MATHEMATICAL MODELING OF GEOFILTRATION AND GEOMIGRATION PROCESSES IN MULTILAYER SYSTEMS

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Abstract — Numerical methods for simultaneous solution of geofiltration and geomigration problems in multilayer systems in contaminant transport investigation have been developed. A multilayer system consists of several aquifers separated by weakly permeable layers. Mathematical models are constructed under the following assumption: longitudinal flows predominate in the aquifer and crossflows — in the separation layers. The mass transfer is described by the convection and diffusion equations.

The implicit finite volume difference schemes were used. The computational algorithm is based on the concept of splitting the schemes on physical processes of two-dimensional filtration and contaminant transport along aquifers and vertical transport through the separation levels.

An iterative method of the block Gauss — Seidel type for the realization of implicit finite difference schemes for geofiltration and geomigration problems in the presence of wells and contaminant sources has been constructed. The method is based on the perturbation transfer from cells with sources (wells and sources of contaminant). The iterative process for update of unknowns has been constructed taking into account the position of a cell relative to the calculated cells.

The results of the numerical experiment on modeling groundwater flows redistribution and contaminant migration in system of two aquifers with operating wells are presented.

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1. Introduction

Estimation of the influence of a groundwater intake on the hydrogeological conditions of the adjoining territory is an important problem. As a result of intensive groundwater withdrawal, extensive depression cones are generated in ground and confined aquifers, and natural underground flows are deformed. This leads to a change in the water balance of the adjacent territory, groundwater reserve depletion, a reduction of river flows up to the drying up of rivers, pollution of exploitable aquifers, and a deterioration of the water quality at drinking water supply intakes.

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An important part of the groundwater protection problem is the development of computational methods for forecasting the contaminant migration. The geological and hydrogeological features of a territory such as the presence of interconnected aquifers with different filtration properties, superficial reservoirs and infiltration should be taken into account in the numerical investigation.

In modeling a groundwater filtration in multilayer systems with aquifers separated by semipermeable layers, we supposed that the longitudinal flows predominated in the aquifer and the crossflows — in the separation layers (Myatiev — Girinsky model) [8]. In mathematical modeling of filtration in aquifers based on plane filtration models, the filtration parameters are averaged over the aquifer thickness.

At present for numerical solution of the mass transfer problem in groundwaters the finite difference and finite element methods are used [2, 3, 6, 11]. For more detailed studies of the flows in the vicinity of well rigorous well models were used for Darcy [9] and Forchheimer [5] flows. In [4], an upscaling technique was proposed for steady flow transport through highly heterogeneous porous media driven by extraction wells.

The absolutely stable additive difference schemes with splitting according to physical processes were applied to the problem of plane filtration in a multilayer system [1]. Parallel algorithms connected with the filtration problem solution (one water-carrying layer per processor) were constructed.

In this paper, for solving the problem of long-term forecast of contaminant migration in multi-aquifer systems, implicit finite volume difference schemes are proposed. The computational algorithm is based on the splitting of the schemes on two physical processes (plane filtration in the aquifers and vertical transport through semipermeable separation levels).

An iterative method for the realization of the implicit finite difference schemes for geofiltration and geomigration problems in the presence of wells and contaminant sources has been developed. The method is based on the perturbation transfer from cells with sources (wells and sources of contaminant). The iterative process with implicit approximation of fluxes in cells with sources are used. For the other cells the iterative process takes into account their locations with respect to the calculated ones.

The results of the numerical experiment on the modeling of groundwater flows redistribution and contaminant migration in system of two aquifers with operating wells are presented.

2. Geofiltration problem in multiaquifer system

The governing equations of the groundwater flow in a multilayer system (p aquifers are divided by $p - 1$ weakly penetrating layers) can be written as the following system of partial differential equations:

$$\mu_1 \frac{\partial H_1}{\partial t} = \frac{\partial}{\partial x} \left(T_{11} \frac{\partial H_1}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_{12} \frac{\partial H_1}{\partial y} \right) + G_r (H_r - H_1) + \omega + \varepsilon - G_{12} (H_1 - H_2) - Q_{1w}, \quad (2.1)$$

$$\begin{aligned} \mu_\alpha \frac{\partial H_\alpha}{\partial t} = & \frac{\partial}{\partial x} \left(T_{\alpha 1} \frac{\partial H_\alpha}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_{\alpha 2} \frac{\partial H_\alpha}{\partial y} \right) + G_{\alpha-1, \alpha} (H_{\alpha-1} - H_\alpha) - \\ & - G_{\alpha, \alpha+1} (H_\alpha - H_{\alpha+1}) - Q_{\alpha w}, \quad \alpha = \overline{2, p-1}, \end{aligned} \quad (2.2)$$

$$\mu_p \frac{\partial H_p}{\partial t} = \frac{\partial}{\partial x} \left(T_{p1} \frac{\partial H_p}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_{p2} \frac{\partial H_p}{\partial y} \right) + G_{p, p-1} (H_{p-1} - H_p) - Q_{pw},$$

$$Q_{aw} = \sum_k Q_{\alpha k}(t) \delta(x - x_{\alpha k}^*) \delta(y - y_{\alpha k}^*), \quad (x, y) \in D_{xy}, \quad t \geq 0. \quad (2.3)$$

