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Model of Solute Transport in a Porous Medium with Multi-Term Time Fractional Diffusion Equation

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Abstract. The manuscript considers the numerical solution of the multi-term time fractional diffusion equations in a finite region. We know that anomalous solute transport is modeled by differential equations with a fractional derivative. The profiles of changes in the concentration of the solute were determined. The influence of the order of the derivative with respect to the coordinate and time is estimated, i.e. fractal dimension of the medium, on the characteristics of the solute transport. The influence of the anomalous convective-diffusion on the transport characteristics is also studied. The results are analyzed for the case when the diffusion equation contains the sum of terms with different orders of time derivative.

INTRODUCTION

Recently, questions of mathematical modeling of processes of anomalous solute transport in porous media have attracted much attention. In principle, modeling approaches are based on the law of mass balance in a certain control volume using additional phenomenological relationships. The process of transfer of substances in a porous medium is determined by many factors, such as convective transfer, diffusion, hydrodynamic dispersion, adsorption, deposition in pores, their release with transition to a mobile state, etc. Convective transfer, diffusion, hydrodynamic dispersion, local changes in concentration can be described by the equation conservation of mass [1-5].

In [6-8], the problem was solved for the one-dimensional advection-dispersion equation with variable coefficients using an explicit finite-difference scheme, then the results were extended to the case of a two-dimensional equation in semi-infinite media [9-12]. It is known that hydrodynamic dispersion depends on the flow velocity [13]. In [14-16] a mathematical model is presented for two-dimensional solute transport in a semi-infinite inhomogeneous porous medium.

In one approach to modeling anomalous phenomena during the solute transport in porous media, the local time derivative in the diffusion equation is replaced by a fractional derivative α. Typically the order of the derivative can vary from 0 to 1, i.e. $0<\alpha<1$. There are known works where α it is taken from the interval from 0 to 2, i.e. $0<\alpha<2$. In the general case , the order of the derivative can be a variable quantity, depending on both time and spatial coordinates [17, 18]. As an alternative approach, it was proposed to use multi-term time fractional diffusion equations [19-23].

In [19], a multi-term time fractional diffusion wave equation with homogeneous and nonhomogeneous boundary conditions was solved using the method of separation of variables. It is noted that, in contrast to the single-term case, the solution to the polynomial fractional-wave diffusion equation is not necessarily non-negative and, therefore, does not represent anomalous diffusion of any kind.

In [20], the method of separation of variables is used to solve the multi-term time fractional diffusion wave equation. The fractional derivative with respect to time is defined in Caputo's definition.

In [21], multi-term time fractional derivatives of the wave diffusion equation were considered. Multi-term time fractional derivatives are defined in the Caputo definition, the orders of which belong to the interval [0,1], [1,2], [0,2],

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[0,3), [2,3) and [2, 4) accordingly. From a computational point of view, efficient numerical methods for modeling polynomial wave diffusion equations with fractional time derivatives are proposed. These methods and techniques can also be extended to other types of multi-term fractional space-time models.

In [22], initial boundary value problems for a generalized multi-term time fractional diffusion equation in an open bounded domain are considered $G \times (0,T)$, $G \in R^n$. Based on the corresponding maximum principle, which is also formulated and proven, some a priori estimates of the solution are established, and then its uniqueness. To show the existence of a solution, a formal solution is first constructed using the Fourier variable separation method. The time-dependent components of the solution are specified in terms of the Mittag-Leffler polynomial function. It is shown that, under certain conditions, the formal solution is a generalized solution of the initial boundary value problem for the generalized polynomial diffusion equation with fractional time derivatives, which under some additional conditions turns out to be a classical solution. Another important consequence of the maximum principle is the continuous dependence of the solution on the data of the problem (initial and boundary conditions and source function), which, together with the results of uniqueness and existence, turns the problem under consideration into a well-posed problem in the sense of Hadamard.

In this work, the problem solute transport in a porous medium is formulated and numerically solved based on the multi-term time fractional diffusion equation. The influence of the orders of fractional derivatives with respect to time on the transport characteristics, in particular, on the distribution of the concentration of the substance at different times, is shown.

