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Numerical Solution of Anomalous Solute Transport in a Two-Zone Fractal Porous Medium

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Abstract. The process of anomalous solute transport in a porous medium is modeled by differential equations with a fractional derivative. The problem of the solute transport in a two-zone porous medium consisting of macropores and micropores. The profiles of changes in the concentrations of suspended particles in the macropore and micropore were determined. The influence of the order of the derivative with respect to the space and time coordinates is estimated, i.e. fractal dimension of the medium, on the characteristics of the solute transport in both zones.

Keywords: filtration · fractal structure · fractional derivative · solute transport · porous medium

1 Introduction

The problem of solute transport in porous media occurs in many technical processes. Mathematical models are widely used in the design and analysis of the solute transport in porous media [1, 2]. If the porous medium is nonhomogeneous (at the micro- and macrolevels), the process of solute transport can be anomalous, i.e., the solute transport does not obey Fick's law [3–5]. In most cases, an nonhomogeneous medium has a fractal dimension, and Fick's law is also written as a fractional derivative depending on the fractal dimension of the medium. This confirms that the process of solute transport proceeds anomally. Solute transport equations based on Fick's law with fractional derivatives have the form of differential equations with fractional derivatives [7–10]. Such equations are not yet well understood. The equations have been studied only in some simple cases. Solving the equations of fractional derivatives by the finite difference method also has its own difficulties [11, 12].

The complex trajectories of liquid and solute particles in aggregates, fracture and porous blocks cause anomalous transport, and the conventional convective transport equation cannot adequately describe anomalous transport. Therefore, such media can be called fractal media. Recently, the interest of researchers in the anomalous solute transport has increased significantly. First of all, this is dictated by the relevance of the problem in terms of applications in various industries and technology. On the other hand, there are many unresolved theoretical issues, in particular, the question of the influence

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of the anomalous nature of the transport on the hydrodynamic parameters has not been fully clarified [13, 14].

The rocks of many oil fields tend to be heterogeneous on both microscopic and macroscopic scales. A typical example of nonhomogeneous porous media are aggregated and fractured-porous media [15–17].

The equations for the solute transport in fractals were first proposed in [18]. In fractured-porous media, the transport equations were analyzed in [20, 21]. It is shown that the order of the fractional derivative in the equations depends on the fractal dimension of the medium.

2 Statement and Numerical Solution of the Problem

In the problem under consideration, the porous medium is divided into two zones, in one zone where the liquid is considered to be mobile, and in the second zone the liquid is considered immobile, but the movement of the solute is observed due to diffusion. Solute transport between these two zones is usually described by a first order kinetic equation. Such a process in the one-dimensional case (a semi-infinite medium) can be written by the following equations

$$\theta_m \frac{\partial c_m}{\partial t} + \gamma \theta_{im} \frac{\partial^\alpha c_{im}}{\partial t^\alpha} = \theta_m D_m \frac{\partial^\beta c_m}{\partial x^\beta} - v_m \theta_m \frac{\partial c_m}{\partial x}, \tag{1}$$

$$\gamma \theta_{im} \frac{\partial^\alpha c_{im}}{\partial t^\alpha} = \omega (c_m - c_{im}), \tag{2}$$

where $\theta_m, \ \theta_{im}$ are the porosity coefficient, $c_m, \ c_{im}$ are the volumetric concentration of the solute, v_m is the average velocity of the solution, γ is the mass transfer coefficient, $[\gamma] = T^{\alpha-1}, \quad [\omega] = T^{-1}$.

The initial and boundary conditions have the form:

$$c_m(0, \ x) = 0, \qquad c_{im}(0, \ x) = 0, \tag{3}$$

$$c_m(t, \ 0) = c_0, \qquad c_m(t, \ \infty) = 0. \tag{4}$$

The orders of fractional derivatives α and β changes in the following interval: $0 < \alpha < 1, \quad 1 < \beta \le 2$.

For the numerical solution of problem (1)–(4), we use the method of finite differences [22]. In the domain, $\Omega = \{0 \le x \le \infty, \ \ 0 \le t \le T\}$ we introduce a uniform grid $\omega_{h\tau} = \left\{(x_i, t_j), \ \ x_i = ih, \ \ i = \overline{0, N}, \ \ h = L/N, \ \ t_j = j\tau, \ \ j = \overline{0, M}, \ \ \tau = T/M\right\}$, where h is the grid step in coordinate x, where τ is the grid step in time, L is the characteristic length of the porous medium.