Here $H_\alpha(x, y, t)$ is the groundwater level at point (x, y) of the aquifer α , $\alpha = 1, \dots, p$ at time t ; $T_{\alpha 1}(x, y)$, $T_{\alpha 2}(x, y)$ are the hydraulic conductivities (aquifer transmissivity) in the directions x, y ; $\mu_\alpha(x, y)$ is the specific yield; $G_{\alpha, \beta}(x, y) = k_{\alpha, \beta} m_{\alpha, \beta}$, $\beta = \alpha \pm 1$ is the vertical conductivity of a semipermeable separation layer ($G_{\alpha, \beta} = G_{\beta, \alpha}$); $k_{\alpha, \beta}$, $m_{\alpha, \beta}$ are the filtration coefficient and the thickness of the separation layer, $Q_{\alpha k}(t)$ are the rates of wells, G_r is the vertical conductivity of underchannel deposits, H_r is the water level in the river, ω , ε are the infiltration and evaporation rates.

The specific yields and transmissivities of aquifers depend on the filtration regime (see Fig. 2.1). For the confined filtration $T_{\alpha 1} = k_{\alpha 1} m_\alpha$, $T_{\alpha 2} = k_{\alpha 2} m_\alpha$, $\mu_\alpha = \mu_\alpha^*$, $s_\alpha < M_{\alpha-1}$, and for the unconfined filtration $T_{\alpha 1} = k_{\alpha 1} (m_\alpha - (s_\alpha - M_{\alpha-1}))$, $T_{\alpha 2} = k_{\alpha 2} (m_\alpha - (s_\alpha - M_{\alpha-1}))$, $\mu_\alpha = \mu_\alpha^{**}$, $M_{\alpha-1} < s_\alpha \leq M_{\alpha-1} + m_\alpha$. Here $k_{\alpha 1}$, $k_{\alpha 2}$ are the filtration coefficients in the x and y directions, m_α is the aquifer thickness, $s_\alpha = H_\alpha(x, y, 0) - H_\alpha(x, y, t)$ is the recession of the level, $M_{\alpha-1} = \sum_{p=1}^{\alpha-1} (m_p + m_{p-1, p})$.

Fig. 1.1. Filtration regimes

For the system of equations (2.1) – (2.3), the distribution of groundwater levels in aquifers at the initial instant of time $t = 0$ is given by

$$H_\alpha(x, y, 0) = H_\alpha^0(x, y), \quad (x, y) \in D_{xy}.$$

In the part Γ_1 of the boundary ∂D_{xy} one can give the levels (Dirichlet type boundary conditions)

$$H_\alpha(x, y, t) = f_\alpha(x, y, t), \quad (x, y) \in \Gamma_1,$$

and in the other part Γ_2 the fluxes (Neumann type boundary conditions)

$$T_\alpha \frac{\partial H_\alpha}{\partial n}(x, y, t) = g_\alpha(x, y, t), \quad (x, y) \in \Gamma_2,$$

where n is the external normal to Γ_2 .

3. Difference schemes for the geofiltration problem

In the domain $\bar{D}_{xy} \times [0, T]$, let us introduce a rectangular difference grid $\omega_\tau \times \omega_h$ with space steps h_x, h_y and a time step τ

$$\omega_\tau = \{t^n : t^n = n\tau, n = 0, 1, \dots\},$$

$$\omega_h = \{(x_i, y_j) : x_{i+1} = x_i + h_{x,i}, i = \overline{1, N_x}, y_{j+1} = y_j + h_{y,j}, j = \overline{1, N_y}\}.$$

