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THE INVERSE PROBLEM OF FINDING THE RETARDATION FACTOR a₂ AND THE DIFFUSION COEFFICIENT D IN A SUBSTANCE TRANSPORT EQUATION IN A HOMOGENEOUS POROUS MEDIUM

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The equations of solute transport in the one-dimensional case are written in the form

$$\rho \frac{\partial S_{a1}}{\partial t} + \rho \frac{\partial S_{s1}}{\partial t} + \theta_1 \frac{\partial c_1}{\partial t} + a_2 \frac{\partial^{\gamma} c_1}{\partial t} = \theta_1 D_1 \frac{\partial^2 c_1}{\partial x^2} - \theta_1 v_1 \frac{\partial c_1}{\partial x},$$
(1)

where $a_2 - is$ the coefficient due to the solute transport into the second medium, $[s] ^{(\beta-1)}$, γ -is the order of the derivative.

Let the problems of finding coefficients a_2 and D_1 from (1) be given.

The sedimentation of matter in each of the sections of the zones occurs reversibly in accordance with the kinetic equations

$$\rho \frac{\partial S_{a1}}{\partial t} = \theta_1 k_{a1} c_1 - \rho k_{ad1} S_{a1}, \tag{2}$$

$$\rho \frac{\partial S_{s1}}{\partial t} = \theta_1 k_{s1} c_1 - \rho k_{sd1} S_{s1},\tag{3}$$

where k_{a1} , k_{s1} – coefficients of deposition of matter from the fluid phase to the solid phase, $s^{(-1)}$; k_{ad1} , k_{sd1} -the coefficients of separation of the substance from the solid phase and the transition to the fluid, $s^{(-1)}$.

Let a fluid with a constant concentration of a substance be pumped into a medium initially saturated with a pure (without substance) fluid from the initial moment of





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time c_0. Let us consider such periods of time where the concentration field does not reach the right boundary of the medium $x \rightarrow \infty$. Under these assumptions, the initial and boundary conditions for the problem have the form

$$c_1(0,x) = 0, \ S_{a1}(0,x) = 0, \ S_{s1}(0,x) = 0,$$
 (4)

$$c_1(t,0) = c_0,$$
 (5)

$$\frac{\partial c_1}{\partial x}(t,\infty) = 0. \tag{6}$$

Problem (4) – (9) is solved by the finite difference method [21]. In the considered area $\Omega = \{(t,x), 0 \le t \le T, 0 \le x \le \infty\}$ introduced a grid uniform in directions

$$\overline{\omega_{\tau h}} = \begin{cases} (t_j, x_i); \ t_j = \tau j, x_i = ih, \\ \tau = \frac{T}{J}, i = \overline{0, I}, j = \overline{0, J} \end{cases}$$

where I-is a sufficiently large integer selected so that segment $[0,x_I],x_I=ih$, overlaps the area of the calculated change in fields c_1,S_a1 and $[S] _s1,h-$ the grid step in the direction of x, - is the grid step in time .

In the open grid area

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$$\omega_{\tau h} = \begin{cases} (t_j, x_i); \ t_j = \tau j, x_i = ih, \\ \tau = \frac{T}{J}, i = \overline{1, I - 1}, j = \overline{1, J} \end{cases}$$

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i+1

equations (4), (5), (6) were approximated as follows



$$\rho \frac{(S_{a1})_{i}^{j+1} - (S_{a1})_{i}^{j}}{\tau} + \rho \frac{(S_{s1})_{i}^{j+1} - (S_{s1})_{i}^{j}}{\tau} + \theta_{1} \frac{(c_{1})_{i}^{j+1} - (c_{1})_{i}^{j}}{\tau} \\ + \frac{a_{2}\tau^{1-\gamma}}{\Gamma(2-\gamma)} \Biggl[\sum_{k=0}^{j-1} \frac{(c_{1})_{i}^{k+1} - (c_{1})_{i}^{k}}{\tau} ((j-k+1)^{1-\gamma} - (j-k)^{1-\gamma}) \\ + \frac{((c_{1})_{i}^{j+1} - (c_{1})_{i}^{j})\tau^{1-\gamma}}{\tau} \Biggr] \\ = \theta_{1}D_{1} \frac{(c_{1})_{i-1}^{j+1} - 2(c_{1})_{i}^{j+1} + (c_{1})_{i+1}^{j+1}}{h^{2}} \\ - \theta_{1}v_{1} \frac{(c_{1})_{i}^{j+1} - (c_{1})_{i-1}^{j+1}}{h}$$
(7)

