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A Problem of Solute Transport in a Cylindrical Porous Media with a Fractal Structure Taking Into Account Nonequilibrium Adsorption Phenomena

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ABSTRACT: The process of anomalous solute transport in a coaxial cylindrical porous media is modeled by differential equations with a fractional derivative. A problem of solute transport in a two-zone cylindrical media consisting of macro- and micropores, with considering adsorption effects, is posed and numerically solved. The profiles of changes in the concentrations of suspended particles and adsorbed solute in macropore and micropore, the surface of local concentration in micropore are determined. The influence of adsorption phenomena and the order of the derivative with respect to the space coordinate, i.e. fractal dimension of the media, on the characteristics of the solute transport in both zones is established.

KEYWORDS: porous media, solute transport, adsorption, fractional derivatives, macropore, micropore.

I. INTRODUCTION

The problems of solute transport and filtration of nonhomogeneous liquids are of great practical importance in many branches of engineering and technology. Oil reservoirs and aquifers may contain areas with a stationary or inactive fluid where fluid filtration and solute transport occurs with the manifestation of several features. Many works have been published where on the basis of experimental studies, several novel effects are revealed. In theoretical works, research is based mainly on phenomenological mathematical models.

Conceptually, models can be divided into two large groups. In the first group of models, the process is described from a microscopic point of view. The solute transport is considered in a single pore or channel with a certain geometry or in a hollow media between aggregates of a certain type. The transfer from macropores to the environment is described by the diffusion equation. Such types of models were analyzed, in particular, in [1,2, 3, 4, 5, 6, 7, 8].

In the second group of models, the geometry of macropores and their environment is not considered explicitly, but instead, channels of various sizes and surrounding rocks are considered as a whole and are studied from a macroscopic point of view. The medium is divided into two parts, in one of which the liquid is considered as active, i.e. mobile, and in the other part - immobile or inactive. Mass transport between two parts (or zones) is usually described by a first order kinetic equation. Models of this type are commonly referred to as “mobile-immobile” type models. As one of the first models of this type, one can indicate the work [9], where the concepts of mobile and immobile parts (zones) of the environment are introduced. This approach was further developed in [10, 11, 12, 13, 14, 15, 16].

In fractals, one of the first, transport equations were proposed in [17]. In fractured-porous media, the transport equations were analyzed in [18, 19, 20]. It is shown that the order of the fractional derivative in the equations depends on the fractal dimension of the media.

In this paper, we numerically investigated the problem of anomalous solute transport in a two-zone cylindrical media, taking into account the phenomenon of adsorption. In both macropores and micropores, the fractal dimension in the diffusion terms is taken into account. The role of adsorption and transport anomalies in changes in concentration fields in both zones is estimated.

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II. FORMULATION OF THE PROBLEM

A cylindrical porous media with a cylindrical macropore in the center is considered, i.e. a research area of the problem consists of two parts: 1) Macroporous media (macropore), having a radius a (zone $\Omega_1\{0 \le x < \infty, 0 \le r \le a\}$), with large pores, characterized by a relatively high porosity and average velocity of the liquid in it, 2) Surrounding cylindrical microporous media (micropore), occupying zone $\Omega_2\{0 \le x < \infty, a \le r \le b\}$, having low or zero porosity and, accordingly, the flow rate (Fig.3.1) [1].

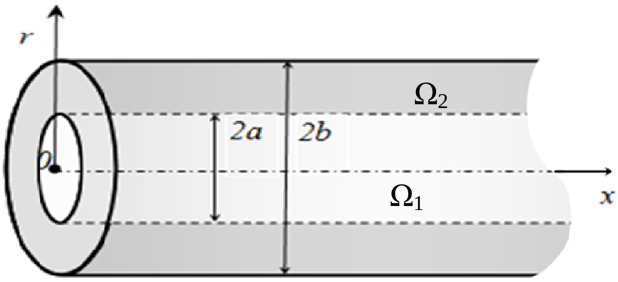

Fig.1. Cylindrical media with cylindrical macropore.

