MATHEMATICAL SIMULATION AND NUMERICAL METHOD FOR SOLVING GEOMIGRATION PROBLEM

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ABSTRACT

In the present paper a two-dimensional boundary value problem of geomigration taking into account convection transfer, hydrodynamic dispersion, molecular diffusion and absorption is considered. The problem is described by the system of two differential equations for the level of ground water [3] and the concentration of the contaminant in ground water [4]. For numerical solving we used the finite difference schemes taking into account the characteristic properties of the problem. The calculations were produced in conformity with concrete hydro-geological conditions. The obtained solutions are used for prognosis of contaminant migration in ground water.

Key words: mathematical simulation, numerical methods, geomigration problem, finite difference schemes

1. INTRODUCTION

The geomigration problem is a difficult problem of mathematical physics [4; 5; 7; 8; 9]. It describes main properties of the interconnected processes of the movement of ground water and contaminants caused by convective transfer, dispersion, diffusion, absorption, etc. For its solving it is necessary to investigate the system of multi-dimensional partial differential equations in the domains composite geometry and in the complex composite domains. Using the standard implicit sequential methods for non-stationary problems is inconvenient and non-perspective. Therefore for such problems it is necessary to build economic and perspective algorithms including those oriented on the parallel computers. In this paper the class of the algorithms, by which the numerical solving of geomigration problem is reduced to the realization of more
simple algorithms for simple weakly connected with each other problems in more simple subdomains is proposed in [1; 2]. Each of these algorithms is realized either sequentially or in parallel.

In this paper the absolutely stable schemes of complete approximation are proposed. Iterative and non-iterative methods for the algorithms in subdomains based on the principle of the domain decomposition are constructed.

These algorithms are explicit by virtue of a method of their implementation. The stability and the rate of the convergence of the iterative methods don’t yield analogous characteristics of the implicit algorithms.

A minimum subdomain on which the quadratic form of initial equation is written is a grid stencil. In each subdomain such important properties as approximation and conservation laws take place. The number of the equations, which are required to be solved in such subdomain, coincides with the number of the points of the stencil (boundary subdomains are excluded). The main reason of the choice of such algorithms is that many numerical methods for solving the composite problems of mathematical physics are developed for the case of simple subdomains. We note that the algorithm is essentially simplified, but the stability domain and the accuracy are not changed.

2. MATHEMATICAL MODEL

Let us consider the boundary value problem of geomigration, we take into account convective transfer, hydrodynamic dispersion, molecular diffusion, absorption.

The two-dimensional movement of ground water of constant density may be described by the partial-differential equation which has been obtained by the balance method [5; 7; 8]:

$$\frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left( T \frac{\partial H}{\partial x} \right) + \frac{\partial}{\partial y} \left( T \frac{\partial H}{\partial y} \right) + Q(H),$$

(2.1)

where $H = H(x, y, t)$ is ground-water level; $T = T(x, y, t)$ is the value of hydraulic conductivity coefficient; $\mu$ is water loss coefficient; $Q(H) = Q_R - Q_{well} + Q_a + Q_{v}$ represents sources and/or sinks of water such as flow through the river beds $Q_R$, the discharge of wells $Q_{well}$, the atmospheric precipitation $Q_a$, the deep-water circulation $Q_v$; $Q_R = T_R(H_R - H)$ ( $T_R = k_R/m_R$ is the vertical hydraulic conductivity coefficient of the river-bed deposits, $H_R$ is the water level in the river, $k_R$ and $m_R$ are the filtration coefficient and thickness of the river-bed deposits accordingly); $Q_a = Q_{inf} - Q_{evap}$ ($Q_{inf}$ is infiltration and $Q_{evap}$ is evaporation through an aeration zone); $Q_v = Q_{v}$ ( $Q_{v} = T_v(H_v - H)$ is flow from the underlying seam and $Q_v = T_v(H_v - H)$ is flow from superstratum).