i+1

$$\rho \frac{(S_{a1})_i^{j+1} - (S_{a1})_i^j}{\tau} = \theta_1 k_{a1} (c_1)_i^j - \rho k_{ad1} (S_{a1})_i^{j+1}, \tag{8}$$

$$\rho \frac{(S_{s1})_i^{j+1} - (S_{s1})_i^j}{\tau} = \theta_1 k_{s1} (c_1)_i^j - \rho k_{sd1} (S_{s1})_i^{j+1}, \tag{9}$$

where $(c_1)_i^j, (S_{a1})_i^j, (S_{s1})_i^j$ – grid function values $c_1(1, x), S_{a1}(t, x), S_{s1}(t, x),$ at the point (t_j, x_i) .

From explicit grid equations (11), (12) we determine $(S_{a1})_i^{j+1}$, $(S_{s1})_i^{j+1}$

$$(S_{a1})_i^{j+1} = p_{b1}(S_{a1})_i^j + p_{b2},$$
(10)

$$(S_{s1})_i^{j+1} = q_{b1}(S_{s1})_i^j + q_{b2},$$
(11)

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Where

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$$p_{b1} = \frac{1}{1 + \tau k_{ad1}}, \quad p_{b2} = \frac{\tau \theta_1 k_{a1}}{\rho + \rho \tau k_{ad1}} (c_1)_i^j,$$

$$q_{b1} = \frac{1}{1 + \tau k_{sd1}}, \qquad q_{b2} = \frac{\tau \theta_1 k_{s1}}{\rho + \rho \tau k_{sd1}} (c_1)_i^j.$$

Grid equations (7) are reduced to the form

$$A_1(c_1)_{i-1}^{j+1} - B_1(c_1)_i^{j+1} + E_1(c_1)_{i+1}^{j+1} = -(F_1)_i^j,$$
(12)

where
$$A_1 = \frac{\theta_1 D_1 \tau}{h^2} + \frac{\theta_1 v_1 \tau}{h}$$
, $B_1 = \theta_1 + \frac{2\theta_1 D_1 \tau}{h^2} + \frac{\theta_1 v_1 \tau}{h} + \frac{a_2 \tau^{1-\gamma}}{\Gamma(2-\gamma)}$, $E_1 = \frac{\theta_1 D_1 \tau}{h^2}$,
 $(F_1)_i^j = \left(\theta_1 + \frac{a_2 \tau^{1-\gamma}}{\Gamma(2-\gamma)}\right) B_1(c_1)_i^j - \rho\left((S_{a1})_i^{j+1} - (S_{a1})_i^j\right) - \rho\left((S_{s1})_i^{j+1} - (S_{s1})_i^j\right)$
 $- \frac{a_2 \tau^{1-\gamma}}{\Gamma(2-\gamma)} \left[\sum_{k=0}^{j-1} ((j-k+1)^{1-\gamma} - (j-k)^{1-\gamma})(c_1)_i^{k+1} - ((j-k+1)^{1-\gamma} - (j-k)^{1-\gamma})(c_1)_i^k\right]$.

$$I_1 = \alpha (C_2 - C_1), \quad I_2 = a_2 \frac{\partial^{\gamma} C_1}{\partial t^{\gamma}}.$$

The following procedure for calculating the solution is established. By (10), (11) $(S_a1)_i^{(j+1)}, (S_s1)_i^{(j+1)}$, are determined, then the system of linear equations (12) is solved by the Thomas' algorithm with respect to $(c \ 1)$ i^(j+1). Since p_b1,q_b1<1, schemes (10), (11) are stable, and for (12) the stability conditions of the Thomas' algorithm are satisfied.

we minimize the function using the above,

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Values describe the standard deviation for the entire time period. I_1 and I_2 the performed calculations show that the minimum value of 1 is reached



The closeness of the flow times should guarantee the closeness of the concentration fields determined using the proposed approach . I_1 and I_2 and the model [4]. To quantitatively estimate their closeness, we use the standard deviation of type (14), which is determined based on only two models, i.e.

$$F(a_2,\gamma) = \int_0^T \int_0^L \left(C_1^{(1)} - C_1^{(2)}\right)^2 dx dt,$$

where $C_1^{(1)}$ is the concentration field C_1 (t,x) at a given t, defined according to [4], and $C_1^{(2)}$ is the same here. The following minimum value was obtained for the cases analyzed above

 $F(a_2, D) = 0.002347387654452$ for $a_2 = 0.0006, D = 10^{-6}$.

The inverse problem of finding a_2 retardation factor and D diffusion coefficient was numerically solved in the given model of substance transport.

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