Modeling the Process of Anomalous Solute Transport in a Porous Medium based on a Fractional Balance Equation

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Abstract: - The paper explores a mathematical model for the anomalous solute transport within a porous medium. This model encompasses the mass balance equation and the kinetic equation. To solve the problem, a numerical algorithm for computer experimentation is developed on the basis of the finite difference method. Based on numerical results, the main characteristics of solute transport in a porous medium are established. Influences of model parameters on the transport and deposition of suspended particles of suspension in porous media are analysed. The anomalies of solute transport and the multi-stage nature of deposition kinetics can induce effects that differ from those typically observed in the normal solute transport with single-stage particle deposition kinetics.

Key-Words: - deep bed filtration, finite difference method, multistage deposition, porous media, mathematical model, two-component suspension.

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1 Introduction

Understanding the dynamics of solute transport in a porous medium is essential for addressing environmental concerns and optimizing industrial processes, [1]. Modeling and simulation are among the most widely used approaches for analyzing such problems, [2], [3].

The hydrodynamic dispersion theory stands out as one of the frequently used frameworks for describing the solute transport in porous media, [4]. The equation governing the transport of nonreactive contaminants, known as the advection-dispersion equation, can be formulated as follows, [4]:

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) - v\frac{\partial c}{\partial x}$$

where c is the solute concentration, D is the hydrodynamic dispersion (diffusion) coefficient, and v is the average pore velocity of solute transport.

Traditional modeling of solute transport in porous media is often characterized by Fick's rule of diffusion and the classical advection–dispersion equation, [5], [6]. These models presume that solute transport adheres to standard diffusion, defined by a linear correlation between mean square displacement and time. Numerous experimental and field studies have shown that solute transport in heterogeneous and broken porous media frequently diverges from Fickian behavior, [7], [8], [9]. Anomalous transport, resulting from pore-scale variability, preferential flow channels, and long-tailed residence time distributions, cannot be sufficiently represented by the advection–dispersion equation. As investigations into real-world porous media systems have advanced, it has become increasingly evident that this classical theories may not adequately describe the complexity of transport phenomena, particularly in heterogeneous environments, [10]. In the last decades, there has been a growing doubt regarding the application of the traditional advection-dispersion equation based on Fickian-type dispersion. This has led to the introduction of alternative non-Fickian dispersion models. Researchers such as [11] proposed that anomalous transport in a sand bed can be better explained by the continuous time random walk theory. Building on Lévy motion theory [12], developed the fractional advection-dispersion equation to capture non-Fickian transport. Studies as [13] demonstrated that the fractional advection-dispersion equation outperforms the advection-dispersion equation in modeling breakthrough curves, especially in representing the long tails.

Significant results were achieved in the research of problems of mathematical modeling of anomalous solute transport processes in porous media and in solving actual theoretical and practical issues. The purpose of the research is to improve mathematical models of the process of solute transport in porous media, taking into account the multi-stage process of deposition formation due to different phenomena, and to develop a numerical algorithm for solving the problem.

2 Problem Formulation

We consider a finite layer with porosity m at the initial value of time and filled with a homogeneous liquid (that is, a liquid without suspended particles). Starting from $t > 0$ at the point $x = 0$, an inhomogeneous liquid with concentration c_0 injected with filtration velocity $v(t) = v_0 = \text{const}$.

The model of inhomogeneous liquid filtration in a porous medium usually consists of the balance and kinetic equations of suspended particles, [14].

The balance equation for the one-dimensional case is as follows, [14], [15]:

$$m\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} + \frac{\partial \rho}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \qquad (1)$$

where c is suspension concentration, v is filtration velocity, m is porosity, ρ is concentration of deposition, D is diffusion coefficient.

In recent years, the kinetics of multi-stage sediment formation have been widely used to fully describe these processes, [15], [16].

$$\frac{\partial \rho}{\partial t} = \begin{cases} k_r v c, & 0 < \rho \le \rho_1 \\ k_a v c - k_d \rho, & \rho_1 < \rho < \rho_0 \\ 0, & \rho = \rho_0 \end{cases} \qquad (2)$$

where ρ_0 is the total capacity of the filter, ρ_1 is the parameter characterizing the "charging" limit of ρ, k_r Is the kinetic coefficient related to the "charging" effect, k_a is the coefficient characterizing the deposition of solid particles, k_d Is the coefficient characterizing the release of solid particles.