When the filtration velocity is small, the velocity vector of the ground-water
Numerical simulation of the geomigration problem

Flow in a porous media is expressed by Darcy’s Law [8]

\[ \mathbf{v} = (v_x, v_y) = -k \nabla H = \left( -k \frac{\partial H}{\partial x}, -k \frac{\partial H}{\partial y} \right), \tag{2.2} \]

where \( v_x, v_y \) are components of the velocity vector; \( k \) is the filtration coefficient.

As a mathematical model of the contaminant migration we use the following equation obtained by the balance method. It describes the concentration of the contaminant in the ground-water flow:

\[ \frac{\partial C}{\partial t} + \frac{1}{\sigma} \frac{\partial N}{\partial t} = \frac{1}{\sigma} \left[ \frac{\partial}{\partial x} \left( D \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( D \frac{\partial C}{\partial y} \right) - v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} \right] + P(H), \tag{2.3} \]

where \( C = C(x, y, t) \) is the concentration of the contaminant; \( \sigma \) is the porosity; \( D = D(x, y, t) \) is the convection-diffusion coefficient which is equal

\[ D = D_m + \lambda |\mathbf{v}|, \tag{2.4} \]

here \( D_m \) is the coefficient of a molecular diffusion, \( \lambda \) is the coefficient of a hydrodynamic dispersion, \( P = P_{mf} + P_{well} + P_R \) represents sources and/or sinks of the contaminant by infiltration \( P_{mf} \), by water intake wells \( P_w \), by rivers \( P_R \). Let us suppose that

\[ P_{mf} = 0, \quad P_{well} = 0, \quad P_R = T_R(H_R - H)C_R/(\sigma_R m), \]

where \( C_R \) is the concentration of the contaminant in the river, \( H(R) \) is the water level in the river, \( m \) is the thickness of an aquifer, \( \sigma_R \) is the river porosity.

\( N \) is the concentration of the contaminant in a solid phase of a porous media and it is determined by the formula [4]

\[ \frac{\partial N}{\partial t} = \alpha(C - \beta N), \]

where \( \alpha \) is a sorption velocity coefficient, \( \beta \) is a contaminant distribution coefficient.

Taking into account the formula [4]

\[ \frac{\partial N}{\partial t} = \alpha \int_0^t \frac{\partial C}{\partial t} \exp(-\alpha \beta (t - \tau)) d\tau, \]

equation (2.3) can be modified as:

\[ \sigma \frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( D \frac{\partial C}{\partial y} \right) - v_x \frac{\partial C}{\partial x} - v_y \frac{\partial C}{\partial y} + P''(H), \tag{2.5} \]
where \( \sigma^* = \sigma \left( 1 + 1/(\sigma \beta) \right) \), \( P^*(H) = \sigma P(H) \).

Let us consider system (2.1), (2.2), (2.4), (2.5) along with initial and boundary conditions. We suppose that the aquifer under consideration has arbitrary geometry \( \Omega = \Omega(x,y) \) and open boundaries \( \partial \Omega \). Without loss of generality, boundary conditions can be represented in the following form:

\[
H = H(x,y,t)|_{\partial \Omega} = 0, \quad C = C(x,y,t)|_{\partial \Omega} = 0, \quad t > 0. \tag{2.6}
\]

At the initial time moment \( t = t_0 \) we consider the following conditions:

\[
H = H(x,y,0)|_{\Omega} = 0, \quad C = C(x,y,0)|_{\Omega} = C_0(x,y). \tag{2.7}
\]

Finally, (2.1), (2.2), (2.4), (2.5) – (2.7) lead to the system of equations describing the ground water flow and the contaminant movement in the ground water.

3. NUMERICAL METHOD

The filtration problems have a number of a specific properties [6; 8; 9; 10], which make difficulties for using standard numerical methods well suited themselves for various classes of the problems.

Constructing the difference schemes for the filtration problems we take into account such properties as composite configuration of the domain of calculation and discontinuous coefficients. It is necessary to use economic numerical algorithms in order to obtain long-term prognosis.

To construct the discrete model of system (2.1), (2.2), (2.4), (2.5) – (2.7) we use the integro-interpolational method [11].

The construction of the numerical solution of the stated problem is performed in two stages, namely, the discretization of the domain of calculation (or the construction of the difference grid) and the implementation of the discrete model.