Here, adsorption in a fractal cylindrical media is considered. For this case the transport equations have the form

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

where c_m – average concentration in Ω_1, $\text{м}^3/\text{м}^3$, D_m – diffusion coefficient in macropore, $\text{м}^\beta/\text{c}$, v_m – the average propagation velocity of the substance in Ω_1, $\text{м}/\text{c}$, β – order of derivative ($1 < \beta \le 2$), θ_m, θ_{im} – porosity coefficients of macroporous and microporous media, ρ_m – relative bulk density of the region Ω_1, s_m – concentration of the adsorbed substance in the macropores, c_{im} – average concentration of the substance in the region Ω_2, $\text{м}^3/\text{м}^3$, which is determined from the following relation

$$c_{im} = \frac{2}{b^2 - a^2} \int_a^b r c_a(t,x,r) dr, \tag{2}$$

$$\theta_a \frac{\partial c_a}{\partial t} + \rho_a \frac{\partial s_a}{\partial t} = \theta_a D_a \frac{1}{r^{\beta_1}} \frac{\partial^{\beta_1}}{\partial r^{\beta_1}} \left(r^{\beta_1} \frac{\partial^{\beta_1} c_a}{\partial r^{\beta_1}} \right) \quad a < r < b, \tag{3}$$

where s_a – local concentration of adsorbed substance in the surrounding cylindrical media, ρ_m, ρ_{im} – bulk density of macropores and micropores.

An initial and boundary conditions are taken as:

$$c_m(0,x) = 0, \tag{4}$$

$$c_{im}(0,x) = 0, \tag{5}$$

$$c_a(0,x,r) = 0, \tag{6}$$

$$c_m(t,0) = c_0, \quad c_0 = \text{const}, \tag{7}$$

$$\frac{\partial c_m}{\partial x}(t,\infty) = 0. \tag{8}$$

1. We consider several cases adsorption kinetics. Solute transport a cylindrical media with a cylindrical macropore taking into account nonequilibrium adsorption. In this case, the kinetic adsorption equations are taken as

$$\beta_{ad} \frac{\partial s_m}{\partial t} = k_m c_m - s_m, \tag{9}$$

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$$\beta_{ad}\frac{\partial s_a}{\partial t}=k_d c_a - s_a\,, \qquad (10)$$

where β_{ad} - coefficient of the characteristic transition of time from nonequilibrium to equilibrium adsorption. In general β_{ad} for (4.11) and (4.12) may have different values.

The initial conditions for the concentrations of adsorbed substances are taken in the form

$$s_m(0,x)=0\,, \qquad (11)$$

$$s_a(0,x,r)=0\,. \qquad (12)$$

III. NUMERICAL SOLUTION OF THE PROBLEM

To solve problem (9) - (12), we use the finite difference method [21]. Equations (9) - (10) after approximation take the form

$$(s_m)_i^{k+1}=\frac{\beta_{ad}}{\beta_{ad}+\tau}(s_m)_i^k+\frac{\tau}{\beta_{ad}+\tau}k_m(c_m)_i^k\,, \qquad (13)$$

$$(s_a)_{i,j}^{k+1}=\frac{\beta_{ad}}{\beta_{ad}+\tau}(s_a)_{i,j}^k+\frac{\tau}{\beta_{ad}+\tau}k_a(c_a)_{i,j}^k\,. \qquad (14)$$

In this case, equations (4.1), (4.3) are approximated as follows

$$\frac{(c_m)_i^{k+1}-(c_m)_i^k}{\tau}+\frac{\rho_m}{\theta_m}\frac{(s_m)_i^{k+1}-(s_m)_i^k}{\tau}+\theta\frac{(c_{im})_i^{k+1}-(c_{im})_i^k}{\tau}=$$

$$=\frac{D_m}{\Gamma(3-\beta)h_1^{\beta}}\sum_{l=0}^{i-1}w_{\beta,l}\left((c_m)_{j-(l-1)}^k-2(c_m)_{i-l}^k+(c_m)_{i-(l+1)}^k\right)- \qquad (15)$$

$$-v_m\frac{(c_m)_i^k-(c_m)_{i-1}^k}{h_1},\qquad i=\overline{1,I-1},$$

$$\frac{(c_a)_{i,j}^{k+1}-(c_a)_{i,j}^k}{\tau}+\frac{\rho_a}{\theta_a}\frac{(s_a)_{i,j}^{k+1}-(s_a)_{i,j}^k}{\tau}=$$

$$=D_a\frac{1}{(jh_2)^{\beta_1}}\left\{\frac{h_2^{\beta_1}\left(j+\frac{1}{2}\right)^{\beta_1}-\beta_1 h_2^{\beta_1}\left(j-\frac{1}{2}\right)^{\beta_1}}{\Gamma(2-\beta_1)h_2^{\beta_1}}\cdot\frac{(c_a)_{i,j}^{k+1}-\beta_1(c_a)_{i,j-1}^{k+1}}{\Gamma(2-\beta_1)h_2^{\beta_1}}+\right. \qquad (16)$$

