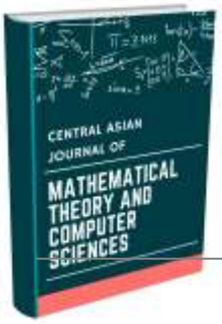

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Numerical Solution of the Inverse Problem of Solute Transport in Non-Homogeneous Porous Media

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Abstract

In this paper, a solute transport problem with non-equilibrium adsorption in a non-homogeneous porous medium consisting of two zones, one with high permeability (mobile zone) and another one with low permeability (immobile liquid zone) are considered. In the mobile zone, there are two zones in both of which adsorption of solute with reversible kinetics occurs. The results of this approach are compared with known, traditional approaches. It is shown that this method of modeling the process gives a satisfactory result. By appropriate selection of the parameters of the source term, one can obtain results close to those of the well-known bicontinuum approach.

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Introduction

Aquifers, oil, and gas reservoirs, as a rule, have a heterogeneous structure at the micro- and macroscale, [1]. **H**eterogeneous reservoirs on a macro scale consist of different zones with different, sometimes very strong, filtration-capacitive properties, i.e. porosity, permeability, etc. Zones with well porosity and permeability are well conductors for liquids and various substances suspended or dissolved in fluids. A typical example of heterogeneous formations is fractured porous media (FPM), [2,3], the structure of which is represented as a system of fractures surrounded by porous blocks.

In [6] a transport model in a medium with double porosity was considered taking into account the reversible and irreversible deposition of colloid particles in both zones and the first-order equilibrium mass exchange between the zones. In each zona, i.e. in fractures and porous blocks, a reversible and irreversible deposition of particles with various characteristics occurs, described by linear equations. An analytical solution to the problem is obtained, which is used to describe the results of previous experiments, [5]. Coefficients of mathematical models are defined as the solution to the coefficient inverse problems (CIP), known as identification problems, [8]. It is assumed that the coefficients of the equation depend on the spatial coordinates and are independent of time. The statements of the problems are based on the use of uniqueness theorems for the solution of the CIP proved in [7], [11], [12], [15]. To obtain a unique solution of the CIP, it is required to set an overdetermined set of boundary conditions on the boundary of the zone: the function for which the equation is written or its normal derivative.

Coefficient inverse problems (identification problems) have become the subject of intensive study, especially in recent years. Interest in them is caused primarily by their important applications. They find applications in solving problems of designing oil reservoir development (determining the filtration parameters of reservoirs), [10,10,14,16,17,18] in solving problems of environmental monitoring, etc. The standard CIP statement contains a residual function, which depends on the solution of the corresponding problem of mathematical physics, [14]. Methods for numerical solution of CIP in connection with their applications in underground hydrodynamics were developed in [7], [8], [9], [11], [13].

In this paper, an inhomogeneous two-zone medium is considered a single-zone medium with a source (sink). The second zone is modeled through the source (sink). This approach is fundamentally new because, in fact, the bicontinual medium is presented as monocontinual one. The validity of this approach is justified by the convergence of the results on the basis of the mono-continuous approach to the corresponding results of the bicontinuous approach. In the work, this is done by minimizing the residual function. In addition, it is assumed that in both parts of the first zone there is reversible adsorption of particles with the corresponding kinetic equations. Identification of parameters in the source (sink) term in the mass balance equation is carried out by solving the corresponding CIP using data from [4].