For the simplicity of presentation without loss of generality, we shall consider a uniform grid: \( h_{x,i} = h_{y,j} = h \).

Integrating equations (2.1) and (2.5) over the control volume \( \int_{x_{i-0.5}}^{x_{i+0.5}} \int_{y_{j-0.5}}^{y_{j+0.5}} \) and using the notation from [11] it is easy to obtain the following system of difference equations:

\[
\mu H_i = (T_{-0.5x} H_x)_z + (T_{-0.5y} H_y)_y + Q_i(H), \tag{3.1}
\]

\[
\sigma^* C_i = (D_{-0.5x} C_x)_z + (D_{-0.5y} C_y)_y - v_x C_z - v_y C_y + P^*(H). \tag{3.2}
\]

Let us construct a multi-component iterative method for implementation of scheme (3.1) – (3.2), which is based on the method of domain decomposition, when grid cells are chosen as subdomains [12].
Let the grid vector-functions $W_{i,j}, \Psi_{i,j}$ are the components of the unknown functions $C$ and $H$, accordingly. These grid vector-functions are defined in the nodes of the grid cell:

$$W_{i,j} = (w_{i,j}(x_i,y_j), w_{i,j}(x_{i+1},y_j), w_{i,j}(x_{i+1},y_{j+1}), w_{i,j}(x_i,y_{j+1}))^T$$

$$= (w_{i,j}^1, w_{i,j}^2, w_{i,j}^3, w_{i,j}^4)^T,$$

$$\Psi_{i,j} = (\psi_{i,j}(x_i,y_j), \psi_{i,j}(x_{i+1},y_j), \psi_{i,j}(x_{i+1},y_{j+1}), \psi_{i,j}(x_i,y_{j+1}))^T$$

$$= (\psi_{i,j}^1, \psi_{i,j}^2, \psi_{i,j}^3, \psi_{i,j}^4)^T.$$

The elements of components are numbered from the bottom left node of the cell anticlockwise.

Numerical solving equation (3.2) presents major difficulties. Therefore, let us consider in more details the description of this part of the geomigration problem. According to the technique of MMDT [1; 2], we construct the following explicit iterative procedure

$$\sigma \left( \frac{w^{n+1}}{w^n} - w \right) / \tau + \delta A_n \left( \frac{w^{n+1}}{w^n} - w \right) + A_n w + A_{n+2} \hat{w}^*_n = P^n(\Psi), \quad (3.3)$$

$$w^0 = w_{i,j}, w^1 = w_{i+1,j}, w^2 = w_{i+1,j+1}, w^3 = w_{i,j+1}, \quad n = 1, 4,$$

where $\delta > 0$ is some iterative parameter,

$$A_1 W = 0.5h^{-1} (v_x w^0 + v_y w^1) - h^{-2} \left( \tilde{D}_{+0.5} w^2 - 2\tilde{D} w^1 + \tilde{D}_{+0.5} w^4 \right),$$

$$A_2 W = -0.5h^{-1} (v_x w^1 - v_y w^0) - h^{-2} \left( \tilde{D}_{-0.5} w^1 - 2\tilde{D} w^2 + \tilde{D}_{-0.5} w^3 \right),$$

$$A_3 W = -0.5h^{-1} (v_x w^4 + v_y w^2) - h^{-2} \left( \tilde{D}_{-0.5} w^3 - 2\tilde{D} w^4 + \tilde{D}_{-0.5} w^1 \right),$$

$$A_4 W = 0.5h^{-1} (v_x w^3 - v_y w^4) - h^{-2} \left( \tilde{D}_{-0.5} w^1 - 2\tilde{D} w^4 + \tilde{D}_{+0.5} w^3 \right),$$