$$\left.+\frac{(jh_2)^{\beta_1}}{\Gamma(3-2\beta_1)h_2^{\beta_1}}\sum_{l=0}^{j-1}w_{2\beta_1,l}\left((c_a)_{i,j-(l-1)}^k-2(c_a)_{i,j-l}^k+(c_a)_{i,j-(l+1)}^k\right)\right\},$$

$$i=\overline{0,I},\; j=\overline{1,J-1}.$$

where $(c_m)_i^k$, $(c_{im})_i^k$, $(c_a)_{i,j}^k$ – grid function values of $c_m(t,x)$, $c_{im}(t,x)$, $c_a(t,x,r)$ at the point (t_k,x_i,r_j) , $\theta=\frac{\theta_{im}}{\theta_m}$, $w_{\beta,l}=(l+1)^{2-\beta}-(l)^{2-\beta}$, $w_{2\beta_1,l}=(l+1)^{2-2\beta_1}-(l)^{2-2\beta_1}$, $\Gamma(\cdot)$ – gamma function, I – is taken large enough so that the concentration profiles do not reach the selected conditional boundary of the region.

The calculation of the solution is as follows. By (13), (14) are determined $(s_m)_i^{k+1}$, $(s_a)_i^{k+1}$. After that, the equation is solved (16) and will be determined $(c_{im})_i^{k+1}$ of (2) by numerical integration. Substituting $(c_{im})_i^{k+1}$ in (15) we determine the concentration field $(c_m)_i^{k+1}$.

Here, adsorption is of a kinetic nature, therefore, in the transition period, the transfer will be different from the equilibrium case.

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Fig.2 and 3 show that the decrease in the values of β from 2 leads to intensification of transfer in both zones, Ω_1 и Ω_2. This, in turn, provides for the intensification of adsorption. The effect of change β_1 on the concentration distribution of suspended and adsorbed substances is shown in fig. 4, 6. Here, as in the case of equilibrium adsorption, transport intensification in Ω_2 adversely affects distribution in Ω_1.

