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Mathematical Modelling of the Problem of Solute Transport in a Two-Dimensional Heterogeneous Porous Medium

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ABSTRACT: The problem of solute transport in a two-dimensional inhomogeneous porous medium is formulated and numerically solved. The filtration rate and hydrodynamic dispersion were set by different ratios, nonlinear. On the basis of the numerical results, the concentration fields are determined for different values of the model parameters of the filtration rate and hydrodynamic dispersion.

KEY WORDS: diffusion, hydrodynamic dispersion, solute transport, porous medium.

I. INTRODUCTION.

The problems of solute transport and filtration of heterogeneous fluids are of great practical importance in many branches of engineering and technology. Many natural and technological processes are associated with the filtration of inhomogeneous fluids and the transfer of particles in heterogeneous porous media. In contrast to heterogeneous fluids that are homogeneous during filtration, a number of new phenomena arise, the study of which is very important for understanding the mechanisms of the filtration process. Recently, the issues of mathematical modeling of the processes of transfer of substances have been intensively developed, mainly abroad. In principle, modeling approaches are based on the law of substance balance in a certain control volume using some additional phenomenological relationships. The process of solute transport suspended in a fluid in a porous medium is determined by many factors, such as convective transfer, diffusion, hydrodynamic dispersion, deposition in pores, their release with a transition to a mobile state, etc. Convective transfer, diffusion, hydrodynamic dispersion, local change in concentration can be described by the mass conservation equation [1, 2].

II. RELATED WORK

In [3], the problem for a one-dimensional advection-dispersion equation with variable coefficients was solved using an explicit finite-difference scheme; further, the results were extended to the case of a two-dimensional equation in semi-infinite media [4]. It is known that dispersion generally depends on the flow rate [5]. In [6], it is believed that the dispersion is proportional to the n th power of the velocity with an exponent in the range from 1 to 2. Sometimes the expressions for the velocity and dispersion are written in degenerate form [6]. In the two-dimensional case, the transport of the solute occurs both in the longitudinal and transverse directions. Significant transport of solute is observed along the transverse direction even at very low transverse velocity and dispersion relative to their longitudinal counterparts. This shows that a two-dimensional model is more suitable than a one-dimensional one.

In [7], a mathematical model for a two-dimensional transfer of matter in a semi-infinite inhomogeneous porous medium is presented. The dispersion coefficient is considered as a linear multiple of the space-dependent function and filtering rate. The exponentially decreasing relation of the filtration rate is considered.

This paper considers the solute transport in a two-dimensional porous medium, where the dispersion coefficients and filtration rates are variable in space and time scale.



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III. PROBLEM STATEMENT

Consider a two-dimensional object, the diagram of which is shown in Fig. 1. Let a solution with a certain concentration be supplied at some point in the $(0 \le x < \infty; 0 \le y < \infty)$ medium. From such a point source, the solution spreads into the medium in mutually perpendicular directions x and y.

The components of the flow velocity along x and y directions at a given point of the field (x, y) will be denoted by u(x,t) and v(y,t), respectively. Both of these components satisfy Darcy's law. Across

Fig. 1. Scheme of a two-dimensional medium, x_{∞} and y_{∞} are chosen so that it was, $\frac{\partial c}{\partial x} = 0$, $\frac{\partial c}{\partial y} = 0$, respectively [4].

We will denote $D_x(x,t)$ and $D_y(y,t)$ as longitudinal and transverse components of the hydrodynamic dispersion



in the directions x and y [4,5], respectively. Then the linear equation of convective dispersion in the two-dimensional case can be written in the following form:

$$\frac{\partial C(x, y, t)}{\partial t} = \frac{\partial}{\partial x} \left(D_x(x, t) \frac{\partial C(x, y, t)}{\partial x} - u(x, t) C(x, y, t) \right) + \frac{\partial}{\partial y} \left(D_y(y, t) \frac{\partial C(x, y, t)}{\partial y} - v(y, t) C(x, y, t) \right),$$
(1)

where C(x, y, t) is the concentration of the solute transported through the medium at a point (x, y) in time t.

In order to solve the two-dimensional advection-dispersion equation (1), it is necessary to set the initial and boundary conditions.