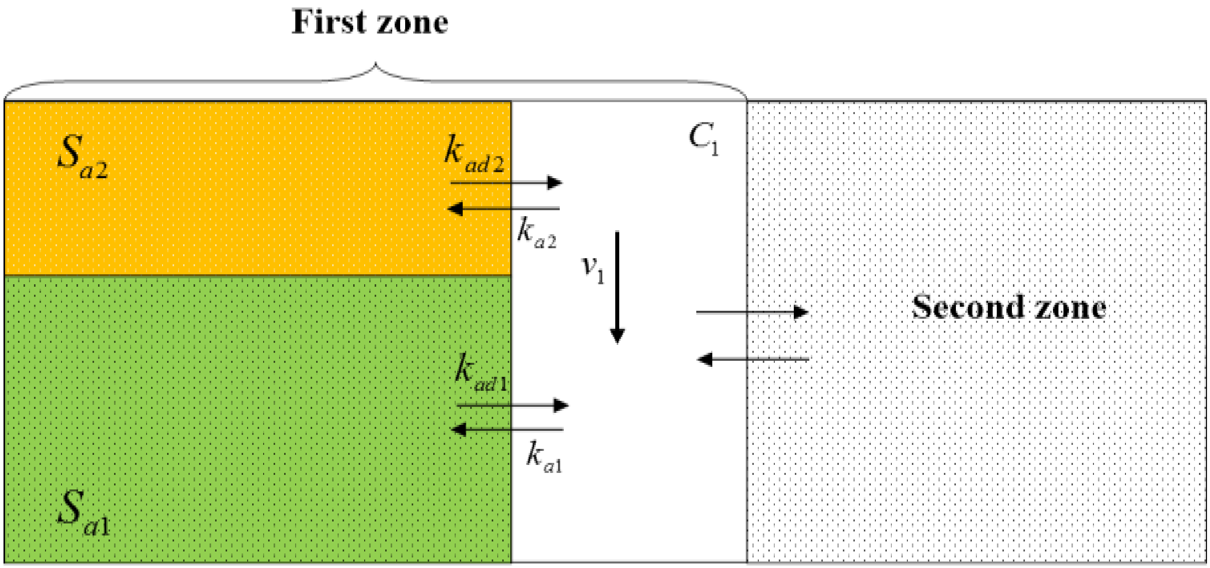

Fig. 1. Scheme of solute transport in a two-zone medium

2. The mathematical model and its numerical implementation

An inhomogeneous porous medium is considered, consisting of well-permeable and relatively low-permeable zones, the diagram of which is shown in Fig. 1. The parameters in the first zone are indicated by index 1. There are two sections in zone 1, in each of which the particle deposition with reversible nonequilibrium nonlinear kinetics occurs. It is believed that such processes also occur in the second zone, but we will not write equations and conditions for it. With the second zone, there is an exchange of substance, which we model by the fractional-order derivative in time of the solute concentration in the first zone. Consequently, in contrast to [4], the concentration field in the second zone is not considered. Note, that the fractional approach was previously used in [19], [20], [21].

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

$$\rho\frac{\partial S_{a1}}{\partial t}+\rho\frac{\partial S_{a2}}{\partial t}+\theta_1\frac{\partial C_1}{\partial t}+a_2\frac{\partial^\gamma C_1}{\partial t^\gamma}=\theta_1 D_1\frac{\partial^2 C_1}{\partial x^2}-\theta_1 v_1\frac{\partial C_1}{\partial x}, \qquad (1)$$

where t **is time**, *s*, *x* **is distance**, m, D_1 **is longitudinal dispersion coefficient**, m^2/s, v_1 **is the fluid velocity**, m/s, C_1 is volume concentration of the solute in the fluid, S_{a1} and S_{a2} are concentrations of deposited particles, m^3/kg, θ_1 is porosity, $\mathrm{m}^3/\mathrm{m}^3$, ρ is medium density, kg/m^3, a_2 *is* **retardation factor related to the mass exchange between two zones,** $s^{\gamma-1}$, γ is the order time derivative with respect to time, $0<\gamma\le 1$.

The deposition of particles in each of the sections of the first zone is reversible with the difference kinetic equations

$$\rho\frac{\partial S_{a1}}{\partial t}=\theta_1 k_{a1}C_1-\rho k_{ad1}S_{a1}, \qquad (2)$$

$$\rho\frac{\partial S_{a2}}{\partial t}=\theta_1 k_{a2}C_1-\rho k_{ad2}S_{a2}, \qquad (3)$$

where k_{a1}, k_{a2} are coefficients of solute deposition from the fluid phase to the solid phase, s^{-1}, k_{ad1}, k_{ad2} are coefficients of substance detachment from the solid phase and transition into liquid, s^{-1}.

Let a fluid with a constant solute concentration c_0 be pumped into the medium initially saturated with pure (without particles) liquid from the initial moment of time. Let us consider such time periods where the concentration field does not reach the right boundary of the medium, $x=\infty$. Under the noted assumptions, the initial and boundary conditions for the problem have the form

$$C_1(0,x)=0,\ S_{a1}(0,x)=0,\ S_{a2}(0,x)=0, \qquad (4)$$

$$C_1(t,0)=c_0, \qquad (5)$$

$$\frac{\partial C_1}{\partial x}(t,\infty)=0. \qquad (6)$$

The problem (1) - (6) although linear, obtaining an analytical solution is difficult, because three concentration fields must be found at the same time. Therefore, to solve the problem, we use the finite difference method. In the considered region $\Omega=\{(t,\ x),\ 0\le t\le T,\ \ 0\le x\le\infty\}$ a uniform grid was introduced

$$\overline{\omega}_{\tau h}=\left\{(t_j,\ x_i);\ t_j=\tau j,\ \ x_i=ih,\ \tau=\frac{T}{J},\ i=\overline{0,I},\ \ j=\overline{0,\ J}\right\},$$

where I is a sufficiently large integer chosen so that segment $[0,\ x_I],\ \ x_i = ih,$ overlaps the area of the calculated change in the fields C_1, S_{a1}, and S_{a2}. h is the grid step in the x direction.