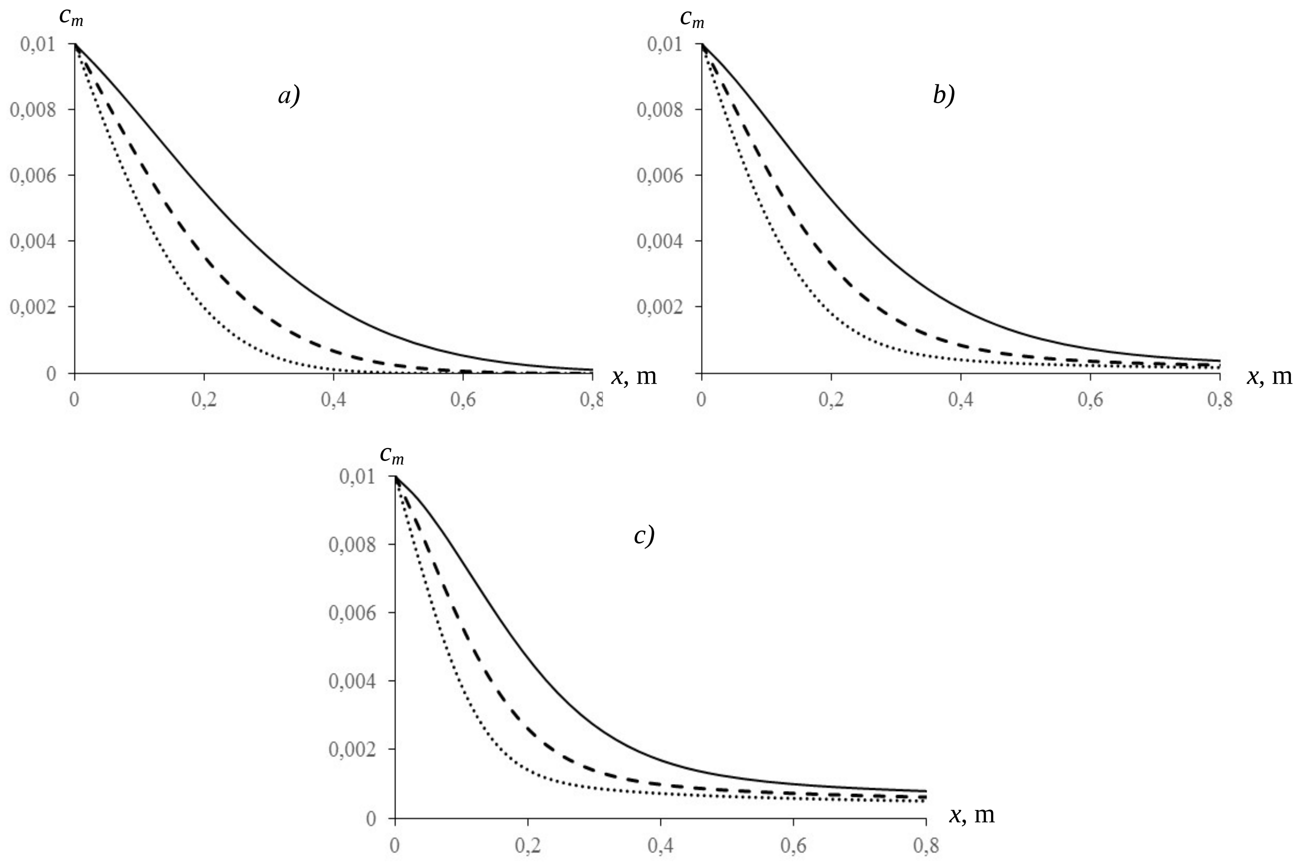

Fig. 2. Concentration profiles c_m at various points in time at $v_m = 10^{-4}$ m/s, $D_a = 10^{-6}$ $\mathrm{m}^{2\beta_1}/\mathrm{s}$, $D_m = 10^{-5}$ $\mathrm{m}^{\beta}/\mathrm{s}$, $k_a = 2{,}5 \cdot 10^{-5}$ m³/kg, $k_m = 10^{-5}$ m³/kg, $\beta_{ad} = 1000$ s, $\beta_1 = 1$, $\beta = 2$ (*a*); $\beta = 1{,}8$ (*b*); $\beta = 1{,}4$ (*c*).

t=900 s, t=1800 s, t=3600 s.

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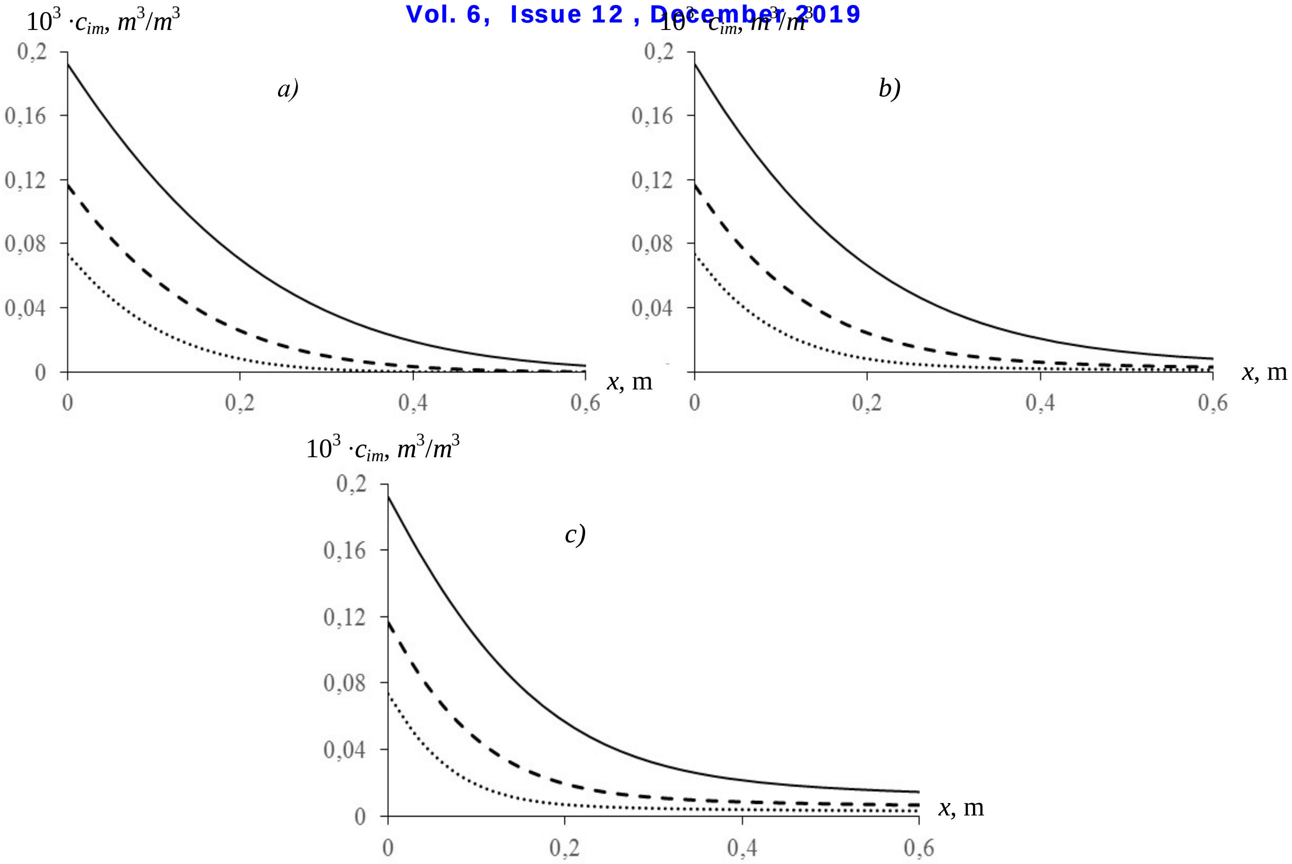