Initially, let the medium be filled with a clean (no substance) fluid. Starting from the initial moment, from the point (0,0), solute with a certain concentration is supplied for a certain time t_0 . At infinity in the directions x and y the conditions of the absence of solute consumption are accepted. Then the initial and boundary conditions can be written in the form

$$C(x, y, t) = 0, \qquad x \ge 0; \quad y \ge 0, \quad t = 0,$$
 (2)

$$C(x, y, t) = \begin{cases} C_0, & x = 0; \quad y = 0; \quad 0 < t \le t_0 \\ 0, & x = 0; \quad y = 0; \quad t > t_0 \end{cases}$$
(3)

$$\frac{\partial C(x, y, t)}{\partial x} = 0, \quad x \to \infty; \quad \frac{\partial C(x, y, t)}{\partial y} = 0, \quad y \to \infty; \quad t \ge 0,$$
(4)



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where C_0 is the concentration of the substance supplied to the medium.

Since the medium is inhomogeneous, two velocity components, i.e. u(x,t) and v(y,t), is considered to be linear functions of the corresponding coordinates x and y. Moreover, the velocities are considered to depend on t, i.e. some functional dependence of the velocity component on t is taken into account. Thus, the components of the fluid velocity are taken in the form [4]

$$u(x,t) = u_0 f_1(mt)(1+ax), \qquad v(y,t) = v_0 f_1(mt)(1+by), \tag{5}$$

where a and b are the parameters of heterogeneity in the longitudinal and transverse directions, $f_1(mt)$ is a known function, m is a parameter, $u_0 = \text{const}$, $v_0 = \text{const}$. Different values a and b express different characteristics of heterogeneity.

It is known that the diffusion (hydrodynamic dispersion) coefficients depend on the fluid velocity. Here the following dependence is accepted [4]

$$D_{x}(x,t) = D_{x0}f_{2}(mt)(1+ax)^{2}, \qquad D_{y}(y,t) = D_{y0}f_{2}(mt)(1+by)^{2}.$$
(6)

where $f_2(mt)$ is a given function, $D_{x0} = \text{const}$, $D_{y0} = \text{const}$. It is guaranteed that f(mt) = 1 for m = 0 or t = 0. In (5), (6) the coefficients u_0 , v_0 , D_{x0} , D_{y0} can be interpreted as homogeneous coefficients of the speed of movement and diffusion coefficients, respectively, in the longitudinal and transverse directions.

IV. NUMERICAL SOLUTION OF THE PROBLEM

System (1) is written as following form

$$\frac{\partial C(x, y, t)}{\partial t} = \left(\frac{\partial D_x(x, t)}{\partial x} \frac{\partial C(c, y, t)}{\partial x} + D_x(x, t) \frac{\partial^2 C(x, y, t)}{\partial x^2}\right) - \left(\frac{\partial u(x, t)}{\partial x} C(x, y, t) + u(x, t) \frac{\partial C(x, y, t)}{\partial x}\right) + \left(\frac{\partial D_y(y, t)}{\partial y} \frac{\partial C(x, y, t)}{\partial y} + D_y(y, t) \frac{\partial^2 C(x, y, t)}{\partial y^2}\right) - \left(\frac{\partial v(x, t)}{\partial y} C(x, y, t) + v(x, t) \frac{\partial C(x, y, t)}{\partial y}\right).$$
(7)

Using expressions for the velocities of motion (5) and diffusion coefficients (6), equation (7) can be written in the form

$$\frac{\partial C(x, y, t)}{\partial t} = D_{x0}e^{mt} (1 + ax)^2 \frac{\partial^2 C(x, y, t)}{\partial x^2} + D_{y0}e^{mt} (1 + by)^2 \frac{\partial^2 C(x, y, t)}{\partial y^2} + \left(D_{x0} \cdot 2a \cdot (1 + ax)e^{mt} - u_0e^{-mt} (1 + ax) \right) \frac{\partial C(x, y, t)}{\partial x} + \left(D_{y0}e^{mt} (1 + by)^2 - v_0e^{-mt} (1 + by) \right) \frac{\partial C(x, y, t)}{\partial y} - \left(au_0e^{-mt} + bv_0e^{-mt} \right) C(x, y, t),$$
(8)

where

$$u(x,t) = u_0 f_1(mt)(1+ax), \quad v(y,t) = v_0 f_1(mt)(1+by), \quad D_x(x,t) = D_{x0} f_2(mt)(1+ax)^2,$$

