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SOLUTE TRANSPORT IN A TWO-ZONE MEDIUM WITH NONLINEAR KINETICS

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ABSTRACT
In the paper, solute transport in a two-zone medium with different transport characteristics is considered with reversible deposition of colloid solids on the solid surface of two domains of each zones. In one dimension case mass balance equation and two kinetic equations are numerically solved. Influence of reversibility of deposition on transport characteristics is established.

KEYWORDS: adsorption, approximation, fractional derivative, porous media, retardation factor, transit zone.

I. INTRODUCTION

In the process of pumping various mixtures into underground reservoirs, colloidal particles suspended in a liquid can move relatively faster and move long distances in structured media than in media with a homogeneous structure [1-4]. The reason for this is the presence of pathways conducive to the rapid solute transport.

Some mathematical models for describing this phenomenon were presented in works [3,4]. In these models, a two-zone approach was used, where solute transport between zones is modeled by a first-order kinetic equation [5,6].

We use a scheme of a medium with double porosity similar to [7] (Fig. 1). In bicontinuous media, such as fractured porous media, a two-zone approach should be used, but in both zones the fluid is considered mobile. In such media with double porosity or double permeability, the solute transport, like the fluid flow, occurs with different intensities, sometimes contrasting. Note that this approach is also used for macroscopically inhomogeneous media, where convective solute transport can occur in both zones.

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In [8], the solute transport in a medium with double porosity is considered, taking into account the reversible and irreversible deposition of mass in both zones and the first-order equilibrium exchange between the zones. In each zone, i.e. in fractures and porous blocks, there is a reversible and irreversible deposition of a solute with different characteristics described by linear equations. An analytical solution to the problem was obtained, which was used to describe the results of earlier experiments [9].

II. Formulation of the problem.

We use the scheme of a medium with double porosity similar to [7] (Fig. 1). The first zone with index 1 in the designations has a high permeability, and the second zone has a low permeability. In each zones there are two sections, in each of which there is a deposition of mass with irreversible nonequilibrium kinetics.

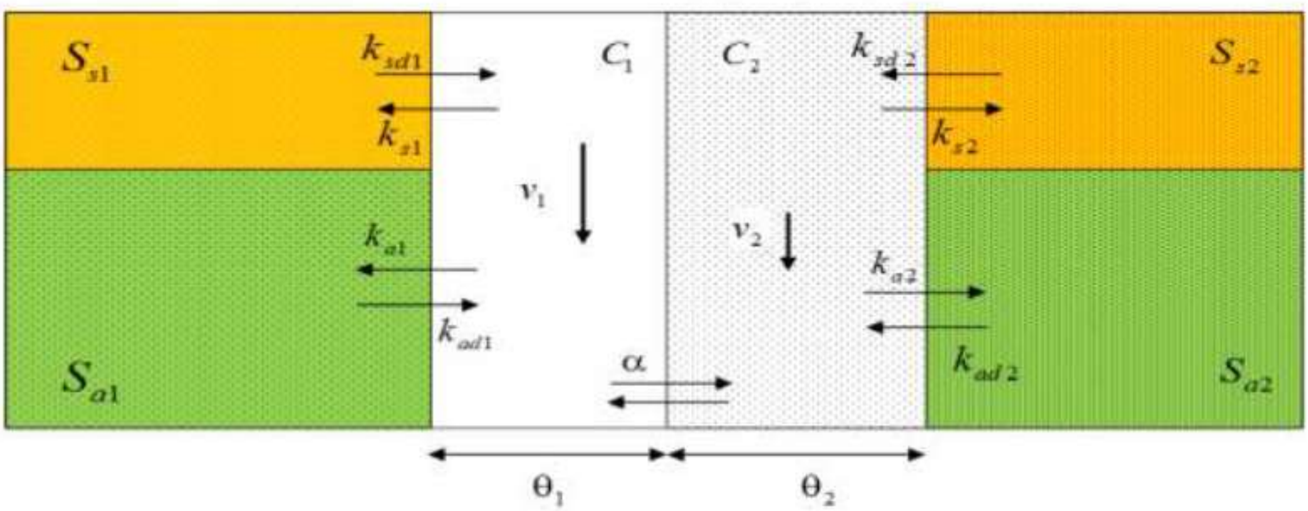

Fig. 1. Scheme of the solute transport in a two-zone medium

Here, in contrast, we will consider nonlinear kinetic equations.
The equations of solute transport in the one-dimensional case are written in the form [10]