Fig.3. Concentration profiles c_{im} at various points in time at $v_m = 10^{-4}$ m/s, $D_a = 10^{-6}$ $\mathrm{m}^{2\beta_1}/\mathrm{s}$, $D_m = 10^{-5}$ $\mathrm{m}^{\beta}/\mathrm{s}$, $k_a = 2{,}5 \cdot 10^{-5}$ m^3/kg, $k_m = 10^{-5}$ m^3/kg, $\beta_{ad} = 1000$ s, $\beta_1 = 1$, $\beta = 2$ (a); $\beta = 1{,}8$ (b); $\beta = 1{,}4$ (c).

……………… t=900 s, – – – – – t=1800 s, ——— t=3600 s.

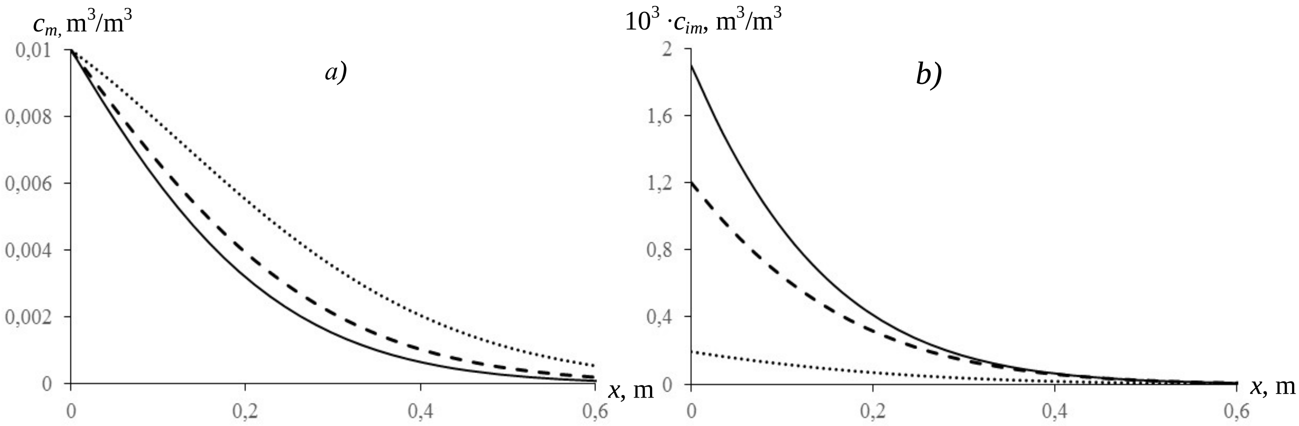

Fig. 4. Concentration profiles c_m (a), c_{im} (b) at $t = 3600$ s, $v_m = 10^{-4}$ m/s, $D_a = 10^{-6}$ $\mathrm{m}^{2\beta_1}/\mathrm{s}$, $D_m = 10^{-5}$ $\mathrm{m}^{\beta}/\mathrm{s}$, $k_a = 2{,}5 \cdot 10^{-5}$ m^3/kg, $k_m = 10^{-5}$ m^3/kg, $\beta_{ad} = 1000$ s,