PROBLEM FORMULATION

The multi-term time fractional diffusion equation is written as [23]

$$\frac{\partial^{\alpha} c}{\partial t^{\alpha}} + \sum_{s=1}^{n} r_s \frac{\partial^{\beta_s} c}{\partial t^{\beta_s}} = D \frac{\partial^{\gamma} c}{\partial x^{\gamma}} + f(t,x), \tag{1}$$

where α, β_s, $s=\overline{1,n}$, $\gamma-$ are the orders of derivatives. $0<\beta_s<\beta_{s-1}<...<\beta_1<\alpha<1$. The orders of fractional derivatives α and γ change in the following range: $0<\alpha\le 1$, $1\le\gamma\le 2$. If c is a dimensionless quantity, then $\left[\frac{\partial^{\alpha} c}{\partial t^{\alpha}}\right]=T^{-\alpha}$, $[r_s]=T^{\beta_s-\alpha}$, $[D]=L^{\gamma}/T^{\alpha}$, $[f(t,x)]=T^{-\alpha}$, $L-$ length dimension, $T-$ time dimension.

The model can be converted to the following simpler form at $n=2$ and $f=0$

$$\frac{\partial^{\alpha} c}{\partial t^{\alpha}} + r_2 \frac{\partial^{\beta_1} c}{\partial t^{\beta_1}} + r_1 \frac{\partial^{\beta_2} c}{\partial t^{\beta_2}} = D \frac{\partial^{\gamma} c}{\partial x^{\gamma}}. \tag{2}$$

The initial and boundary conditions have the form:

$$c_m(0,\ x)=0, \qquad c_m(t,0)=c_0, \qquad c_m(t,\infty)=0. \tag{3}$$

SOLUTION OF THE PROBLEM

To numerically solve problem (2)-(3) we use the finite difference method. In the domain $\Omega=\{0\le x\le\infty,\ 0\le t\le T\}$ we introduce a grid, where h is the grid step in coordinate x, where τ is the grid step in time t, L and is the characteristic length of the porous medium. As a result, we have a grid [24-30] $\omega_{h\tau}=\left\{(x_i,t_j),\ x_i=ih,\ i=\overline{0,N},\ h=L/N,\ t_j=j\tau,\ j=\overline{0,M},\ \tau=T/M\right\}$.

The equations of system (2), (3) are approximated on a grid $\omega_{h\tau}$ in the following form [31-33]

$$\frac{1}{\Gamma(2-\alpha)\tau^{\alpha}}\left[\sum_{l=0}^{j-1}\left((c)_i^{l+1}-(c)_i^{l}\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)-(c)_i^{j}\right]+\frac{1}{\Gamma(2-\alpha)\tau^{\alpha}}(c)_i^{j+1}+$$

$$+\frac{r_1}{\Gamma(2-\beta_1)\tau^{\beta_1}}\left[\sum_{l=0}^{j-1}\left((c)_i^{l+1}-(c)_i^{l}\right)\left((j-l+1)^{1-\beta_1}-(j-l)^{1-\beta_1}\right)-(c)_i^{j}\right]+\frac{1}{\Gamma(2-\beta_1)\tau^{\beta_1}}(c)_i^{j+1}+$$

$$+\frac{r_2}{\Gamma(2-\beta_2)\tau^{\beta_2}}\left[\sum_{l=0}^{j-1}\left((c)_i^{l+1}-(c)_i^{l}\right)\left((j-l+1)^{1-\beta_2}-(j-l)^{1-\beta_2}\right)-(c)_i^{j}\right]+\frac{1}{\Gamma(2-\beta_2)\tau^{\beta_2}}(c)_i^{j+1} \tag{4}$$

$$=D\frac{1}{\Gamma(3-\beta)h^{\gamma}}\left(\sum_{l=0}^{i-1}\left((c)_{i-(l+1)}^{j}-2(c)_{i-l}^{j}+(c)_{i-(l-1)}^{j}\right)\right)\left((l+1)^{2-\gamma}-(l)^{2-\gamma}\right).$$