$$\rho\frac{\partial S_{al}}{\partial t}+\rho\frac{\partial S_{sl}}{\partial t}+\theta_l\frac{\partial C_l}{\partial t}=\theta_l D_l\frac{\partial^2 C_l}{\partial x^2}-\theta_l v_l\frac{\partial C_l}{\partial x}+\alpha(C_m-C_l)\,, \quad (1)$$

$$(l=1,2;\quad m=2,1)\,,$$

where t - time, *c, x*- distance, м, D_l - longitudinal dispersion coefficient, м^2/c, v_l - fluid velocity, m/s,$v_1<v_2$, C_l - volume concentration of a mass in a liquid,S_{al} и S_{sl} - concentration of deposited mass,m^3/kg, θ_l - porosity of zone, m^3/m^3, ρ - medium density, kg/m^3,α - coefficient of exchange mass between zones, s^{-1}.

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The deposition of mass in each of the sections of the zones occurs reversibly in accordance with the kinetic equations

$$\rho\frac{\partial S_{al}}{\partial t}=\theta_l k_{al}C_l^n-\rho k_{adl}S_{al},\quad (l=1,2)\,, \tag{2}$$

$$\rho\frac{\partial S_{sl}}{\partial t}=\theta_l k_{sl}C_l^n-\rho k_{sdl}S_{sl},\quad (l=1,2)\,, \tag{3}$$

where k_{al}, k_{sl} - coefficients of deposition of mass from fluid phase l to solid phase, s^{-1}, k_{adl}, k_{sdl} - coefficients of separation of mass from solid phase and transition to fluid, s^{-1} ,Let a fluid with a constant concentration of mass c_0 be injected into a medium initially saturated with pure (without solute) fluid from the initial moment of time. Consider such time periods where the concentration field does not reach the right boundary of the medium, $x=\infty$. Under the assumptions noted, the initial and boundary conditions for the problem have the form

$$C_i(0,x)=0,\ S_{al}(0,x)=0,\ S_{sl}(0,x)=0, \tag{4}$$

$$C_l(t,0)=c_0, \tag{5}$$

$$\frac{\partial C_l}{\partial x}(t,\infty)=0,\quad l=1,2. \tag{6}$$

I. NUMERICAL SOLUTION OF THE PROBLEM

Problem (1) - (6) although it is linear, obtaining an analytical solution is difficult, because it is necessary to find simultaneously three fields in each of the zones. Therefore, to solve the problem, we use the finite difference method [11]. In the considered region $\Omega=\{(t,\ x),\ 0\le t\le T,\ \ 0\le x\le\infty\}$, a grid uniform in directions is introduced

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

where I – a sufficiently large integer chosen so that the segment $[0,\ x_I]$ $x_i=ih$, overlapped the area of calculated field changes *C*i, *S*ai and *S*si, h – grid step in direction x.

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

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

$$\rho\frac{(S_{al})_i^{j+1}-(S_{al})_i^j}{\tau}+\rho\frac{(S_{sl})_i^{j+1}-(S_{sl})_i^j}{\tau}+\theta_l\frac{(C_l)_i^{j+1}-(C_l)_i^j}{\tau}=$$
$$\theta_l D_l\frac{(C_l)_{i-1}^{j+1}-2(C_l)_i^{j+1}+(C_l)_{i+1}^{j+1}}{h^2}--\theta_l v_l\frac{(C_l)_i^{j+1}-(C_l)_{i-1}^{j+1}}{h}+\alpha(C_m)_i^j-\alpha(C_l)_i^j\,, \tag{5}$$

$$(l=1,2;\quad m=2,1)\,,$$

$$\rho\frac{(S_{al})_i^{j+1}-(S_{al})_i^j}{\tau}=\theta_l k_{al}(C_l^n)_i^j-\rho k_{adl}(S_{al})_i^{j+1},\qquad (l=1,2)\,, \tag{6}$$

$$\rho\frac{(S_{sl})_i^{j+1}-(S_{sl})_i^j}{\tau}=\theta_l k_{sl}(C_l^n)_i^j-\rho k_{sdl}(S_{sl})_i^{j+1}, \quad (l=1,2), \qquad (7)$$

where $(C_l)_i^j$, $(S_{al})_i^j$, $(S_{sl})_i^j$ - grid function values $C_l(t,x)$, $S_{al}(t,x)$, $S_{sl}(t,x)$, $(l=1,2)$ at the point (t_j, x_i).