In the open grid area

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

equations (1), (2), (3) were approximated as follows

$$\rho\frac{(S_{a1})_i^{j+1} - (S_{a1})_i^j}{\tau} + \rho\frac{(S_{a2})_i^{j+1} - (S_{a2})_i^j}{\tau} + \theta_1\frac{(C_1)_i^{j+1} - (C_1)_i^j}{\tau} + \frac{a_2}{\Gamma(2-\gamma)} \times$$

$$\times\left[\sum_{k=0}^{j-1}\frac{(C_1)_i^{k+1} - (C_1)_i^k}{\tau}((j-k+1)^{1-\gamma} - (j-k)^{1-\gamma}) + \frac{((C_1)_i^{j+1} - (C_1)_i^j)\tau^{1-\gamma}}{\tau}\right] = \qquad (7)$$

$$= \theta_1 D_1\frac{(C_1)_{i-1}^{j+1} - 2(C_1)_i^{j+1} + (C_1)_{i+1}^{j+1}}{h^2} - \theta_1 v_1\frac{(C_1)_i^{j+1} - (C_1)_{i-1}^{j+1}}{h},$$

$$\rho\frac{(S_{a1})_i^{j+1} - (S_{a1})_i^j}{\tau} = \theta_1 k_{a1}(C_1)_i^j - \rho k_{ad1}(S_{a1})_i^{j+1}, \qquad (8)$$

$$\rho\frac{(S_{a2})_i^{j+1} - (S_{a2})_i^j}{\tau} = \theta_1 k_{a2}(C_1)_i^j - \rho k_{ad2}(S_{a2})_i^{j+1}, \qquad (9)$$

where $(C_1)_i^j$, $(S_{a1})_i^j$, $(S_{a2})_i^j$ are grid values of functions $C_1(t,\ x)$, $S_{a1}(t,\ x)$, $S_{a2}(t,\ x)$ at a given point $(t_j,\ x_i)$.

From the explicit grid equations (8), (9) we determine $(S_{a1})_i^{j+1}$, $(S_{a2})_i^{j+1}$

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

$$(S_{a2})_i^{j+1} = q_{b1}(S_{a2})_i^j + q_{b2}, \qquad (11)$$

where

$$p_{b1} = \frac{1}{1+\tau k_{ad1}},\ \ p_{b2} = \frac{\tau\theta_1 k_{a1}}{\rho + \rho\tau k_{ad1}}(C_1)_i^j,$$

$$q_{b1} = \frac{1}{1+\tau k_{ad2}},\ \ q_{b2} = \frac{\tau\theta_1 k_{a2}}{\rho + \rho\tau k_{ad2}}(C_1)_i^j.$$

The grid equations (7) are reduced to the form

$$A_1(C_1)_{i-1}^{j+1} - B_1(C_1)_i^{j+1} + E_1(C_1)_{i+1}^{j+1} = -(F_1)_i^j, \qquad (12)$$

where

$$A_1 = \frac{\theta_1 D_1\tau}{h^2} + \frac{\theta_1 v_1\tau}{h},$$

$$B_1 = \theta_1 + \frac{2\theta_1 D_1\tau}{h^2} + \frac{\theta_1 v_1\tau}{h} + \frac{a_2\tau^{1-\gamma}}{\Gamma(2-\gamma)}$$

$$E_1 = \frac{\theta_1 D_1 \tau}{h^2},$$

$$(F_1)_i^j = (\theta_1 + \frac{a_2 \tau^{1-\gamma}}{\Gamma(2-\beta)})(C_1)_i^j - \rho((S_{a1})_i^{j+1} - (S_{a1})_i^j) - \rho((S_{a2})_i^{j+1} - (S_{a2})_i^j) - \frac{a_2}{\Gamma(2-\gamma)} \times$$

$$\times \left[\sum_{k=0}^{j-1} ((j-k+1)^{1-\gamma} - (j-k)^{1-\gamma})(C_1)_i^{k+1} - ((j-k+1)^{1-\gamma} - (j-k)^{1-\gamma})(C_1)_i^k \right]$$

The following procedure of computing is used. From (10), (11) $(S_{a1})_i^{j+1}$, $(S_{a2})_i^{j+1}$ are determined, then we solve the system of linear equations (12) by Thomas' algorithm in order to calculate $(C_1)_i^{j+1}$. Since $p_{b1}, q_{b1} < 1$, schemes (10), (11) are stable, and for (12) the stability conditions of the Thomas' algorithm are satisfied.