To approximate fractional time derivatives, we use the following relationship [23–25].

$$\frac{\partial^\alpha c_{im}}{\partial t^\alpha} = \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{l=0}^{j-1}\frac{(c_{im})_i^{l+1}-(c_{im})_i^l}{\tau}\cdot\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)+\frac{(c_{im})_i^{j+1}-(c_{im})_i^j}{\tau}\right].$$

Difference approximations Eq. (1) has the form

$$\begin{aligned}
&\theta_m\frac{(c_m)_i^{j+1}-(c_m)_i^j}{\tau}\\
&\quad+\gamma\theta_{im}\left(\frac{1}{\Gamma(2-\alpha)\tau^\alpha}\left[\sum_{l=0}^{j-1}\left((c_{im})_i^{l+1}-(c_{im})_i^l\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)\right.\right.\\
&+\left.\left.\left((c_{im})_i^{j+1}-(c_{im})_i^j\right)\right]\right)\\
&\quad=\theta_m D_m\frac{1}{\Gamma(3-\beta)*h^\beta}*\left(\sum_{l=0}^{i-1}\left((c_m)_{i-(l+1)}^j-2(c_m)_{i-l}^j+(c_m)_{i-(l-1)}^j\right)\right)\\
&*\left((l+1)^{2-\beta}-(l)^{2-\beta}\right)-v_m\theta_m\frac{(c_m)_{i+1}^j-(c_m)_{i-1}^j}{2h},
\end{aligned}\tag{5}$$

Difference approximations, the kinetics Eq. (2) takes the form

$$\begin{aligned}
&\gamma\theta_{im}\left(\frac{1}{\Gamma(2-\alpha)\tau^\alpha}\left[\sum_{l=0}^{j-1}\left((c_{im})_i^{l+1}-(c_{im})_i^l\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)\right.\right.\\
&\quad+\left.\left.\left((c_{im})_i^{j+1}-(c_{im})_i^j\right)\right]\right)=\omega((c_m)_i^i-(c_{im})_i^{j+1})
\end{aligned}\tag{6}$$

The initial and boundary conditions are approximated as follows

$$(c_m)_i^0=0\qquad(c_{im})_i^0=0\tag{7}$$

$$(c_m)_0^j=0\qquad(c_m)_N^j=0\tag{8}$$

Difference Eq. (5) after some operations takes the form

$$\begin{aligned}
&\theta_m\frac{(c_m)_i^{j+1}-(c_m)_i^j}{\tau}\\
&\quad+\gamma\theta_{im}\left(\frac{1}{\Gamma(2-\alpha)\tau^\alpha}\left[\sum_{l=0}^{j-1}\left((c_{im})_i^{l+1}-(c_{im})_i^l\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)\right.\right.\\
&\quad+\left.\left.\left((c_{im})_i^{j+1}-(c_{im})_i^j\right)\right]\right)\\
&\quad=\theta_m D_m\frac{1}{\Gamma(3-\beta)*h^\beta}*\left(\sum_{l=0}^{i-1}\left((c_m)_{i-(l+1)}^j-2(c_m)_{i-l}^j+(c_m)_{i-(l-1)}^j\right)\right)\\
&\quad*\left((l+1)^{2-\beta}-(l)^{2-\beta}\right)-v_m\theta_m\frac{(c_m)_{i+1}^j-(c_m)_{i-1}^j}{2h},\\
&\quad(c_m)_i^{j+1}=\frac{\tau D_m}{\Gamma(3-\beta)*h^\beta}\left(\sum_{l=0}^{i-1}\left((c_m)_{i-(l+1)}^j-2(c_m)_{i-l}^j+(c_m)_{i-(l-1)}^j\right)\right)
\end{aligned}$$

$$\left((l+1)^{2-\beta}-(l)^{2-\beta}\right)-\tau v_m\frac{(c_m)_{i+1}^j-(c_m)_{i-1}^j}{2h}$$
$$-\frac{\gamma\tau\theta_{im}}{\theta_m\Gamma(2-\alpha)\tau^\alpha}\sum_{l=0}^{j-1}\left((c_{im})_i^{l+1}-(c_{im})_i^l\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)$$
$$+\left((c_{im})_i^{j+1}-(c_{im})_i^j\right)+(c_m)_i^j,$$