From explicit grid equations (6), (7) define $(S_{al})_i^{j+1}$, $(S_{sl})_i^{j+1}$

$$(S_{al})_i^{j+1}=p_{b1}(S_{al})_i^j+p_{b2}, (l=1,2;\ b=1,2), \qquad (8)$$

$$(S_{sl})_i^{j+1}=q_{b1}(S_{sl})_i^j+q_{b2}, \ (l=1,2;\ b=1,2), \qquad (9)$$

where

$$p_{b1}=\frac{1}{1+\tau k_{adl}},\ p_{b2}=\frac{\tau\theta_l k_{al}}{\rho+\rho\tau k_{adl}}(C_l^n)_i^j,\ (l=1,2;\ b=1,2),$$

$$q_{b1}=\frac{1}{1+\tau k_{sdl}},\ q_{b2}=\frac{\tau\theta_l k_{sl}}{\rho+\rho\tau k_{sdl}}(C_l^n)_i^j,\ (l=1,2;\ b=1,2).$$

Grid equations (5) are reduced to the form

$$A_l(C_l)_{i-1}^{j+1}-B_l(C_l)_i^{j+1}+E_l(C_l)_{i+1}^{j+1}=-(F_l)_i^j,\ (l=1,2), \qquad (10)$$

where $A_l=\frac{\theta_l D_l\tau}{h^2}+\frac{\theta_l v_l\tau}{h}$, $B_l=\theta_l+\frac{2\theta_l D_l\tau}{h^2}+\frac{\theta_l v_l\tau}{h}$, $E_l=\frac{\theta_l D_l\tau}{h^2}$,

$(F_l)_i^j=(\theta_l-\alpha\tau)(C_l)_i^j+\alpha\tau(C_m)_i^j-\rho((S_{al})_i^{j+1}-(S_{al})_i^j)-\rho((S_{sl})_i^{j+1}-(S_{sl})_i^j)$,

$(l=1,2;\ m=2,1)$.

The following procedure for calculating solutions is established. According to (8), (9), $(S_{al})_i^{j+1}$, $(S_{sl})_i^{j+1}$ is determined, then solving the system of linear equations (10) by the Thomas' algorithm - $(C_l)_i^{j+1}$, $(l=1,2)$.

Since $p_{b1}, q_{b1}<1$, schemes (8), (9) are stable, and for (10) the stability conditions for the Thomas' algorithm are satisfied $(b=1,2)$.

The calculations used the following values of the initial parameters:

$v_1=10^{-4}m/s$, $v_2=10^{-5}m/s$, $D_1=v_1\cdot\alpha_l$, $D_2=v_2\cdot\alpha_l$, $\theta_1=0{,}1,\ \theta_2=0{,}4$

$k_{a1}=3\cdot10^{-4}s^{-1}$, $k_{ad1}=2{,}5\cdot10^{-4}s^{-1}$,
$k_{s1}=4\cdot10^{-4}s^{-1}$, $k_{sd1}=2\cdot10^{-4}s^{-1}$, $\rho=1800\ kg/m^3$,

$k_{a2}=4\cdot10^{-4}s^{-1}$, $k_{ad2}=2\cdot10^{-4}s^{-1}$,
$k_{s2}=5\cdot10^{-4}s^{-1}$, $k_{sd2}=10^{-4}s^{-1}$,

dispersion $\alpha_l=0{,}005m$.

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IV. RESULTS

Some typical results are shown in Fig. 2-4. It can be seen from Fig. 2 that a decrease in the index n from unity leads to a slowdown in the development of concentration profiles (with the remaining parameters unchanged). At the same time, the concentration of the precipitated mass has an outstripping development (Fig. 3.4). In other words, a decrease in the index *n* with other unchanged values of the remaining parameters leads to an intensification of the deposition of solute in both parts of the zones. As a consequence of this, a lag occurs in the distribution of the concentration of the solute in the mobile fluid of both zones.