The grid functions of levels $H_{\alpha,i,j}^n = H_\alpha(x_{i+0.5}, y_{j+0.5}, t^n)$ are determined at the cell centers, while the grid function of flows are evaluated at the centers of the cell edges

$$W_E = T_{\alpha 1}^+ H_{\alpha,x} = T_{\alpha 1,i,j+0.5} (H_{\alpha,i+1,j} - H_{\alpha,i,j}) / (x_{i+1.5} - x_{i+0.5}),$$

$$W_W = T_{\alpha 1} H_{\alpha,\bar{x}} = T_{\alpha 1,i,j+0.5} (H_{\alpha,i,j} - H_{\alpha,i-1,j}) / (x_{i+0.5} - x_{i-0.5}),$$

$$W_N = T_{\alpha 2}^+ H_{\alpha,y} = T_{\alpha 2,i+0.5,j+1} (H_{\alpha,i,j+1} - H_{\alpha,i,j}) / (y_{j+1.5} - y_{j+0.5}),$$

$$W_S = T_{\alpha 2} H_{\alpha,y} = T_{\alpha 2,i+0.5,j} (H_{\alpha,i,j} - H_{\alpha,i,j-1}) / (y_{j+0.5} - y_{j-0.5}).$$

On the grid $\omega_\tau \times \omega_h$ the differentiation operator from (2.1) – (2.3)

$$LH_\alpha = \frac{\partial}{\partial x} \left(T_{\alpha 1} \frac{\partial H_\alpha}{\partial x} \right) + \frac{\partial}{\partial y} \left(T_{\alpha 2} \frac{\partial H_\alpha}{\partial y} \right)$$

is approximated by the following difference operator:

$$L_h H_\alpha = (W_E - W_W) / (x_{i+1} - x_i) + (W_N - W_S) / (y_{j+1} - y_j).$$

To construct the difference schemes, we used the schemes splitting on the physical processes [1]. At the first half-step we consider the liquid transfer in the aquifers

$$\begin{aligned} \mu_\alpha \frac{H_\alpha^{n+1/2} - H_\alpha^n}{\tau} &= L_h H_\alpha^{n+1/2} + \varphi_\alpha, \quad \varphi_\alpha = \begin{cases} \omega + \varepsilon - Q_{1w,h}, & \alpha = 1, \\ -Q_{\alpha w,h}, & \alpha \neq 1, \end{cases} \\ Q_{\alpha w,h} &= \begin{cases} \sum_k Q_{\alpha k}(t^{n+1}) / h_{x,i} h_{y,j}, & (x_{\alpha k}^*, y_{\alpha k}^*) \in [x_i, x_{i+1}] \times [y_j, y_{j+1}], \\ 0, & (x_{\alpha k}^*, y_{\alpha k}^*) \notin [x_i, x_{i+1}] \times [y_j, y_{j+1}], \end{cases} \end{aligned} \quad (3.1)$$

and at the second vertical transport through dividing layers —

$$\mu_\alpha \frac{H_\alpha^{n+1} - H_\alpha^{n+1/2}}{\tau} = G_{\alpha-1,\alpha} (H_{\alpha-1}^{n+1} - H_\alpha^{n+1}) - G_{\alpha,\alpha+1} (H_\alpha^{n+1} - H_{\alpha+1}^{n+1}), \quad (3.2)$$

for each (i, j) , $i = \overline{1, N_x}$, $j = \overline{1, N_y}$.

The systems of three-point equations (3.2) for $p > 2$ are solved by the Thomas algorithm in the z direction. For implementation of the implicit difference scheme (3.1), the iterative process

$$\mu_\alpha \frac{H_\alpha^{s+1} - H_\alpha^n}{\tau} = \frac{1}{h_{x,i}} \left(T_{\alpha 1}^{s+1} H_{\alpha,x}^s - T_{\alpha 1}^s H_{\alpha,\bar{x}}^{s+1} \right) + \frac{1}{h_{y,j}} \left(T_{\alpha 2}^{s+1} H_{\alpha,y}^s - T_{\alpha 2}^s H_{\alpha,\bar{y}}^{s+1} \right) + \varphi_\alpha$$

can be used. It leads to the necessity of solving on each iterative step the five-point system of difference equations. In the present work, for solving (3.1) an iteration algorithm has been developed. The algorithm takes into account the particularities of the problem (the presence of wells in the computational domain). At each iteration step of the proposed algorithm the systems of three-point equations are solved by the Thomas algorithm.

4. Computational algorithm

The proposed algorithm belongs to the block iteration methods for solving systems of difference equations. In such algorithms, the subgroups of unknowns are chosen. The values of these unknowns are determined from the systems of equations by the elimination method. If ordering of the unknowns along the coordinate lines is used, the systems of three-point equations are solved sequentially.

In the proposed algorithm, the block includes the grid functions in cells combined in contour. These contours surrounding the cells with perturbations sequentially. For geofiltration problems the computational contours are constructed from cells with wells.