After some simple arithmetic operations, the difference kinetics Eq. (6) has the form

$$\sum_{l=0}^{j-1}\left((c_{im})_i^{l+1}-(c_{im})_i^l\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)+\left((c_{im})_i^{j+1}-(c_{im})_i^j\right)$$
$$=\frac{\Gamma(2-\alpha)\tau^\alpha}{\gamma\theta_{im}}\omega((c_m)_i^j-(c_{im})_i^{j+1})$$
$$(c_{im})_i^{j+1}+\frac{\omega\Gamma(2-\alpha)\tau^\alpha}{\gamma\theta_{im}}(c_{im})_i^{j+1}=\frac{\omega\Gamma(2-\alpha)\tau^\alpha}{\gamma\theta_{im}}(c_m)_i^j+(c_{im})_i^j$$
$$-\sum_{l=0}^{j-1}\left((c_{im})_i^{l+1}-(c_{im})_i^l\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)$$
$$(c_{im})_i^{j+1}(1+\frac{\omega\Gamma(2-\alpha)\tau^\alpha}{\gamma\theta_{im}})=\frac{\omega\Gamma(2-\alpha)\tau^\alpha}{\gamma\theta_{im}}(c_m)_i^j+(c_{im})_i^j$$
$$-\sum_{l=0}^{j-1}\left((c_{im})_i^{l+1}-(c_{im})_i^l\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)$$
$$(c_{im})_i^{j+1}=((c_{im})_i^j-\sum_{l=0}^{j-1}\left((c_{im})_i^{l+1}-(c_{im})_i^l\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)$$
$$+\frac{\omega\Gamma(2-\alpha)\tau^\alpha}{\gamma\theta_{im}}(c_m)_i^j)/(1+\frac{\omega\Gamma(2-\alpha)\tau^\alpha}{\gamma\theta_{im}})$$

3 Results and Discussion

For the numerical solution of the problem (1)–(4) the following initial data values were used: $v_m = 10^{-4}\,m/s, D_m = 10^{-5}\,m^\beta/s, \omega = 10^{-6}\,1/s, \tau = 1$, $h = 0.1$, $\theta_m = 0.4\ m^3/m^3$, $\theta_{im} = 0.1\ m^3/m^3$.

Some results of numerical calculations are shown in Fig. 1, 2, 3, 4, 5 and 6. As can be seen from Fig. 1, a decrease in the order of the derivative β from 2 will lead to a more diffuse distribution of the concentration field c_m. Comparing Fig. 1 *a*, *b* one can notice more advanced profiles c_m in the direction of x in case *b*) and *c*). This corresponds to the case of "fast diffusion". This distribution of concentration in the macropore is also reflected in the distribution in the micropore. On Fig. 2 shows the results when decreasing α from 1. This leads to a slowdown in the spread of solute in the zone c_{im} (Fig. 2b). Comparing the Fig. 3a and Fig. 1a one can notice the intensification of the movement of the solute in c_m and c_{im} with a decrease in the values of β. Thus, "fast diffusion" in c_m leads to the same fast diffusion" in c_{im}. Comparing the Fig. 4b and Fig. 2b one can notice a slowdown in the progress of the solute in the micropore with a decrease in the values of α. In Fig. 5 shows the change in the concentration profiles at different values of diffusion coefficient. With an increase in the value of the diffusion coefficient, a wider distribution of the concentration profiles in the zones c_m and, c_{im} respectively, is observed. In Fig. 6 shows the change in concentration profiles at different time points. Based on the results obtained, more widespread concentration profiles were determined with increasing time.