Anomalous (or not obeying Fick's law) transport is recognized as a common phenomenon in porous media, where the extreme complexity of the pore space geometry strongly affects the flow and migration processes in them. The existence of such environments has been confirmed in many field and laboratory experiments, [17]. Problems of anomalous mass transfer in porous media are of great practical importance in many fields of engineering and technology.

The model used here is an improved version of the models available in the literature, [11], [16]:

$$m_0\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} + \frac{\partial \rho}{\partial t} = D\frac{\partial^\alpha c}{\partial x^\alpha} \qquad (3)$$

where α is the order of the derivative $(1 < \alpha \le 2)$.

The initial and boundary conditions are as follows.

$$c(0,t) = c_0 = \text{const}$$
$$\frac{\partial c}{\partial x} = 0, x = L, t > 0$$
$$c(x,0) = 0,$$
$$\rho(x,0) = 0. \qquad (4)$$

3 Problem Solution

To solve the problem (2) - (4), we use the finite differences method, [18]. In the field $D = \{0 \leq x < L, 0 \leq t \leq T\}$, let's enter a net, where T is the maximal value of time in which the process is studied. For this, the interval $[0, L]$ will be divided with step h into N pieces and $[0, T]$ will be divided with step τ. As a result, we obtain the following net.

$$\omega_{h\tau} = \{(x_i, t_j), x_i = ih, i = 0,1,\dots,N, \\ h = L/N, t_j = j\tau, j = 0,1,\dots,J, \tau = T/J\}$$

Instead of functions $c(t,x), \rho(t,x)$ we use net functions, which acceptance values c_i^j, ρ_i^j at the nodes (x_i, t_j).

We approximate the system (2) - (4) in the net. $\omega_{h\tau}$. We use the integral form of the fraction derivative in equation (3). While the integral form can be discretized as follows:

$$\frac{\partial^\alpha c}{\partial x^\alpha} = \frac{1}{\Gamma(3-\alpha) \cdot h^\alpha} \cdot \left(\sum_{k=0}^{i-1} \left((c)_{i-(k+1)}^j - 2(c)_{i-k}^j + (c)_{i-(k-1)}^j \right) \right) \left((k+1)^{2-\alpha} - (k)^{2-\alpha} \right) \quad (5)$$

where $\Gamma(\cdot)$ is the Gamma function.

$$m\frac{c_i^{j+1} - c_i^j}{\tau} + v\frac{c_i^{j+1} - c_{i-1}^{j+1}}{h} + \frac{\rho_i^j - \rho_i^{j-1}}{\tau} = \frac{1}{\Gamma(3-\alpha) \cdot h^\alpha} \left(\sum_{k=0}^{i-1} \left((c)_{i-(k+1)}^j - 2(c)_{i-k}^j + (c)_{i-(k-1)}^j \right) \right) \quad (6)$$

$$\frac{\rho_i^{j+1} - \rho_i^j}{\tau} = \begin{cases} k_r v c_i^j, & 0 < \rho_i^j \leq \rho_1 \\ k_a v c_i^j - k_d \rho_i^j, & \rho_1 < \rho_i^j < \rho_0 \\ 0, & \rho_i^j = \rho_0 \end{cases} \quad (7)$$

Initial and boundary conditions (3) are also expressed in the net form.

$$\begin{aligned} & c_i^j = 0, \rho_i^j = 0, i = \overline{0,I}, j = 0 \\ & c_i^j = c_0, i = 0, j = \overline{0,J} \\ & c_{i+1}^j - c_i^j = 0, i = I, j = \overline{0,J} \end{aligned} \quad (8)$$

Calculations are carried out in the following sequence: from relations (8), the values of c_i^j, and ρ_i^j will be found in the zero layer. Then, from the Equation (7), we will find ρ_i^j In the next layer. Finally we we will find. c_i^j at the corresponding points in the higher layer.

4 Results and Discussion

To solve the problem (2)-(4), using approximations and the algorithm given above, a software tool has been created in Python. Numerical results obtained for different parameter values. Received results analysis done, evaluated the effect of the anomaly on transport characteristics. During the solving of the problem following values of parameters were used: $\rho_0 = 0.1, \rho_1 = 0.005,\ c_0 = 0{,}05, m_0 = 0.3, v = 10^{-4}$ m/s, $D = 10^{-5}$ m^2/s, $k_r = 32$ s^{-1}, $k_a = 42$ s^{-1}, $k_d = 0.002$ s^{-1}. Values of other parameters are given under the graphics.

Figure 1, Figure 2 and Figure 3 show the changing profiles of the relative concentration of suspended particles (c/c_0) and the deposition concentration (ρ) over time.