$$(c)_i^{j+1}=\left(\begin{array}{l}D\frac{1}{\Gamma(3-\beta)h^{\gamma}}\left(\sum_{l=0}^{i-1}\left((c)_{i-(l+1)}^{j}-2(c)_{i-l}^{j}+(c)_{i-(l-1)}^{j}\right)\right)\left((l+1)^{2-\gamma}-(l)^{2-\gamma}\right)\\ -\frac{1}{\Gamma(2-\alpha)\tau^{\alpha}}\left[\sum_{l=0}^{j-1}\left((c)_i^{l+1}-(c)_i^{l}\right)\left((j-l+1)^{1-\alpha}-(j-l)^{1-\alpha}\right)-(c)_i^{j}\right]\\ -\frac{r_1}{\Gamma(2-\beta_1)\tau^{\beta_1}}\left[\sum_{l=0}^{j-1}\left((c)_i^{l+1}-(c)_i^{l}\right)\left((j-l+1)^{1-\beta_1}-(j-l)^{1-\beta_1}\right)-(c)_i^{j}\right]\\ -\frac{r_2}{\Gamma(2-\beta_2)\tau^{\beta_2}}\left[\sum_{l=0}^{j-1}\left((c)_i^{l+1}-(c)_i^{l}\right)\left((j-l+1)^{1-\beta_2}-(j-l)^{1-\beta_2}\right)-(c)_i^{j}\right]\end{array}\right) \tag{5}$$

$$/\left(\frac{1}{\Gamma(2-\alpha)\tau^{\alpha}}+\frac{1}{\Gamma(2-\beta_1)\tau^{\beta_1}}+\frac{1}{\Gamma(2-\beta_2)\tau^{\beta_2}}\right)$$

where $\Gamma(\cdot)$ is the Euler Gamma function, c_i^j is the grid function defined at the point (t_j, x_i).

The initial and boundary conditions are approximated as follows :

$$c_i^j=0\,,\qquad c_0^j=0\,,\qquad c_N^j=0\,. \tag{6}$$

Where N is a sufficiently large number for which the equation $c_N^j=0$ is approximately satisfied.

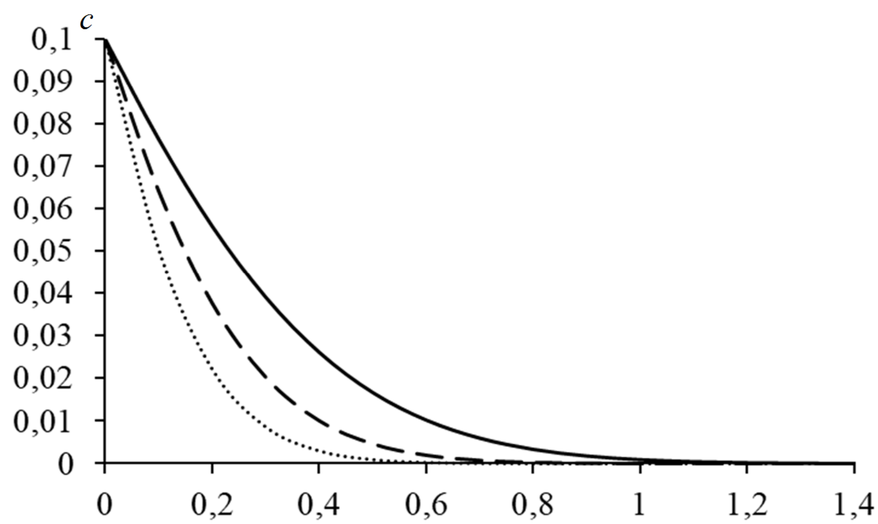
RESULTS AND DISCUSSION

The following values of the initial parameters were used in the calculations: $D=10^{-5}\,м^{\gamma}/c$, $c_0=0{,}1$.