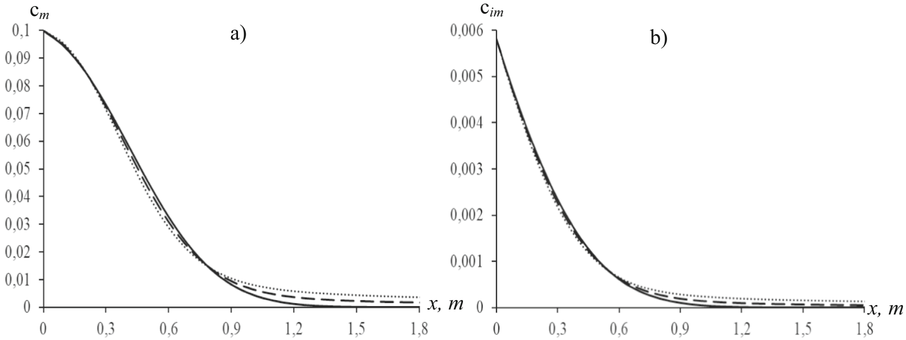

Fig. 1. Concentration c_m (a) and c_{im}, *(b)* profiles at $v_m = 10^{-4}\, m/s$, $D_m = 10^{-5}\, m^{\beta}/s$, $t = 3600\, s$,$\omega = 10^{-6}\, 1/s$, $\gamma = 0.6$,$\alpha = 1$, ·············, $\beta = 1.6$ – – – – , $\beta = 1.8$, ———— $\beta = 2$.

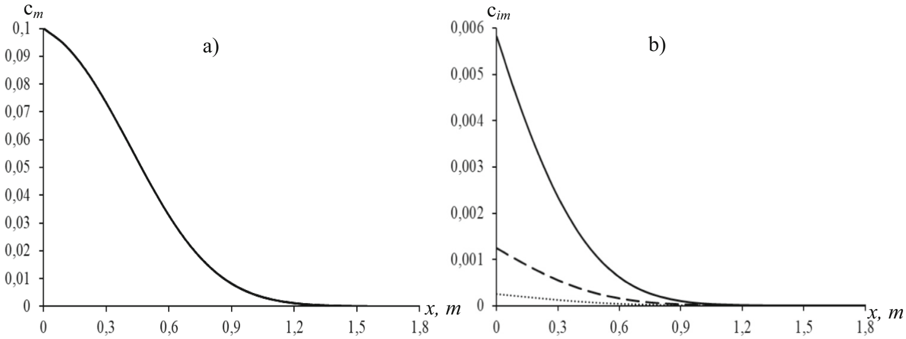

Fig. 2. Concentration c_m (a) and c_{im}, *(b)* profiles at $v_m = 10^{-4}\, m/s$, $D_m = 10^{-5}\, m^{\beta}/s$, $t = 3600\, s$,$\omega = 10^{-6}\, 1/s$, $\gamma = 0.6$,$\beta = 2$ ·············, $\alpha = 0.6$ – – – – -, $\alpha = 0.8$, ———— $\alpha = 1$.

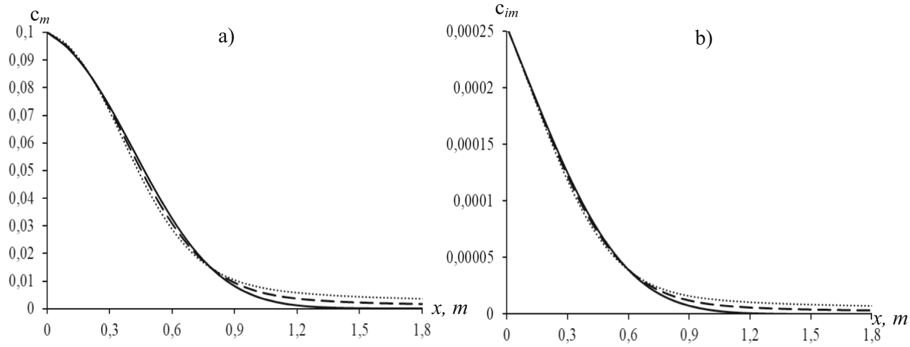

Fig. 3. Concentration c_m (a) and c_{im},, (*b)* profiles at $v_m = 10^{-4}\,m/s$, $D_m = 10^{-5}\,m^{\beta}/s$, $t = 3600\,s$, $\omega = 10^{-6}\,1/s$, $\gamma = 0.6$,$\alpha = 0.6$, ··············, $\beta = 1.6$ – – – – , $\beta = 1.8$, ———— $\beta = 2$.