It can be seen from the graphs that over time, both fields move towards the inner part of the porous media, and at the same time, their values increase at fixed points (Figure 1, Figure 2 and Figure 3).

At $\alpha = 2$ when $t = 1600$ s from the time starting only at the point $x = 0$, deposition concentration reached its own maximum (Figure 1 b). At the larger values of time in the point near $x = 0$, deposition concentration also reached its own maximum value of achieving as shown (Figure 1b).

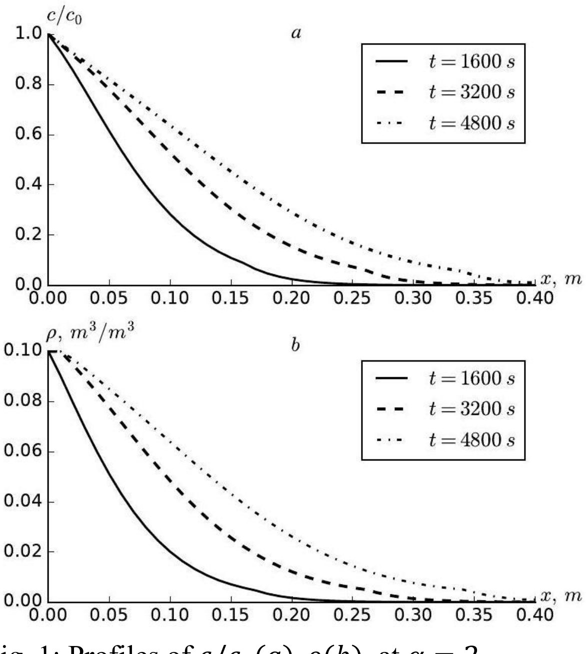

Fig. 1: Profiles of $c/c_0(a), \rho(b)$, at $\alpha = 2$
Source: Created by the authors

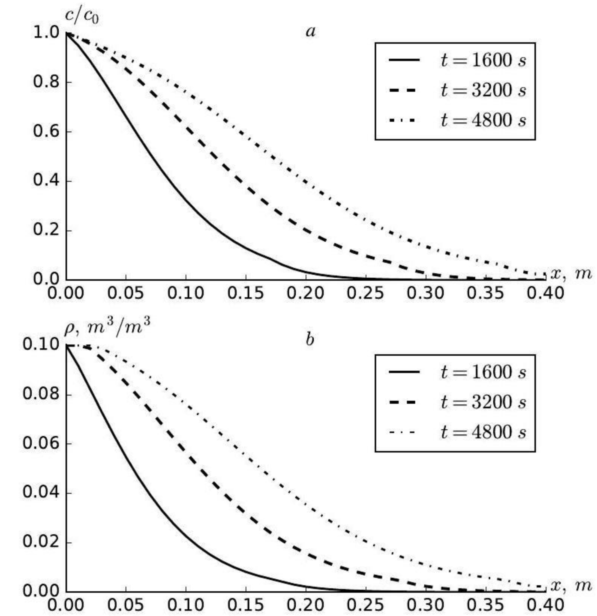

Fig. 2: Profiles of $c/c_0(a), \rho(b)$, at $\alpha = 1.8$
Source: Created by the authors

At $\alpha = 2$ the concentration of suspended particles in the liquid at $t = 1600$ s has reached 0.25 m of the medium, at $t = 3200$ s, this indicator is in 0.35 m, at $t = 4800$ s can be observed that it has reached the end of the porous medium (Figure 1a).

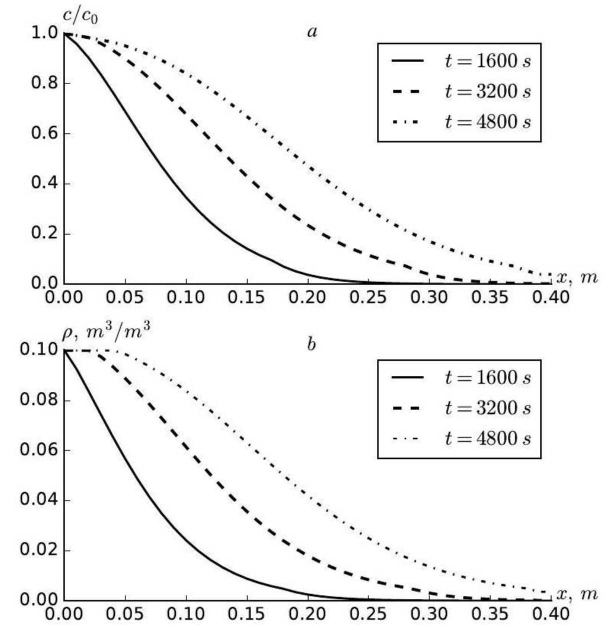

Fig. 3: Profiles of $c/c_0(a), \rho(b)$, at $\alpha = 1.6$
Source: Created by the authors