$v_x = v_x(i,j), v_y = v_y(i,j); A_{i+4} = A_i, W = W_{i,j}$, the component $W_n^*$ is diagonally opposite to $W_{i,j}$ with respect to the node, in which the element $w^0$ of the component $W_{i,j}$ is defined (for example, $W_1 = W_{i-1,j-1}, W_2^* = W_{i+1,j-1}$ and etc),

$$\tilde{D}_{+0.5} = \tilde{D}_{i+0.5,j} = 0.5(D(x_{i+1},y_j) + D(x_i,y_{j+1})), \quad \tilde{D}_{-0.5} = \tilde{D}_{i-0.5,j} = 0.5(D(x_{i-1},y_j) + D(x_i,y_{j+1})),

\tilde{D}_{+0.5} = \tilde{D}_{i+0.5,j} = 0.5(D(x_{i+1},y_{j+1}) + D(x_i,y_{j-1})), \quad \tilde{D}_{-0.5} = \tilde{D}_{i-0.5,j} = 0.5(D(x_{i-1},y_{j+1}) + D(x_i,y_{j-1})),

\tilde{D} = 0.5(\tilde{D}_{i+0.5,j} + \tilde{D}_{i-0.5,j}), \quad \tilde{D} = 0.5(\tilde{D}_{i+0.5,j} + \tilde{D}_{i-0.5,j}).
In the case of two-dimensional domain $\Omega = \Omega \cup \partial \Omega$ there are 15 types of the grid cells (see Fig.1).

In the case of the internal cell (see Fig.1 I) for finding $\hat{w}_{i,j}^{+1}$ from equations (3.3) we obtain the system of four linear algebraic equations for the unknowns $w^1, w^2, w^3, w^4$:

$$M^{+1} \hat{w} = F,$$

(3.4)

where

$$m_{11} = \sigma^*/\tau + 2\hat{D}_{i,j}\delta/h^2, \quad m_{22} = \sigma^*/\tau + 2\hat{D}_{i+1,j}\delta/h^2,$$

$$m_{33} = \sigma^*/\tau + 2\hat{D}_{i+1,j+1}\delta/h^2, \quad m_{44} = \sigma^*/\tau + 2\hat{D}_{i,j+1}\delta/h^2,$$

$$m_{13} = m_{31} = m_{24} = m_{42} = 0, \quad m_{12} = \delta(-\hat{D}_{i-0.5,j}/h + 0.5v_x)/h,$$

$$m_{21} = \delta(-\hat{D}_{i+0.5,j}/h - 0.5v_x)/h, \quad m_{23} = \delta(-\hat{D}_{i+1,j+0.5}/h + 0.5v_y)/h,$$

$$m_{32} = \delta(-\hat{D}_{i+1,j+0.5}/h - 0.5v_y)/h, \quad m_{14} = \delta(-\hat{D}_{i,j-0.5}/h + 0.5v_y)/h,$$

$$m_{41} = \delta(-\hat{D}_{i,j+0.5}/h - 0.5v_y)/h, \quad m_{34} = \delta(-\hat{D}_{i+0.5,j+1}/h - 0.5v_x)/h,$$

$$m_{43} = \delta(-\hat{D}_{i+0.5,j+1}/h + 0.5v_x)/h,$$

$$f_1 = P^*(w^1) + \sigma^* w^1/\tau + 2\hat{D}_{i,j}\delta w^1/h^2 + m_{12} w^2 + m_{14} w^4$$

$$+ L_1(i,j) + L_3(i,j),$$

$$f_2 = P^*(w^2) + \sigma^* w^2/\tau + 2\hat{D}_{i+1,j}\delta w^2/h^2 + m_{21} w^1 + m_{23} w^3,$$
Numerical simulation of the geomigration problem

\[ f_3 = P^* (w^3) + \sigma^* w^3 / \tau + 2 \tilde{D}_{t+1, j+1} \delta w^3 / h^2 + m_{32} w^2 + m_{34} w^4 \\
+ L_1 (i + 1, j + 1) + L_3 (i + 1, j + 1), \]

\[ f_4 = P^* (w^4) + \sigma^* w^4 / \tau + 2 \tilde{D}_{t,j+1} \delta w^4 / h^2 + m_{41} w^1 + m_{43} w^3 \\
+ L_2 (i, j + 1) + L_4 (i, j + 1), \]