$$D_y(y,t) = D_{y0} f_2(mt)(1+by)^2, \quad \frac{\partial u}{\partial x} = a u_0 e^{-mt}, \quad \frac{\partial v}{\partial y} = b v_0 e^{-mt}$$

$$\frac{\partial D_x}{\partial x} = D_{x0} \cdot 2a(1+ax) \cdot e^{mt}, \qquad \frac{\partial D_y}{\partial y} = D_{y0} \cdot 2b(1+by) \cdot e^{mt}.$$

$$f_1(mt) = e^{-mt}, \quad f_2(mt) = e^{mt}.$$

The following designations are introduced



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$$L_{1} = D_{x0}e^{mt} (1+ax)^{2}, \quad L_{2} = D_{y0}e^{mt} (1+by)^{2}, \quad L_{3} = D_{x0} 2a (1+ax)e^{mt} - u_{0} (1+ax)e^{-mt},$$

$$L_{4} = D_{y0} 2b (1+by)e^{mt} - v_{0} (1+by)e^{-mt}, \quad L_{5} = -(au_{0}+bv_{0})e^{-mt}.$$
Using notation (9), we write equation (8) in the form
$$\frac{\partial C(x, y, t)}{\partial t} = L_{1} \frac{\partial^{2} C(x, y, t)}{\partial x^{2}} + L_{2} \frac{\partial^{2} C(x, y, t)}{\partial y^{2}} + L_{3} \frac{\partial C(x, y, t)}{\partial x} + L_{4} \frac{\partial C(x, y, t)}{\partial y} - L_{5} C(x, y, t).$$
(10)
To solve equation (10), we use the finite difference method. For this, we introduce the following grid [8]

To solve equation (10), we use the finite difference method. For this, we introduce the following grid [8] $\omega_{\tau h_i h_2} = \{(x_i, y_j, t_k), i = \overline{0, N}, j = \overline{0, R}, k = \overline{0, K}, x_i = ih_1, k = \overline{0, N}\}$

$$y_j = jh_2, \ t_k = k\tau, \ h_1 = \frac{x_\infty}{N}, \ h_2 = \frac{y_\infty}{R}, \ \tau = \frac{T}{K} \bigg\},$$

where τ , h_1 , h_2 are the grid steps in time, coordinates x and y, respectively.

To approximate (10), the Crank-Nicholson scheme was used [8]

$$\begin{cases} \frac{C_{i,j}^{k+\frac{1}{2}} - C_{i,j}^{k}}{\tau/2} = L_{1} \frac{C_{i-1,j}^{k+\frac{1}{2}} - 2 \cdot C_{i,j}^{k+\frac{1}{2}} + C_{i+1,j}^{k+\frac{1}{2}}}{h_{1}^{2}} + L_{2} \frac{C_{i,j-1}^{k} - 2 \cdot C_{i,j}^{k} + C_{i,j+1}^{k}}{h_{2}^{2}} + L_{2} \frac{L_{1}^{k} + L_{2}^{k} + L_$$

where C_{ij}^k is the grid function corresponding to the nodal point (x_i, y_j, t_k) .

It can be seen from (11) that the approximation error for scheme (11) is of the order $O(\tau, h_1^2, h_2^2)$.

The system of equations (11) is written in the form

$$\begin{cases} A_{1}C_{i-1,j}^{k+\frac{1}{2}} - B_{1}C_{i,j}^{k+\frac{1}{2}} + C_{1}C_{i+1,j}^{k+\frac{1}{2}} = -F_{1i}, \\ A_{2}C_{i,j-1}^{k+1} - B_{2}C_{i,j}^{k+1} + C_{2}C_{i,j+1}^{k+1} = -F_{2j}, \end{cases}$$
(12)