All cells $\Omega_{ij} = \{(x_j, y_j) : i = \overline{1, N_x}, j = \overline{1, N_y}\}$ are grouped into closed and open contours $L_k = \{\vec{x}_l\}, x_l \in \Omega_{ij}, l = \overline{1, N_k}$ and $\Omega_{ij} = \bigcup_k L_k$. The problem solution is reduced to the successive determination of the unknowns on the contours L_k .

We introduce cell codes in order to denote the type of approximation of flows through the cell edges. The flows belonging to current or previous contours are approximated implicitly.

Depending on the cell code k_{cell} , the difference operator $L_h^{s+1} H_\alpha$ is given by the following expressions for the nonboundary cells:

$$L_h^{s+1} H_\alpha = \begin{cases} (\bar{W}_E^{s+1} - \bar{W}_W^s)/(x_{i+1} - x_i) + (\bar{W}_N^{s+1} - \bar{W}_S^s)/(y_{j+1} - y_j), & k_{\text{cell}} = 1, \\ (\bar{W}_E^{s+1} - \bar{W}_W^s)/(x_{i+1} - x_i) + (\bar{W}_N^{s+1} - \bar{W}_S^s)/(y_{j+1} - y_j), & k_{\text{cell}} = 2, \\ (\bar{W}_E^{s+1} - \bar{W}_W^{s+1})/(x_{i+1} - x_i) + (\bar{W}_N^{s+1} - \bar{W}_S^s)/(y_{j+1} - y_j), & k_{\text{cell}} = 3, \\ (\bar{W}_E^s - \bar{W}_W^{s+1})/(x_{i+1} - x_i) + (\bar{W}_N^{s+1} - \bar{W}_S^s)/(y_{j+1} - y_j), & k_{\text{cell}} = 4, \\ (\bar{W}_E^s - \bar{W}_W^{s+1})/(x_{i+1} - x_i) + (\bar{W}_N^{s+1} - \bar{W}_S^{s+1})/(y_{j+1} - y_j), & k_{\text{cell}} = 5, \\ (\bar{W}_E^s - \bar{W}_W^{s+1})/(x_{i+1} - x_i) + (\bar{W}_N^s - \bar{W}_S^{s+1})/(y_{j+1} - y_j), & k_{\text{cell}} = 6, \\ (\bar{W}_E^{s+1} - \bar{W}_W^{s+1})/(x_{i+1} - x_i) + (\bar{W}_N^s - \bar{W}_S^{s+1})/(y_{j+1} - y_j), & k_{\text{cell}} = 7, \\ (\bar{W}_E^{s+1} - \bar{W}_W^s)/(x_{i+1} - x_i) + (\bar{W}_N^s - \bar{W}_S^{s+1})/(y_{j+1} - y_j), & k_{\text{cell}} = 8, \\ (\bar{W}_E^{s+1} - \bar{W}_W^{s+1})/(x_{i+1} - x_i) + (\bar{W}_N^{s+1} - \bar{W}_S^{s+1})/(y_{j+1} - y_j), & k_{\text{cell}} = 13. \end{cases} \quad (4.1)$$

For the approximation of flows in the boundary cells ($k_{\text{cell}} \neq 1, \dots, 8, 13$), the approximation of the boundary conditions is used. Figure 4.1 presents the cell codes on the contours surrounding the cell with a well (code 13).

Fig. 4.1. The first four contours $L_1, \dots, L_4$ around the perturbation source

For the solution of equation (3.1) in accordance with approximation (4.1) for cells of contour $L_k = \{x_l = (x_i, y_j) \in \Omega_{ij}, l = \overline{1, N_k}\}$ we have the iterative process

$$\mu_\alpha H_{\alpha t}^{s+1} = L_h H_\alpha^{s+1} + F_\alpha^s,$$

which can be written in the index form

$$a_l^{s, s+1} H_{\alpha, l-1}^{s+1} - c_l^{s, s+1} H_{\alpha, l}^{s+1} + b_l^{s, s+1} H_{\alpha, l+1}^{s+1} = -f_l^s, \quad l = \overline{1, N_k}. \quad (4.2)$$

The matrix of system (4.2) has a three-diagonal form with diagonal predominance. In the case of an open contour, the solution of system (4.2) with the boundary conditions for $l = 1$ and $l = N_k$ is determined by the Thomas algorithm, and in the case of a closed contour, the cyclic variant of the Thomas algorithm is used [10].

Introducing vector $\vec{H}_{\alpha k} = \{H_{\alpha 1}, H_{\alpha 2}, \dots, H_{\alpha N_k}\}^\top$ we write system (4.2) in following matrix form:

$$C_{\alpha k} \vec{H}_{\alpha k}^{s+1} + A_{\alpha k} \vec{H}_{\alpha k-1}^{s+1} + B_{\alpha k} \vec{H}_{\alpha k+1}^s = \vec{F}_{\alpha k}, \quad k = \overline{1, K},$$

where $C_{\alpha k}, A_{\alpha k}, B_{\alpha k}$ are $N_k \times N_k, N_k \times N_{k-1}, N_k \times N_{k+1}$ matrices respectively.