To assess the performance of the proposed model, it is important to compare the results with the corresponding results, [4]. To do this, we compare the source (stock) terms $\alpha(C_2 - C_1)$ in [4] and $a_2 \frac{\partial^\gamma C_1}{\partial t^\gamma}$ in (1). To quantify the proximity of the results based on the curves was calculated

$$\delta_1 = \int_0^L (I_1 - I_2)^2 dx \qquad (13)$$

for a given value of *t*, where *L* is the conditional boundary of the medium to which the concentration profiles extend,

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

The proximity of the terms I_1 and I_2 should guarantee the proximity of the concentration fields C_1 determined using the proposed approach and the model, [4]. To estimate their proximity, we use the standard deviation (13), only for C_1 determined on the basis of two models, i.e.

$$\delta_2 = \int_0^L \left(C_1^{(1)} - C_1^{(2)}\right)^2 dx,$$

where $C_1^{(1)}$ – concentration field $C_1(t,x)$ for a given *t*, determined according to [4], and $C_1^{(2)}$ – the same as defined here.

For other moments t and α, a_2, γ different estimates can be obtained for δ_1 and δ_2. In principle, to approximate the two models, it is important to set and solve the corresponding coefficient inverse problems by determining of a_2, γ for a given value of α or, conversely, determining of α for a given α and γ.

3.Numerical results and their analysis

In the calculations following initial values of parameters are used:

$c_0 = 0$, $v_1 = 10^{-4}\,\mathrm{m}/s$, $D_1 = v_1 \cdot \alpha_l$, $\alpha_l = 0{,}005$ m, $\rho = 1800\,kg/m^3$, $\theta_1 = 0{,}1$,

$k_{a1} = 3 \cdot 10^{-4} s^{-1}$, $k_{ad1} = 2{,}5 \cdot 10^{-4} s^{-1}$, $k_{a2} = 4 \cdot 10^{-4} s^{-1}$, $k_{ad2} = 2 \cdot 10^{-4} s^{-1}$ and various a_2, γ.

We minimize the functional

$$\Phi(a_2,\gamma)=\int_0^T\int_0^L (I_1-I_2)^2\,dxdt \quad , \qquad (14)$$

that characterizes the standard deviation of I_1 from I_2 for the entire time period. The calculations show that the minimum value of $\Phi(a_2,\gamma)$ is achieved at $a_2=0{,}0006,\ \gamma=0{,}8$.

The proximity of the terms I_1 and I_2 should guarantee the proximity of the concentration fields C_1, determined using the proposed approach and model, [4]. For this, the corresponding profiles are plotted for the data, obtained through minimization of $\Phi(a_2,\gamma)$ (Fig. 2). As can be seen from the graphs, the solutions are close to each other.

For a numerical estimation of their proximity, we use the standard deviation of the type (14), only for the one determined on the basis of two models, i.e.

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

where $C_1^{(1)}$ is the concentration field $C_1(t,x)$ for a given *t*, determined according to [4]. $C_1^{(2)}$ is the same defined here. For the cases analyzed above, the following minimum value of $F(a_2,\gamma)$ was obtained 0,002347387654452 for $a_2=0{,}0006,\ \gamma=0{,}8$.

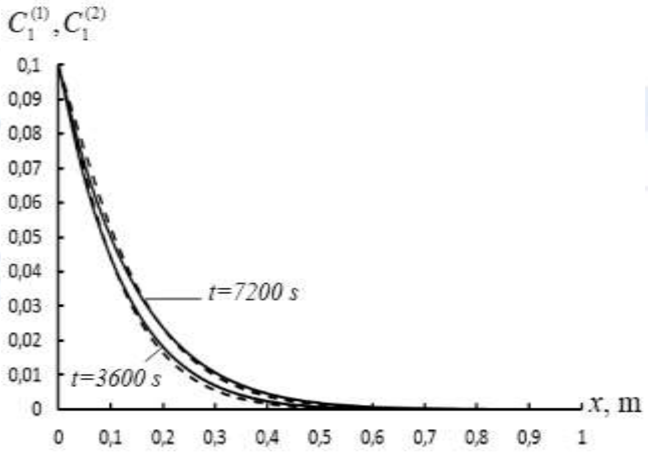

Fig. 2. Comparison of concentration profiles obtained on the basis of two models $a_2=0{,}0006$, $\gamma=0{,}8$, $C_1^{(1)}$ (————), $C_1^{(2)}$ (- - - - - -).

The analysis shows that the simpler model proposed here, with an appropriate choice of parameters, can satisfactorily describe the results of a more complex model, [4].

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