Some results are presented in Fig. 1-6. In Fig. 1 and 2 show graphics of changes in concentration profiles in the case when the time fractional derivative on the left side of the equation consists of the sum of 3 terms. Here the order of the fractional derivative is chosen in decreasing order ($\alpha=0.9$, $\beta_1=0.8$, $\beta_2=0.7$). The results show that adding additional terms with fractional time derivatives to the diffusion equation slows down the dynamics of the distribution of concentration profiles. In other words, with the addition of additional fractional time derivatives to the diffusion equation, the effect of a delay in the development of concentration fields is manifested. In difference to Fig. 1, Fig. 2 shows the results when γ is reduced from 2. Comparing Fig. 1 with Fig. 2 shows that the decrease of γ is effective in the opposite direction than a , β_1 , β_2 , i.e. with the decrease of γ from 2 the called "fast diffusion" is observed. Thus, we can conclude that the multi-term of the local fractional time derivative and the reduction of the order of the derivative in the diffusion term have mutually opposite effects.

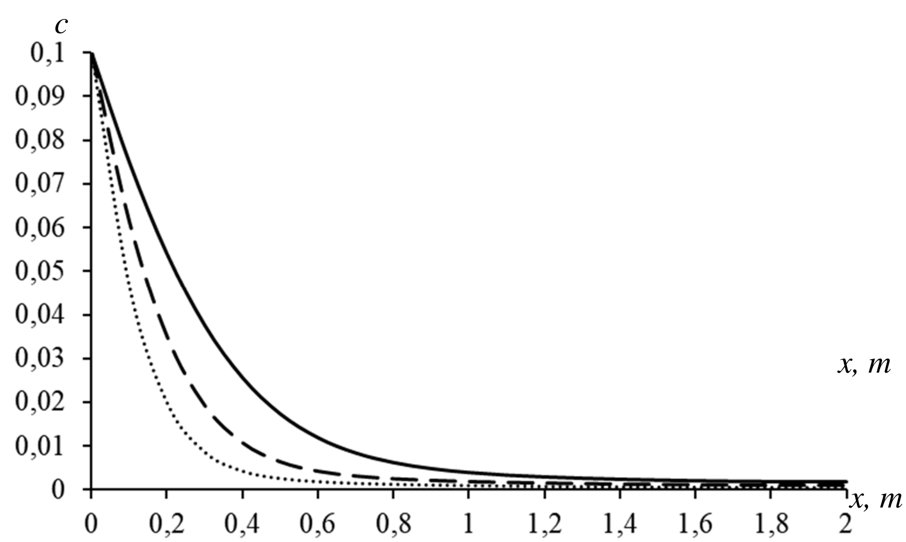
In Fig. 3, 4 show the change in the concentration of a substance over time for different values of the parameter r_1 and r_2. As can be seen from the figures, with increasing coefficients r_1 and r_2 at the same values of γ , β_1 , β_2 the development of substance concentration profiles slows down. Thus, both the increase of the number of terms with fractional time derivatives and the increase of their coefficients in the multi-term diffusion equation leads to the slowed dynamics of changes in the concentration profiles. Decreasing the order of the γ derivative in the diffusion equation, as in the previous case, leads to "fast diffusion" (Figs. 3,4).

Calculations with reduced orders of time derivatives were also given β_1, β_2 compared to previous cases. Some results are shown in Fig.5,6. As can be seen from the figures, decreasing the value β_1 from *0.8* to *0.7* and decreasing the value β_2 from *0.7* to *0.5* leads to an increase in the effect of retardation in the development of concentration profiles. In particular, a comparison of Fig. 3 with Fig. 5 shows that if the leading concentration front in the first case reached approximately 0.55 m (Fig. 3), then in the second case this value is ~ 0.35 m. Therefore, we can conclude that a decrease in the orders of multi-term time fractional diffusion equation enhances the effects of retardation in the development of concentration profiles.