The convergence of the algorithm can be accelerated by alternating the computation along contours from wells to boundaries and from boundaries to wells. In this case, for the solution of (3.1) we have the following two-step algorithm:

$$a_l^{s, s+0.5} H_{\alpha, l-1}^{s+0.5} - c_l^{s, s+0.5} H_{\alpha, l}^{s+0.5} + b_l^{s, s+0.5} H_{\alpha, l+1}^{s+0.5} = -f_l^s, \quad l = \overline{1, N_k}, \quad x_l \in L_k, \quad k = \overline{1, K},$$

$$a_l^{s, s+1} H_{\alpha, l-1}^{s+1} - c_l^{s, s+1} H_{\alpha, l}^{s+1} + b_l^{s, s+1} H_{\alpha, l+1}^{s+1} = -f_l^s, \quad l = \overline{N_k, 1}, \quad x_l \in L_k, \quad k = \overline{K, 1},$$

where N_k is the number of cells on contour L_k and K is the number of contours.

5. Geomigration problem in a multiaquifer system

The processes of contaminant migration in multilayer systems are described by the equations of transfer and diffusion in aquifers

$$\begin{aligned} \sigma_1 m_1 \left(\frac{\partial C_1}{\partial t} + \frac{\partial N_1}{\partial t} \right) + \frac{\partial}{\partial x} \left(v_{x1} m_1 C_1 - D_{x1} \frac{\partial (m_1 C_1)}{\partial x} \right) + \frac{\partial}{\partial y} \left(v_{y1} m_1 C_1 - D_{y1} \frac{\partial (m_1 C_1)}{\partial y} \right) = \\ = -W_{1,2} + W_r + W_{\text{inf}} - W_{1w} + W_s, \end{aligned}$$

$$\begin{aligned}
 \sigma_\alpha m_\alpha \left(\frac{\partial C_\alpha}{\partial t} + \frac{\partial N_\alpha}{\partial t} \right) + \frac{\partial}{\partial x} \left(v_{x\alpha} m_\alpha C_\alpha - D_{x\alpha} \frac{\partial (m_\alpha C_\alpha)}{\partial x} \right) + \frac{\partial}{\partial y} \left(v_{y\alpha} m_\alpha C_\alpha - D_{y\alpha} \frac{\partial (m_\alpha C_\alpha)}{\partial y} \right) = \\
 = W_{\alpha-1,\alpha} - W_{\alpha,\alpha+1} - W_{\alpha w}, \quad \alpha = \overline{2, p-1}, \\
 \sigma_p m_p \left(\frac{\partial C_p}{\partial t} + \frac{\partial N_p}{\partial t} \right) + \frac{\partial}{\partial x} \left(v_{xp} m_p C_p - D_{xp} \frac{\partial (m_p C_p)}{\partial x} \right) + \frac{\partial}{\partial y} \left(v_{yp} m_p C_p - D_{yp} \frac{\partial (m_p C_p)}{\partial y} \right) = \\
 = W_{p-1,p} - W_{pw}, \quad (x, y) \in D_{xy}, \quad t > 0,
 \end{aligned} \tag{5.1}$$

and by the equation of vertical transfer of pollution through weakly permeable separation layers

$$\tilde{\sigma}_\alpha \tilde{m}_\alpha \left(\frac{\partial \tilde{C}_\alpha}{\partial t} + \frac{\partial \tilde{N}_\alpha}{\partial t} \right) + \frac{\partial}{\partial z} \left(v_{z\alpha} \tilde{m}_\alpha \tilde{C}_\alpha - D_{z\alpha} \frac{\partial (\tilde{m}_\alpha \tilde{C}_\alpha)}{\partial z} \right) = 0, \quad \alpha = 1, \dots, p-1.$$

Here C_α , $\tilde{C}_\alpha$ are the contaminant concentrations, m_α , $\tilde{m}_\alpha$, σ_α , $\tilde{\sigma}_\alpha$ are the thicknesses and porosities of the aquifers and separation layers, $v_\alpha = (v_{x\alpha}, v_{y\alpha}, v_{z\alpha})$ is the filtration rate, determined from the solution of the geofiltration problem. The diffusion components in the directions x, y, z are specified by the following equalities:

$$D_{x\alpha} = D_m + \lambda_{x\alpha} \sqrt{v_{x\alpha}^2 + v_{y\alpha}^2}, \quad D_{y\alpha} = D_m + \lambda_{y\alpha} \sqrt{v_{x\alpha}^2 + v_{y\alpha}^2}, \quad D_{z\alpha} = D_m + \lambda_{z\alpha} |v_{z\alpha}|,$$

where D_m is the molecular diffusion, $\lambda_{x\alpha}$, $\lambda_{y\alpha}$, $\lambda_{z\alpha}$ are the hydrodynamic dispersion coefficients.