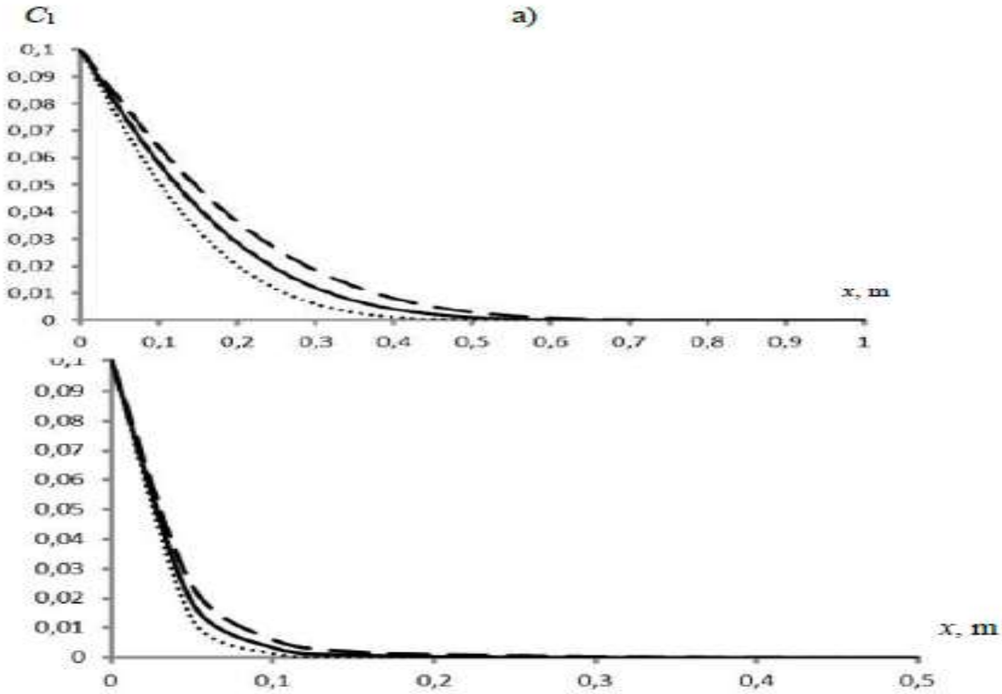
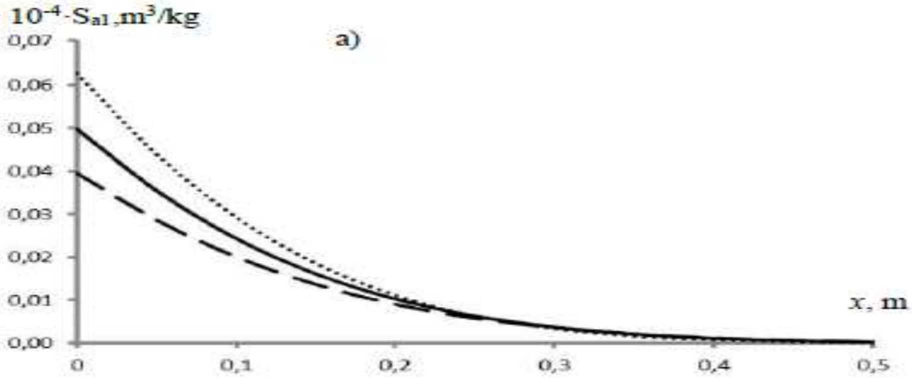


Fig. 2. Concentration profiles C_i at $\alpha=10^{-5}s^{-1}$, t=3600 s,
.... n=0,8, ———— n=0,9, — — n=1,0.