\[
L_1 (i, j) = \left( \tilde{D}_{t+0.5,j} w_{i,j}^2 - 2 \tilde{D}_{t,j} w_{i,j}^1 + \tilde{D}_{t,j+0.5} w_{i,j}^1 \right) / h^2 \\
- 0.5 h^{-1} (v_x (i + 0.5, j) w_{i,j}^2 + v_y (i, j + 0.5) w_{i,j}^1),
\]

\[
L_2 (i, j) = \left( \tilde{D}_{t+0.5,j} w_{i+1,j}^2 - 2 \tilde{D}_{t,j} w_{i+1,j}^1 + \tilde{D}_{t,j+0.5} w_{i+1,j}^1 \right) / h^2 \\
+ 0.5 h^{-1} (v_x (i - 0.5, j) w_{i+1,j}^2 + v_y (i, j + 0.5) w_{i+1,j}^1),
\]

\[
L_3 (i, j) = \left( \tilde{D}_{t+0.5,j} w_{i-1,j}^2 - 2 \tilde{D}_{t,j} w_{i-1,j}^1 + \tilde{D}_{t,j+0.5} w_{i-1,j}^1 \right) / h^2 \\
+ 0.5 h^{-1} (v_x (i - 0.5, j) w_{i-1,j}^2 + v_y (i, j - 0.5) w_{i-1,j}^1),
\]

\[
L_4 (i, j) = \left( \tilde{D}_{t+0.5,j} w_{i,j-1}^2 - 2 \tilde{D}_{t,j} w_{i,j-1}^1 + \tilde{D}_{t,j+0.5} w_{i,j-1}^1 \right) / h^2 \\
- 0.5 h^{-1} (v_x (i + 0.5, j) w_{i,j-1}^2 - v_y (i, j - 0.5) w_{i,j-1}^1),
\]

\[
v_z (i \pm 0.5, j) = 0.5 (v_x (i \pm 1, j) + v_x (i, j)), v_y (i \pm 0.5, j) = 0.5 (v_y (i \pm 1, j) + v_y (i, j)),
\]

\[
v_z (i, j \pm 0.5) = 0.5 (v_x (i, j \pm 1) + v_x (i, j)), v_y (i, j \pm 0.5) = 0.5 (v_y (i, j \pm 1) + v_y (i, j)).
\]

The solution of system (3.4) can be written in the form

\[
\frac{w^1_{i+1}}{w^1} = \frac{\Delta}{\Delta}, \quad \frac{w^2_{i+1}}{w^2} = \frac{\Delta}{\Delta},
\]

\[
\frac{w^3_{i+1}}{w^3} = p_0 - p_1 \cdot \frac{\Delta}{\Delta} - p_2 \Delta^2 / \Delta, \quad \frac{w^4_{i+1}}{w^4} = t_0 - t_1 \cdot \frac{\Delta}{\Delta} - t_2 \Delta^2 / \Delta,
\]

where \( \Delta = ad - cb, \Delta_1 = ed - fb, \Delta_2 = af - ce, \)

\[
a = -m_{33} p_1 - m_{34} t_1, b = m_{32} - m_{33} p_2 - m_{34} t_2, c = m_{41} - m_{43} p_1 - m_{44} t_1,
\]

\[
d = -m_{43} p_2 - m_{44} t_2, e = f_3 - m_{33} p_0 - m_{34} t_0, f = f_4 - m_{43} p_0 - m_{44} t_0,
\]

\[
p_0 = f_2 / m_{33}, p_1 = m_{21} / m_{23}, p_2 = m_{22} / m_{23},
\]

\[
t_0 = f_1 / m_{44}, t_1 = m_{11} / m_{14}, t_2 = m_{12} / m_{14}.
\]

We get a similar system for finding the elements of the component \( \tilde{w}^{i+1}_{i,j} \) for any internal cell.

In the case of boundary cells \((i,j)\) (Fig. 1, II-IV) the values of the elements of the component \( \tilde{w}^{i+1}_{i,j} \) in the boundary nodes are determined from
the boundary conditions. Here the dimension of the system of equations for
determination of the unknown elements of the component \( \bar{W}_{i,j} \) is reduced to
3 for cells of the IV-kind, to 2 for cells of the II-kind and to 1 for cells of the
III-kind.