The seepage velocities are computed using the Darcy law $v_{l\alpha} = -\sigma_\alpha^{-1} k_{\alpha l} \partial H_\alpha / \partial l$, where $k_{\alpha l}$ are the filtration coefficients in the x, y and z directions. For non-Darcy flows, the Forchheimers quadratic relations between the pressure gradient and the flow velocity can be applied [6].

Equations (5.1) take into account the contaminant inflow into the aquifers from rivers $W_r = m_r^{-1} k_r (H_r - H_1) C_r$ and contaminant source $W_s = \sum_k Q_{sk}(t) C_s \delta(x - x_k^*) \delta(y - y_k^*)$, and due to the infiltration $W_{\text{inf}} = \varepsilon_{\text{inf}} C_{\text{inf}}$. These equations also take into account the contaminant cross flows through the separation layers $W_{\alpha,\alpha+1} = -D_{z\alpha} \partial C_\alpha / \partial z + v_{z\alpha} C_\alpha$ and its outflow due to the operation of wells

$$W_{\alpha w} = \sum_k Q_{\alpha k}(t) C_\alpha \delta(x - x_{\alpha k}^*) \delta(y - y_{\alpha k}^*).$$

Here $Q_s(t)$ and C_s are the intake intensity and the contaminant concentration in the pollution source; m_r , k_r , C_r are the thickness of the underchannel deposit, the filtration coefficient, and the contaminant concentration in river; ε_{inf} and C_{inf} are the infiltration rate and the contaminant concentration in the infiltration.

Contaminant concentrations in a solid N_α are determined by the sorption kinetic equation

$$\frac{\partial N_\alpha}{\partial t} = \gamma(C_\alpha - \beta N_\alpha), \tag{5.2}$$

where γ and β are the coefficients of kinetic sorption and effective porosity. For the problems of long-term forecast, the asymptotic form of (5.2)

$$\frac{\partial N_\alpha}{\partial t} = \frac{1}{\beta} \frac{\partial C_\alpha}{\partial t} \tag{5.3}$$

was used in [3, 7].

6. Difference schemes for the geomigration problem

On the difference grid introduced in Section 3, the grid functions of the concentration $C_{\alpha,ij}^n = C_\alpha(x_{i+0.5}, y_{j+0.5}, t^n)$ are determined at the cell centers. The grid functions of flows are evaluated at the centers of the cell edges. Now we approximate the differentiate operator from (5.1)

$$LC_\alpha = -\frac{\partial}{\partial x} \left(v_{x\alpha} m_\alpha C_\alpha - D_{x\alpha} \frac{\partial (m_\alpha C_\alpha)}{\partial x} \right) - \frac{\partial}{\partial y} \left(v_{y\alpha} m_\alpha C_\alpha - D_{y\alpha} \frac{\partial (m_\alpha C_\alpha)}{\partial y} \right)$$

on the grid $\omega_\tau \times \omega_h$ by the difference operator

$$L_h C_\alpha = (W_E - W_W)/(x_{i+1} - x_i) + (W_N - W_S)/(y_{j+1} - y_j),$$

where

$$\begin{aligned} W_E &= -v_{x\alpha, i+1, j+0.5}^+ (mC)_{\alpha, i, j} - v_{x\alpha, i+1, j+0.5}^- (mC)_{\alpha, i+1, j} + \\ &+ D_{x\alpha, i+1, j+0.5} ((mC)_{\alpha, i+1, j} - (mC)_{\alpha, i, j}) / (x_{i+1.5} - x_{i+0.5}), \\ W_W &= -v_{x\alpha, i-1, j+0.5}^+ (mC)_{\alpha, i-1, j} - v_{x\alpha, i-1, j+0.5}^- (mC)_{\alpha, i, j} + \\ &+ D_{x\alpha, i-1, j+0.5} ((mC)_{\alpha, i, j} - (mC)_{\alpha, i-1, j}) / (x_{i+0.5} - x_{i-0.5}), \\ W_N &= -v_{y\alpha, i+0.5, j+1}^+ (mC)_{\alpha, i, j} - v_{y\alpha, i+0.5, j+1}^- (mC)_{\alpha, i, j+1} + \\ &+ D_{y\alpha, i+0.5, j+1} ((mC)_{\alpha, i, j+1} - (mC)_{\alpha, i, j}) / (y_{j+1.5} - y_{j+0.5}), \\ W_S &= -v_{y\alpha, i+0.5, j-1}^+ (mC)_{\alpha, i, j-1} - v_{y\alpha, i+0.5, j-1}^- (mC)_{\alpha, i, j} + \\ &+ D_{y\alpha, i+0.5, j-1} ((mC)_{\alpha, i, j} - (mC)_{\alpha, i, j-1}) / (y_{j+0.5} - y_{j-0.5}). \end{aligned}$$