……………………… $\beta = 2$, $\beta_1 = 1$; – – – – – – – $\beta = 2$, $\beta_1 = 0{,}9$; ——————— $\beta = 2$, $\beta_1 = 0{,}8$.

c_m c_m

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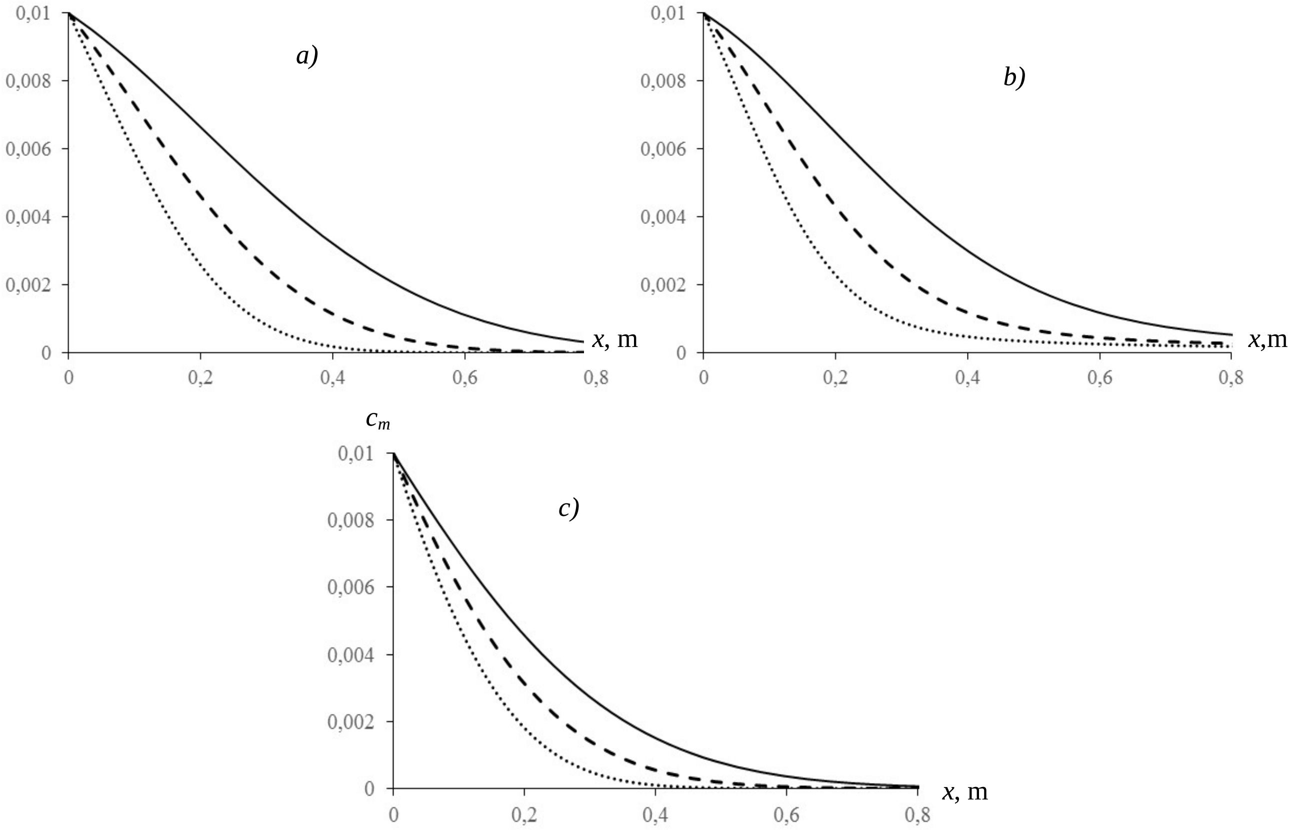
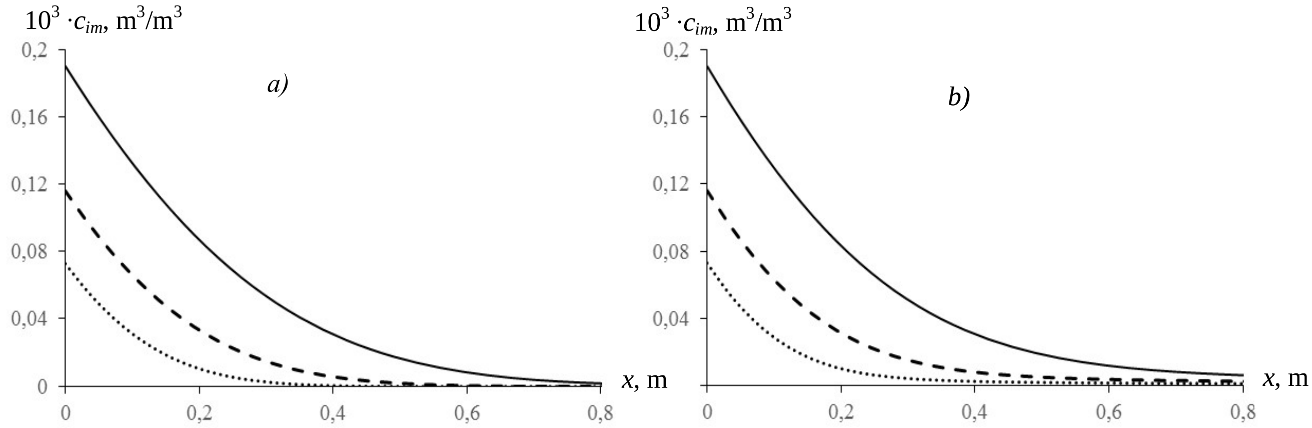


