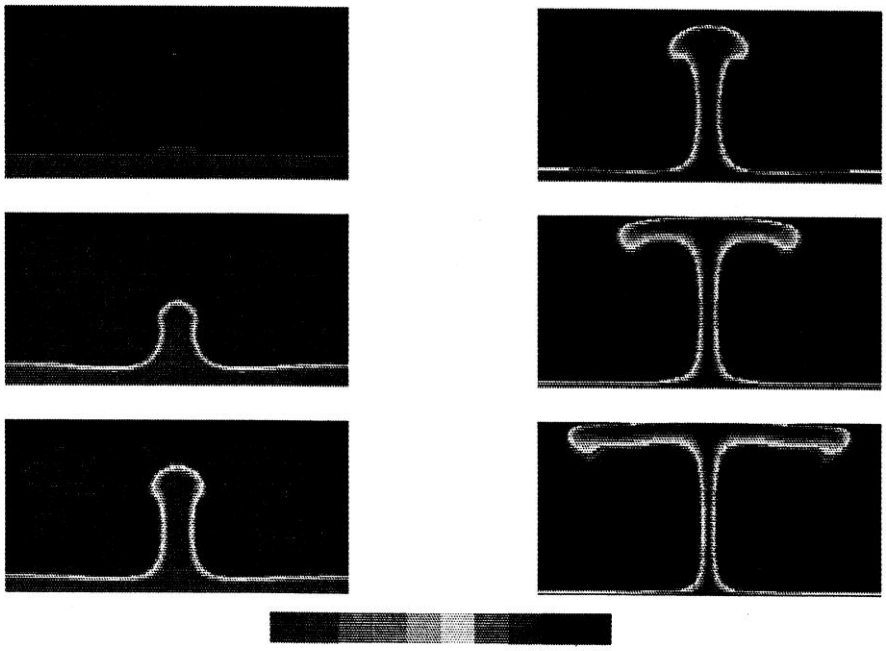


Figure 4. The concentration levels: $t = 0$, 30.3, 40.5, 49.1, 67.4, 94.4 m.y.

In Figure 4, the process of upwelling of the light fluid is shown, where it is possible to observe the creation of the plume near the symmetry axis and its spreading along the upper boundary of the domain.

References

[1] Loitsyanskii L.G. Fluid and gas mechanics. – Moscow: Nauka, 1987 (in Russian).

[2] Trubitsyn V.P., Harybin E.V. A convective instability of the sedimentation mode in the mantle // Physics of the Earth. – 1987. – № 8. – P. 21–30 (in Russian).

[3] Samarskii A.A., Nikolayev E.C. Methods of solution of grid equations. – Moscow: Nauka, 1978 (in Russian).

[4] Samarskii A.A., Gulin A.V. Numerical methods. – Moscow: Nauka, 1989 (in Russian).

[5] Godunov S.K. Solution of linear equations systems. – Novosibirsk: Nauka, 1980 (in Russian).

[6] Liapidevskaya Z.A. A complex of procedures on linear algebra. – Novosibirsk, 1980. – (Preprint / SO AN SSSR. Computing Center; 259) (in Russian).

[7] Liapidevskaya Z.A. Solution of linear algebraic equations systems by orthogonal transformations of reflection. – Novosibirsk, 1981. – (Preprint / SO AN SSSR. Computing Center; 279) (in Russian).

[8] Godunov S.K., Zabrodin A.V., Ivanov M.I., Kraiko A.N., Prokopov G.P. Numerical solution of the gas dynamics multidimensional problems. – Moscow: Nauka, 1976 (in Russian).

[9] Turkotte D., Schubert G. Geodynamics. – Moscow: Nauka, 1985 (in Russian).