Here $v_\alpha^+ = 0.5(v_\alpha + |v_\alpha|)$, $v_\alpha^- = 0.5(v_\alpha - |v_\alpha|)$.

As for the solution of the filtration problem, difference schemes based on splitting on physical processes have been constructed. At the first half-step the contaminant transfer in the aquifers

$$\left(1 + \frac{1}{\beta}\right) \sigma_\alpha m_\alpha \frac{C_\alpha^{n+1/2} - C_\alpha^n}{\tau} = L_h C_\alpha^{n+1/2} + \varphi_\alpha, \quad (6.1)$$

where

$$\begin{aligned} \varphi_\alpha &= \begin{cases} W_{r,h} + W_{\text{inf}} - W_{1w,h} + W_{s,h}, & \alpha = 1, \\ -W_{\alpha w,h}, & \alpha \neq 1, \end{cases} \\ W_{\alpha w,h} &= \begin{cases} \sum_k Q_{\alpha k}(t^{n+1}) C_\alpha / h_{x,i} h_{y,j}, & (x_{\alpha k}^*, y_{\alpha k}^*) \in [x_i, x_{i+1}] \times [y_j, y_{j+1}], \\ 0, & (x_{\alpha k}^*, y_{\alpha k}^*) \notin [x_i, x_{i+1}] \times [y_j, y_{j+1}], \end{cases} \\ W_{s,h} &= \begin{cases} \sum_k Q_{sk}(t^{n+1}) C_{sk} / h_{x,i} h_{y,j}, & (x_k^{**}, y_k^{**}) \in [x_i, x_{i+1}] \times [y_j, y_{j+1}], \\ 0, & (x_k^{**}, y_k^{**}) \notin [x_i, x_{i+1}] \times [y_j, y_{j+1}], \end{cases} \\ W_{r,h} &= G_r (H_r - H_1) \cdot C_{1r}, \quad G_r = \frac{k_r}{m_r}, \quad C_{1r} = \begin{cases} C_r, & H_r > H_1, \\ C_1, & H_r \leq H_1, \end{cases} \end{aligned}$$

and at the second vertical transport of the contaminant through separation layers

$$\begin{aligned} \left(1 + \frac{1}{\beta}\right) \sigma_{\alpha} m_{\alpha} \frac{C_{\alpha}^{n+1} - C_{\alpha}^{n+1/2}}{\tau} &= W_{\alpha-1,\alpha,h}^{n+1} - W_{\alpha,\alpha+1,h}^{n+1}, \\ \left(1 + \frac{1}{\tilde{\beta}}\right) \tilde{\sigma}_{\alpha} \tilde{m}_{\alpha} \frac{\tilde{C}_{\alpha}^{n+1} - \tilde{C}_{\alpha}^n}{\tau} &= W_{\alpha-1,\alpha,h}^{n+1} - W_{\alpha,\alpha+1,h}^{n+1}, \end{aligned} \quad (6.2)$$

was considered. Here

$$W_{\alpha,\alpha+1,h} = v_{z\alpha}^+ C_{\alpha} + v_{z\alpha}^- \tilde{C}_{\alpha} + D_{z\alpha} (\tilde{C}_{\alpha} - C_{\alpha}) / 0.5 \tilde{m}_{\alpha}, \quad v_{z\alpha}^+ = 0.5(v_{z\alpha} + |v_{z\alpha}|), \quad v_{z\alpha}^- = 0.5(v_{z\alpha} - |v_{z\alpha}|).$$

From (6.2) we have the systems of three-point equations

$$a_{\alpha} C_{\alpha-1}^{n+1} - c_{\alpha} C_{\alpha}^{n+1} + b_{\alpha} C_{\alpha+1}^{n+1} = -f_{\alpha}, \quad \alpha = \overline{1, p},$$

which are solved by the Thomas algorithm in the z direction for all (i, j) , $i = \overline{1, N_x}$, $j = \overline{1, N_y}$ when $p > 2$.