Fig. 5. Concentration profiles c_m at various points in time at $v_m = 10^{-4}$ m/c, $D_a = 10^{-6}$ $\text{m}^{2\beta_1}/\text{s}$, $D_m = 10^{-5}$ $\text{m}^{\beta}/\text{s}$, $k_a = 2{,}5 \cdot 10^{-5}$ m^3/kg, $k_m = 10^{-5}$ m^3/kg, $n = 0{,}9$, $\beta_1 = 1, \beta = 2$ (a); $\beta_1 = 1, \beta = 1{,}8$ (b); $\beta = 2, \beta_1 = 0{,}9$ (c).

.... t=900 s, – – – – – t=1800 s, ——— t=3600 s.



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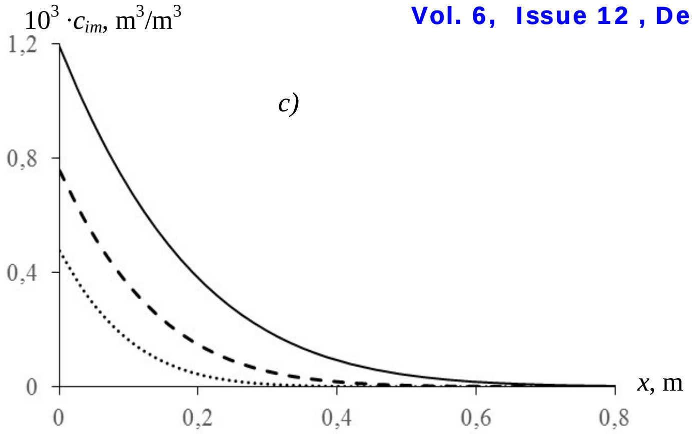

Рис. 6. Concentration profiles c_{im} at various points in time at $v_m = 10^{-4}$ m/s, $D_a = 10^{-6}$ $\mathrm{m}^{2\beta_1}/\mathrm{s}$, $D_m = 10^{-5}$ $\mathrm{m}^{\beta}/\mathrm{s}$, $k_a = 2{,}5 \cdot 10^{-5}$ m³/kg, $k_m = 10^{-5}$ m³/kg, $n = 0.9$, $\beta_1 = 1, \beta = 2$ (a); $\beta_1 = 1, \beta = 1{,}8$ (b); $\beta = 2, \beta_1 = 0{,}9$ (c).

.... t=900 s, — — — — — t=1800 s, ———— t=3600 s.