where

$$\begin{aligned} A_{1} &= \frac{\tau L_{1}}{2h_{1}^{2}} - \frac{\tau \cdot L_{3}}{4h_{1}}, \quad B_{1} = 1 - \frac{\tau \cdot L_{2}}{2} + \frac{\tau \cdot L_{1}}{h_{1}^{2}}, \quad C_{1} = \frac{\tau \cdot L_{1}}{2h_{1}^{2}} + \frac{\tau \cdot L_{3}}{4h_{1}}, \\ F_{1i} &= \frac{\tau \cdot L_{2}}{2h_{2}^{2}} \left(C_{i,j-1}^{k} - 2 \cdot C_{i,j}^{k} + C_{i,j+1}^{k} \right) + \frac{\tau \cdot L_{4}}{4h_{2}} \left(C_{i,j+1}^{k} - C_{i,j-1}^{k} \right) + C_{i,j}^{k}, \\ A_{2} &= \frac{\tau \cdot L_{4}}{2h_{2}^{2}} - \frac{\tau \cdot L_{2}}{4h_{2}}, \quad B_{2} = 1 - \frac{\tau \cdot L_{5}}{2} + \frac{\tau \cdot L_{2}}{h_{2}^{2}}, \quad C_{2} = \frac{\tau \cdot L_{2}}{2h_{2}^{2}} + \frac{\tau \cdot L_{4}}{4h_{2}}, \\ F_{2j} &= \frac{\tau \cdot L_{4}}{2h_{1}^{2}} \left(C_{i-1,j}^{k+\frac{1}{2}} - 2 \cdot C_{i,j}^{k+\frac{1}{2}} + C_{i+1,j}^{k+\frac{1}{2}} \right) + \frac{\tau \cdot L_{3}}{4h_{1}} \left(C_{i+1,j}^{k+\frac{1}{2}} - C_{i-1,j}^{k+\frac{1}{2}} \right) + C_{i,j}^{k+\frac{1}{2}}. \end{aligned}$$
We use the following relations to solve (12) by the sweep method

 $C_{i,j}^{k+\frac{1}{2}} = \alpha_{1i,j+1}C_{i,j+1}^{k+\frac{1}{2}} + \beta_{1i,j+1},$ $C_{i,j}^{k+1} = \alpha_{2,i+1,j}C_{i+1,j}^{k+\frac{1}{2}} + \beta_{2,i+1,j},$

where $\alpha_{1i,j+1}$, $\beta_{1i,j+1}$, $\alpha_{2,i+1,j}$, $\beta_{2,i+1,j}$ are coefficients of Thomas' algorithm

(14)



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Then from (12) we obtain the following recursive formulas for the coefficients of Thomas' algorithm.

$$\begin{cases} \alpha_{1i+1,j} = \frac{C_1}{B_1 - A_1 \alpha_{1i,j}}, \qquad \beta_{1i+1,j} = \frac{F_{1i} + A_1 \beta_{1i,j}}{B_1 - A_1 \alpha_{1i,j}}, \\ \alpha_{2i,j+1} = \frac{C_2}{B_2 - A_2 \alpha_{2i,j}}, \qquad \beta_{2i,j+1} = \frac{F_{2j} + A_2 \beta_{2i,j}}{B_2 - A_2 \alpha_{2i,j}}. \end{cases}$$
(15)

The initial condition in the difference form is

$$C_{i,j}^{0} = 0, \quad x \ge 0; \quad y \ge 0; \quad t = 0.$$
(16)

From the boundary conditions we have

$$\begin{cases} C_{0,j}^{k+\frac{1}{2}} = \left(\overline{\alpha}_{1}\right)_{j+1} C_{0,j+1}^{k+\frac{1}{2}} + \left(\overline{\beta}_{1}\right)_{j+1}, \\ C_{i,0}^{k+1} = \left(\overline{\alpha}_{2}\right)_{i+1} C_{i+1,0}^{k+1} + \left(\overline{\beta}_{2}\right)_{i+1}, \end{cases}$$
(17)

from which we obtain

$$C_{i,R}^{k+\frac{1}{2}} = \frac{(\beta_{1})_{i,R}}{1-(\alpha_{1})_{i,R}}; \qquad C_{N,j}^{k+1} = \frac{(\beta_{2})_{N,j}}{1-(\alpha_{2})_{N,j}}$$