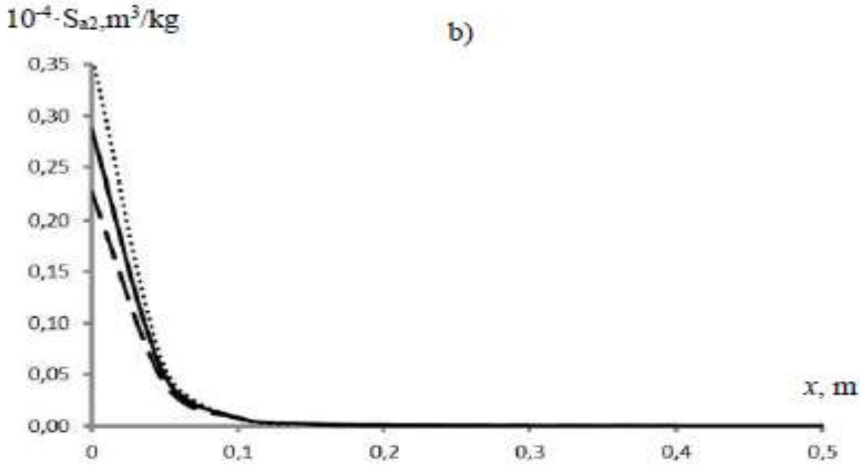


Fig. 3. Concentration profiles S_{a} at $\alpha=10^{-5}s^{-1}$, t=3600 s,
………. n=0,8, ——— n=0,9, — — n=1,0.

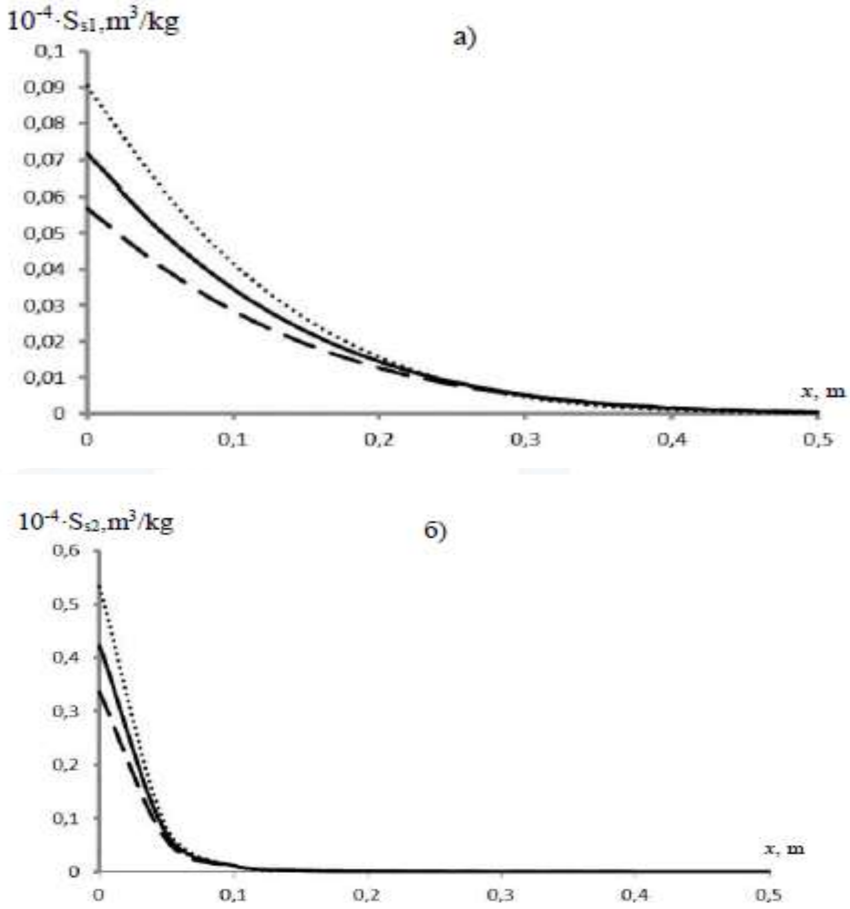


Fig. 3. Concentration profiles S_{a} at $\alpha=10^{-5}s^{-1}$, t=3600 s,
………. n=0,8, ——— n=0,9, — — n=1,0.

V. CONCLUSION

In this paper a solute transport model in a two-zone medium with different transport characteristics is considered with reversible deposition of colloid solids on the solid surface of two domains of each zones. In one dimension case mass balance equation end two kinetic equations are numerically solved. Comparison of the calculation results with case $n=1$ shows that the nonlinear kinetics of adsorption, all other things being equal, leads to an intensification of the adsorption processes of the mass. In this case, the less n is from 1, the more intensive the adsorption occurs. As a consequence of this, a lag occurs in the distribution of the concentration of the substance in the mobile liquid of both zones.

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