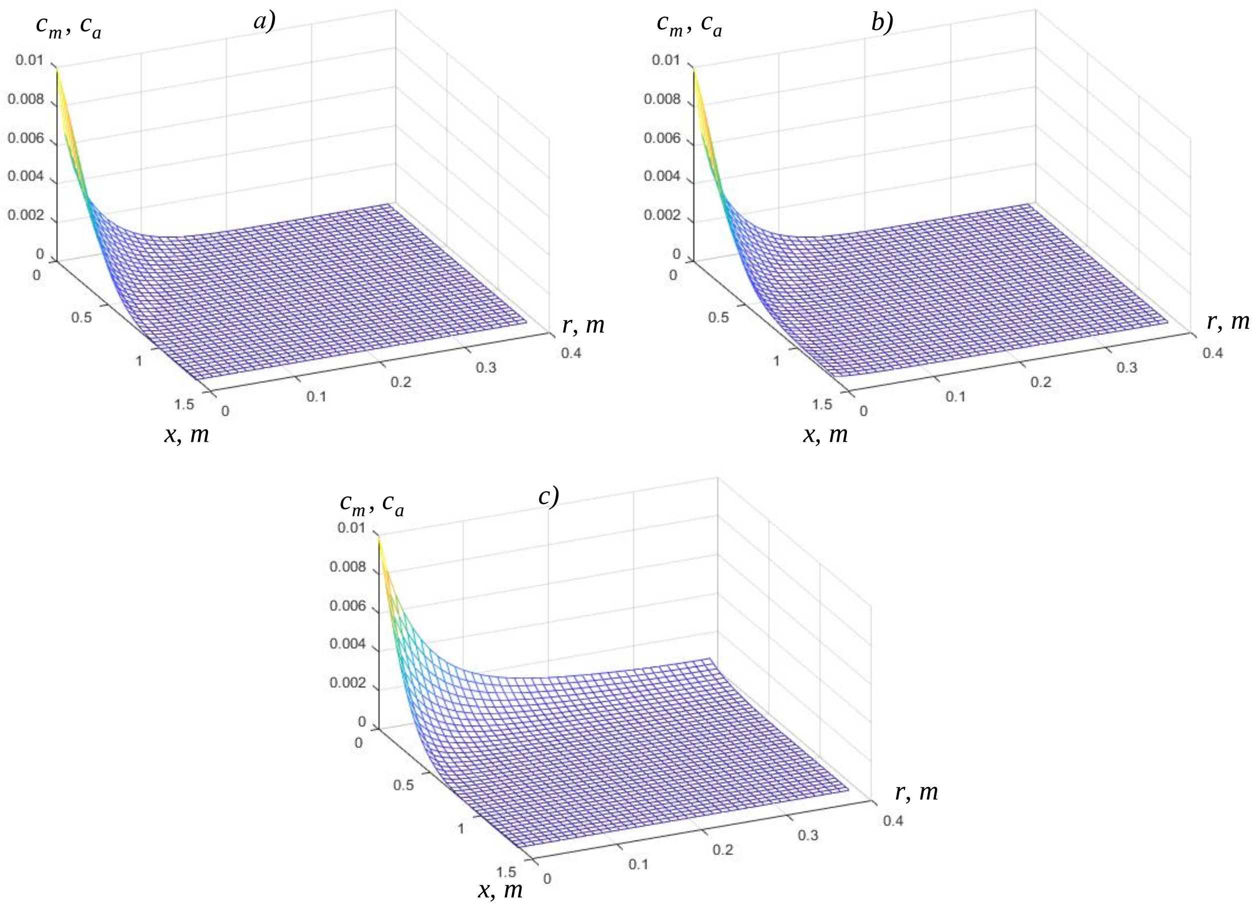

Fig. 7. Surface c_a at t=3600 s, $n = 0{,}9$, $v_m = 10^{-4}$ m/s, $D_a = 10^{-6}$ $\mathrm{m}^{2\beta_1}/\mathrm{s}$, $D_m = 10^{-5}$ $\mathrm{m}^{\beta}/\mathrm{s}$, $k_a = 2{,}5 \cdot 10^{-5}$ м³/kg, $k_m = 10^{-5}$ m³/kg, $\beta_1 = 1, \beta = 2$ (a); $\beta_1 = 1, \beta = 1{,}8$ (b); $\beta = 2, \beta_1 = 0{,}9$ (c).

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IV. CONCLUSIONS

On the basis of computer experiments it is shown that adsorption phenomena lead to a slow propagation of solute concentration profiles in both zones. Nonlinear adsorption with $n<1$ at all other some parameters intensifies adsorption, which affects the general characteristics of the transport. Fractal structure of zones considerably influences on solute transport, leads to “slow” or “fast” diffusion according to where it is taken into account, in diffusion term or in local temporal derivative term in the transport equation.

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