For each aquifer α , the system of difference equations (6.1) is a five-point system. The iterative algorithm proposed in Section 4 is used for the solution. The computational contours are constructed from cells with pollution sources.

7. Numerical experiment

For the solution of the problem of groundwater flow and contaminant transport in two aquifers separated by a semipermeable layer, a numerical experiment was carried out. The proposed algorithm was used. The dynamics of the groundwater flow was described by the above mathematical model.

The modelled filtration area in plan and section is presented in Fig. 7.1. The area is bounded above by the subsoil water surface on which the infiltration rate is given, and

Fig. 7.1. Investigated area: plan (a) and hydrogeological section on I—I line (b)

below — by an impermeable bed. The investigated area in plan is the area of the influence of the groundwater intake. It is bounded by the maximal size of the depression cone formed as a result of groundwater withdrawal.

The first aquifer incorporates a subsoil aquifer consisting of sand, sandy loam and loam. In the aquifer, reservoirs (rivers and lakes) and superficial streams are located. The filtration flows from the reservoirs depend on the conductivity of underchannel deposits and the levels of superficial and subsoil waters. In the first aquifer, the filtration regime is unconfined. The pollution source is located in the aquifer. The pollution concentration in the source is 10 mg/dm^3 and the infiltration rate is 69 mm/year .

The second aquifer is separated from the upper aquifer by a layer of semipermeable deposits with low filtration properties. This aquifer consists of sand and chalk. The aquifer is a source of drinking water supply. The groundwater intake consists of five identical wells. The total rate of the groundwater intake is $7500 \text{ m}^3/\text{day}$. The filtration regime in the second aquifer is confined.

The transmissivity and the infiltration rate of the first aquifer are shown in Figs. 7.2,*a* and 7.2,*b*, and the vertical conductivity of the underchannel deposits — in Fig. 7.2,*c*. The transmissivity of the second aquifer is $500 \text{ m}^2/\text{day}$. The specific yields of the first and second aquifers are 0.1 and 0.01 respectively. Thickness of the separation layer is 10 m and the filtration coefficient is 0.05 m/day .

Fig. 7.2. Input data: *a*) transmissivity (m^2/day) and *b*) infiltration rate (mm/year) of the first aquifer, *c*) vertical conductivity of the underchannel deposits ($1/\text{day}$)

The partition of the area into 29×21 computational blocks in plan and on computational horizons in section is presented in Fig. 7.3. At the area boundaries where the aquifer is absent, the boundary conditions of the second kind (the filtration flows are equal to zero) are given (Fig. 7.4). To determine the groundwater levels, contours surrounding well-containing cells have been constructed. For the geomigration problem, the computational contours around the cell with a pollution source have been constructed (Fig. 7.5).

According to the intake design norms, studies of the groundwater drawdown and redistribution of filtration flows at $t = 1$ year and $t = 25$ years have been carried out. The contour plots of the initial and calculated levels are shown in Figs. 7.6, 7.7.

Fig. 7.3. Spatial discretization of the area

Fig. 7.4. Difference grid and boundary conditions

Fig. 7.5. Contours with cell codes: a) the first aquifer; b) the second aquifer

Fig. 7.6. Initial groundwater levels at $t = 0$: the first (a) and second (b) aquifers

Fig. 7.7. Forecast of groundwater levels at $t = 25$ years: the first (a) and second (b) aquifers

The absolute mark of the groundwater level in the vicinity of intake has been lowered from 160 m to 156.2 m in 25 years. The maximal drawdown of the second aquifer is 2.1 m for 1 year and 3.8 m for a 25-year intake operation (Fig. 7.8).

Fig. 7.8. Drawdown of groundwater levels in the second aquifer at $t = 1$ year (a) and at $t = 25$ years (b)

The piezometric surfaces and groundwater flow vectors of the first aquifer are presented in Fig. 7.9. The operation of an intake leads to a change of the direction of flows and to a break of the levels of superficial and subsoil waters in the reach of the river near the intake.

The results of the computational experiment on contaminant migration under intake operation for different instants of time are presented in Fig. 7.10.

Due to the vertical mass transfer the contaminant penetrates into the second aquifer. At $t=0.5$ year the size of the pollution plume reaches its maximum and the contaminant concentration in the intake is 0.0005 mg/dm^3 . This is 20000 times less than the concentration in the source. Further the contaminant concentration decreases. At $t = 2$ years the plume practically vanishes.

The proposed algorithm can be used for estimating the influence of the possible pollution sources on the groundwater quality in the intake area.

Fig. 7.9. Groundwater surfaces: initial (a), under the operation of an intake (b)

Fig. 7.10. Contaminant concentration in the groundwater of the first and second aquifers

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