When the order of the fractional derivative in equation (3) is reduced to $\alpha = 1.8$, it can be seen that the profiles of (c/c_0) and (ρ) are spread wider (Figure 2) and their values at fixed points are larger than when $\alpha = 2$. This is explained by the fact that fast diffusion (superdiffusion) is observed, and therefore, the concentration profiles spread more widely.

Decreasing the value of α up to 1.6 provides to relatively more wider to spread of (c/c_0) and (ρ) concentrations than $\alpha = 1.8$ (Figure 3). This is especially so for deposition concentration ρ of in their profiles $t = 3200$ s and $t = 4800$ s, when it is more obvious (Figure 3b). $t = 3200$ s when almost $x = 0.035$ m to the distance has been pore environment in the part sediment concentration his own maximum to the value achieved, $t = 4800$ s, and - this indicator 0,05 m that it also passed to see possible (Figure 3b).

Figure 4 compares the distribution profiles of (c/c_0) and (ρ) concentrations at $t = 4800$ s for different values of the fractional derivative α. It can be observed that decreasing the values of α leads to an increase in the values of both concentrations at all points of the layer (Figure 4). It is observed that the deposition concentration reaches its maximum value at points close to the point $x = 0$ and is further shifted towards the inner side of the porous medium with increasing value of α. We can see that the occurrence of the fast diffusion phenomenon also increases the intensity of sediment formation.

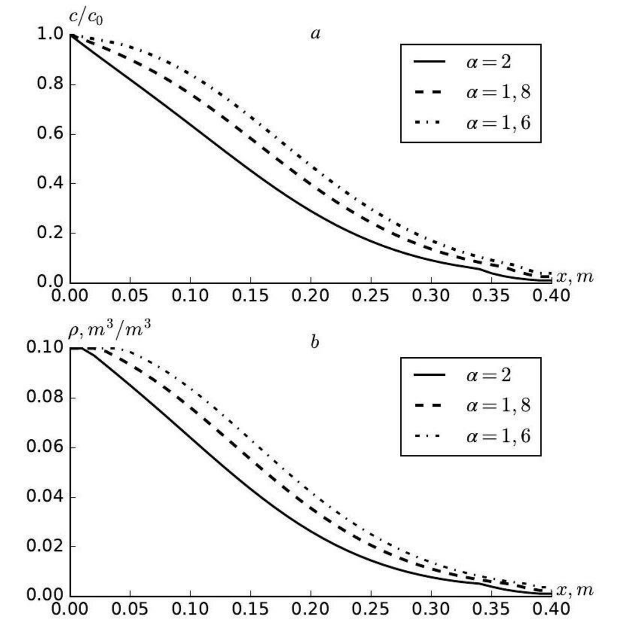

Fig. 4: Profiles of $c/c_0(a), \rho(b)$, at $t = 4800s$ and different values of α
Source: Created by the authors

Figure 5 shows the changing dynamics of deposition concentration ρ at fixed points at different values of α. Figure 5a shows the results for the point $x = 0.02$ m and Figure 5b $-$ for $=$

0.04 m. Here, also, it can be observed that at both points and at all values of time, decreasing the order of the derivative α leads to an increase in the value of ρ. It can be seen from the graphs that at $\alpha = 2$ even at $t = 5000$ s at the point $x = 0.02m$, the deposition concentration has not reached its maximum value of 0.01, that is, the depositing process is still ongoing (Figure 5a). At $\alpha = 1.8$ approximately ≈ 3500 s, and at $\alpha = 1.6$ at $t \approx 3200s$ the concentration of deposition reached its maximum value at the point $x = 0.02m$ (Figure 5a). At the point $x = 0.4$ during the studied time, it can be observed that the deposition reaches its maximum value, and the formation of deposition has stopped only at $\alpha = 1.6$, and at $\alpha = 1.8$ and $\alpha = 2$, formation of deposition is still ongoing.