$$\begin{cases} (\bar{\alpha}_{1})_{j+1} = \frac{\bar{C}_{1}}{\bar{B}_{1}-\bar{A}_{1}(\bar{\alpha}_{1})_{j}}; \qquad (\bar{\beta}_{1})_{j+1} = \frac{(\bar{F}_{1})_{i}+\bar{A}_{1}(\bar{\beta}_{1})_{j}}{\bar{B}_{1}-\bar{A}_{1}(\bar{\alpha}_{1})_{j}} \\ (\bar{\alpha}_{2})_{i+1} = \frac{\bar{C}_{2}}{\bar{B}_{2}-\bar{A}_{2}(\bar{\alpha}_{2})_{i}}; \qquad (\bar{\beta}_{2})_{i+1} = \frac{(\bar{F}_{2})_{j}+\bar{A}_{2}(\bar{\beta}_{2})_{i}}{\bar{B}_{2}-\bar{A}_{2}(\bar{\alpha}_{2})_{i}} \end{cases}$$

where

$$\begin{split} \overline{A}_{1} &= \frac{\tau \cdot M_{1}}{2h_{2}^{2}} - \frac{\tau \cdot M_{2}}{2h_{2}}; \ \overline{B}_{1} = 1 + \frac{\tau \cdot M_{1}}{h_{2}^{2}} - \frac{\tau \cdot M_{3}}{2}; \ \overline{C}_{1} = \frac{\tau \cdot M_{1}}{2h_{2}^{2}} + \frac{\tau \cdot M_{2}}{2h_{2}}; \ \overline{F}_{1j} = C_{0,j}^{k}; \\ \overline{A}_{2} &= \frac{\tau \cdot N_{1}}{2h_{1}^{2}} - \frac{\tau \cdot N_{2}}{2h_{1}}; \ \overline{B}_{2} = 1 + \frac{\tau \cdot N_{1}}{h_{1}^{2}} - \frac{\tau \cdot N_{3}}{2}; \ \overline{C}_{2} = \frac{\tau \cdot N_{1}}{2h_{1}^{2}} + \frac{\tau \cdot N_{2}}{2h_{1}}; \ \overline{F}_{2j} = C_{i,0}^{k+\frac{1}{2}}, \\ M_{1} &= D_{y0}e^{mt} \left(1 + by\right)^{2}; \ M_{2} = (1 + by) \left(2bD_{y0}e^{mt} + v_{0}e^{-mt}\right); \\ M_{3} &= -\left(au_{0} + bv_{0}\right)e^{-mt}; D_{y0}e^{mt} \left(1 + by\right)^{2}; \\ N_{1} &= D_{x0} \left(1 + ax\right)^{2}e^{mt}; \ N_{2} = (1 + ax) \left(2aD_{x0}e^{mt} + u_{0}e^{-mt}\right); \ N_{3} = -\left(au_{0} + bv_{0}\right)e^{-mt}. \end{split}$$

V. RESULTS

Some numerical results are shown in Figure 2-5. The calculations used the following values of the initial parameters:

$$D_{x0} = 2 \cdot 10^{-6} \,\mathrm{m^2/c}; \ D_{y0} = 10^{-6} \,\mathrm{m^2/c}; \ u_0 = 4 \cdot 10^{-6} \,\mathrm{m/c}; \ v_0 = 2 \cdot 10^{-6} \,\mathrm{m/c}; \ a = 10^{-4} \,\mathrm{m^{-1}}; \ b = 10^{-4} \,\mathrm{m^{-1}}; \ C_0 = 0.01 \,.$$



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Fig. 2. Concentration profiles for the exponential form of the functions $f_1(mt)$ and $f_2(mt)$ at t = 9000c (a); 18000c (b); 36000c; (c).





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Fig. 3. Concentration profiles for exponential form functions $f_1(mt)$ and $f_2(mt)$ at $t = 36000c \ m = 10^{-9}$ (a); $m = 10^{-7}$ (b); $m = 10^{-5} \ c^{-1}$; (c).

As can be seen from Figs. 2, 4, with increasing time t, concentration profiles propagate over the region in both directions, i.e. x and y. In this case, the profiles propagate more intensively in the direction x, because values u_0 and D_{x0} more than values v_0 and D_{y0} . This situation corresponds to the case when both convective and diffusion directional transfers x are significantly ahead of the corresponding directional transfers y. However, other situations are also possible when both types of transport along the directions can have different intensities.

VI.CONCLUSION

The problem of material transfer in a two-dimensional porous medium is formulated and numerically solved. It is shown that the concentration propagation at a certain position is higher for the smaller parameter m and lower for the larger parameter m.

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