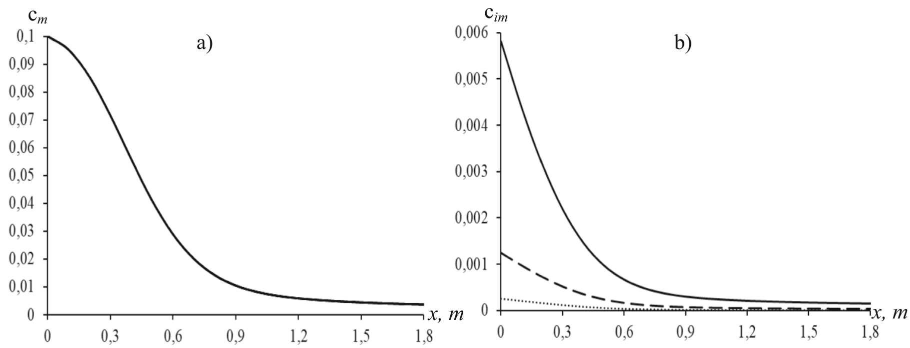

Fig. 4. Concentration c_m (a) and c_{im}, (b*)* profiles at $v_m = 10^{-4}\,m/s$, $D_m = 10^{-5}\,m^{\beta}/s$, $t = 3600\,s$,$\omega = 10^{-6}\,1/s$, $\gamma = 0.6$,$\beta = 1.6$, ··············, $\alpha = 0.6$ – – – – , $\alpha = 0.8$, ———— $\alpha = 1$.

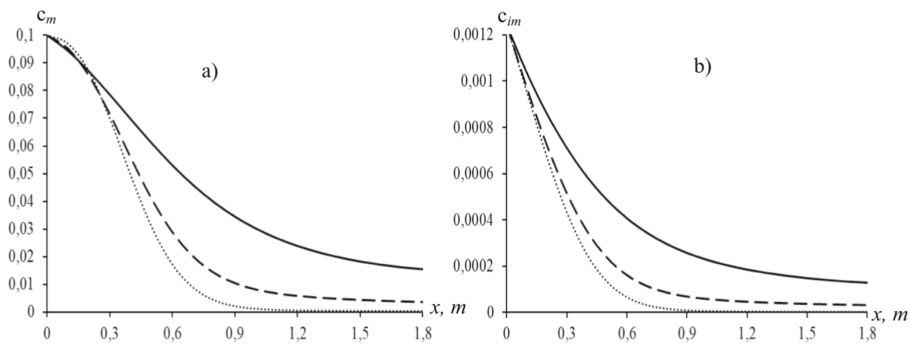

Fig. 5. Concentration c_m (a) and c_{im}, (b) profiles at $\alpha = 0.8$,$\beta = 1.6$,$v_m = 10^{-4}\,m/s$, $t = 3600\,s$,$\omega = 10^{-6}\,1/s$,$\gamma = 0.6$, ················, $D_m = 10^{-6}$ – – – – –, $D_m = 10^{-5}$, ———— $D_m = 5 \cdot 10^{-5}$.

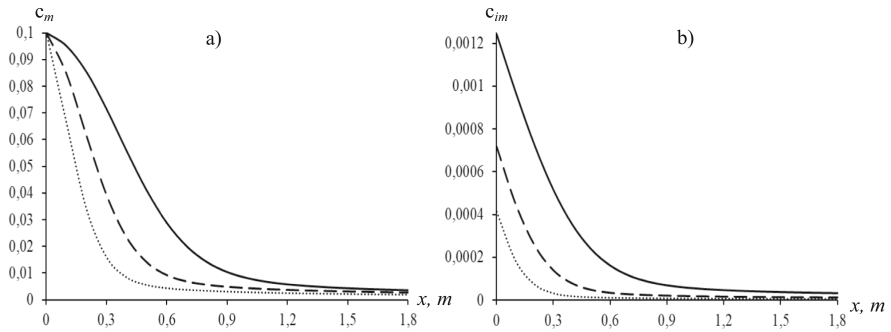

Fig. 6. Concentration c_m (a) and c_{im}, (b) profiles at $\alpha = 0.8, \beta = 1.6, v_m = 10^{-4}\, m/s$, $D_m = 10^{-5}\, m^{\beta}/s$, $\omega = 10^{-6}\, 1/s$, $\gamma = 0.6$, ········t = 900 c, – – – ·t = 1800 c, ——t = 3600 c.

4 Conclusion

In this work, the problem of anomalous transport in porous media with a fractal structure is posed and numerically solved. For the numerical solution of the fractional differential equation, Caputo's definition was used. The numerical analysis shows that the anomalous process significantly affects the characteristics of the solute transport in both zones of the medium, i.e. in both micro and macropores. The anomaly of the transport is characterized by the order of the derivative in the diffusion terms of the transport equations in the macropore (β) and micropore (α). Reducing the order of the derivative in the diffusion terms of the transport equations in both zones leads to "fast diffusion". The decrease in α leads to "slow diffusion" in the micropore.

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