After calculations at all cells of the grid domain (including the boundary
cells) as a solution on \( k + 1 \) time step we can take arithmetic mean of the
elements of the solution components related with the same node of the grid:

\[
\bar{w}^{k+1} = w(x_i, y_j, t_{k+1}) = \frac{1}{4} \left( w^{k+1}_{i,j} + w^{k+1}_{i-1,j} + w^{k+1}_{i-1,j-1} + w^{k+1}_{i,j-1} \right).
\]

A method for numerical solving (3.1) is constructed similarly. Taking into ac-
count the discussion given above, the procedure of finding numerical solution
of the problem consists of the following stages:
1. Solve (2.1) and find the level function \( H \) in the domain of the calculation ;
2. Find the filtration velocity from formula (2.1);
3. Find approximate solution of equation (2.5) for concentration of the conta-
naminant \( C \) in the grid domain using the obtained level function \( H \) and the
filtration velocity \( v \);
4. Transit to the next time level;

<table>
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<td>Hydrogeological and hydrochemical parameters of an aquifer.</td>
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<td><strong>Concentration of contaminant in the river</strong></td>
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<td><strong>River porosity</strong></td>
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</table>

The applied programs have been written in Fortran. Let us formulate some
properties of the described numerical algorithm. Schemes (3.1), (3.2) are abso-
lutely stable and the order of their accuracy is \( O(\tau + h^2) \). The method
is implemented as the explicit algorithm. It has practically unlimited possi-
bilities of parallelization (at each time step all components are calculated inde-
pendently from each other by the explicit formulas). The method can be
used for the domains of arbitrary composite geometry (not only rectangular
and multiply connected) and in the case of the three-dimensional problems.
4. RESULTS AND DISCUSSION

Figure 2. Ground-water level \( H \) at time 5 years.

Figure 3. Forecast of the contaminant migration in ground water after 5 years: a) contaminated domain, b) ground-water contaminant concentration.

The represented model allows us to simulate processes of the movement of ground water and contaminants taking into account advective transfer of chemically non-active contaminants in ground water, percolation through hydrogeological "windows", dispersion, diffusion, evaporation and etc. It takes into account arbitrary geometry of filtration field and arbitrary boundary conditions, various hydrogeological and hydrochemical parameters of calculated aquifer, a variety of features and processes such as rivers, wells, evapotranspiration, recharge from precipitation, information on the sources of contamination, etc. With the help of our model it is possible to forecast the contaminant migration in the ground-water flow at arbitrary time moment.

In Table 1 hydrogeological and hydrochemical parameters of simulated aquifer are presented. Let us present some results of numerical experiments. For example consider the rectangular domain \( 2250 \text{m} \times 2500 \text{m} \) with one water intake well at point \((1125m, 1125m)\) and the river on the line \( y = 500m \). In Fig.2 the results of simulation of the ground-water level are presented. Fig.3 illustrates the distribution of the contaminant in the simulated aquifer system at time 5 years if there is a source of the contaminant with intensity
$C_0 = 0.05g/l$ at the three points of the domain $(875m, 500m)$, $(1125m, 500m)$, $(1425m, 500m)$ at the initial time moment $t = 0$.

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Geomigracijos uždavinio matematinis modeliavimas ir skaitiniai metodai

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Šiame straipsnyje nagrinėjama dvimatis kūrėtis geomigracijos uždavinys, kai atsižvelgiama į konvekcinį perėmimą, hidrodinaminę dispersiją, molekulišką difuziją. Šis uždavinys aptiko dvi dujų differencialinių lyginių sistemų grupę vandenį ir užterštumo koncentracijos vandenyje. Šiam uždavinio spręsti taikomas baigtinių skirtumų metodas atsižvelgiant į uždavinio charakteristikines savybes. Skaičiavimai buvo atlikti su konkrečiomis hidrogeologinėmis sąlygomis. Gauti sprendiniai gali būti naudojami prognozuojant užterštumo judėjimą gruntiniame vandenyje.