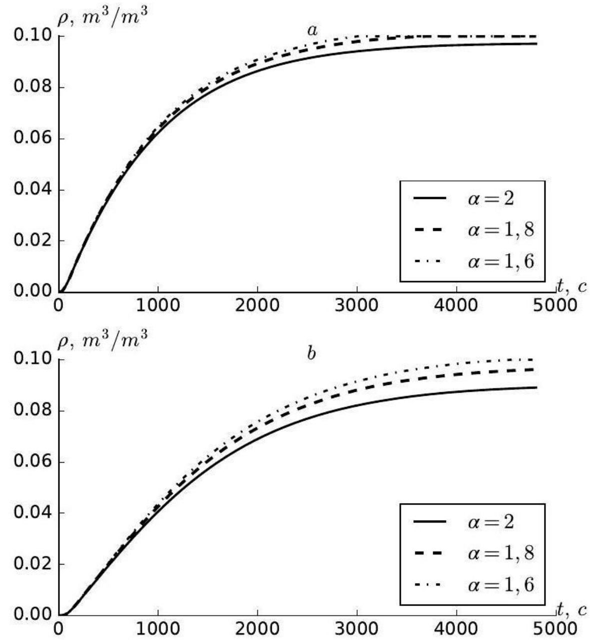

Fig. 5: The dynamics of change of deposition concentration ρ at points $x = 0.02$ (a) and $x = 0.04$ (b) at $t = 4800s$ and different values of α
Source: Created by the authors

Figure 6 shows the changing dynamics of deposition concentration c/c_0 at fixed points at different values of α. Figure 6a shows the results for the point $x = 0.02$ m and Figure 6b – for $=$ 0.04 m. It can be observed that at both points and for all studied times, decreasing the order of the derivative α leads to an increase in the concentration. Some sharp changes can be observed due to the multi-stage characteristics of the deposition kinetics. This behavior is observed at the early stage of the process, as the 'charging' effect is completed very rapidly.

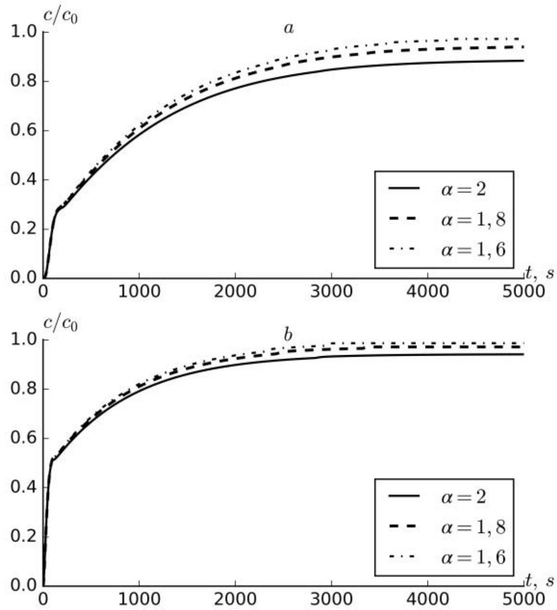

Fig. 6: The dynamics of change of concentration c/c_0 at points $x = 0.02$ (a) and $x = 0.04$ (b) at $t = 4800s$ and different values of α
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5 Conclusion

This paper is aimed at the improvement of mathematical models of the process of anomalous solute transport in porous media and their numerical solution, taking into account the multi-stage process of deposition formation. Mechanisms and kinetics of particle deposition on pore walls, including multi-stage kinetics, were analyzed. Methods of numerical implementation of mathematical models of anomalous solute transport in porous media were analyzed. Unlike the previous scientific works, the influence of anomalous diffusion and fractional derivative multistage kinetics on the process of solute transport was evaluated. The mathematical model of the anomalous solute transport process in the porous medium was improved based on the system of differential equations with fractional derivatives in the balance equation. Based on the improved model, an effective algorithm was developed based on the finite difference method for solving problems numerically, and a software tool was created for conducting computational experiments. It was shown that the decrease of the order of the derivative in the diffusion term in the balance equation from 2 leads to the acceleration of the diffusion of the solute, which, in turn, leads to an increase in the intensity of deposition formation.
Future research may expand the model to incorporate heterogeneous porous media with

spatially variable characteristics and interactions among numerous solute species. Additional optimization of numerical techniques for accelerated and more efficient simulations is also anticipated. Furthermore, doing a sensitivity analysis of model parameters and systematically comparing them with experimental data may yield profound insights into the mechanisms underlying anomalous solute transport and multi-stage deposition processes.

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Conflict of Interest

The authors have no conflicts of interest to declare that are relevant to the content of this article.

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