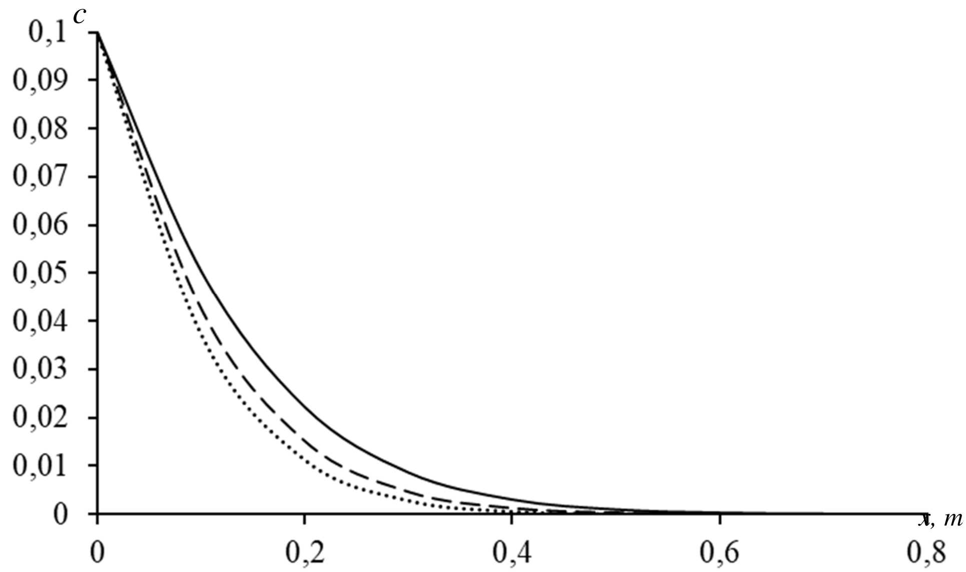
$r_1 = 0$, $r_2 = 0$, $r_1 = 0.6$, $r_2 = 0$, $r_1 = 0.6$, $r_2 = 0.5$

FIGURE. 1. Concentration profiles: $\gamma = 2$, $\alpha = 0.9$, $\beta_1 = 0.8$, $\beta_2 = 0.7$, $t = 3600c$.



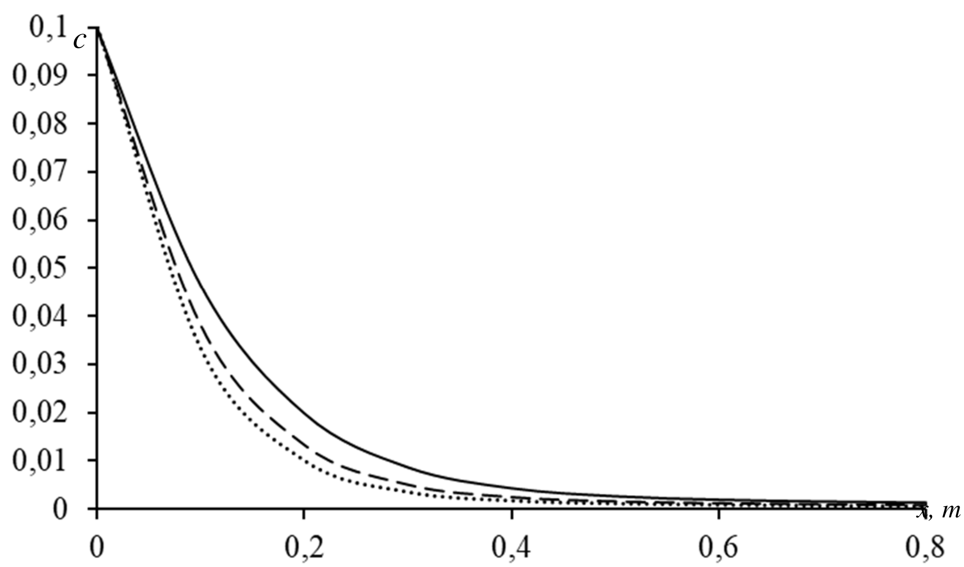
$r_1 = 0$, $r_2 = 0$, $r_1 = 0.6$, $r_2 = 0$, $r_1 = 0.6$, $r_2 = 0.5$

FIGURE. 2. Concentration profiles: $\gamma = 1.9$, $\alpha = 0.9$, $\beta_1 = 0.8$, $\beta_2 = 0.7$, $t = 3600c$



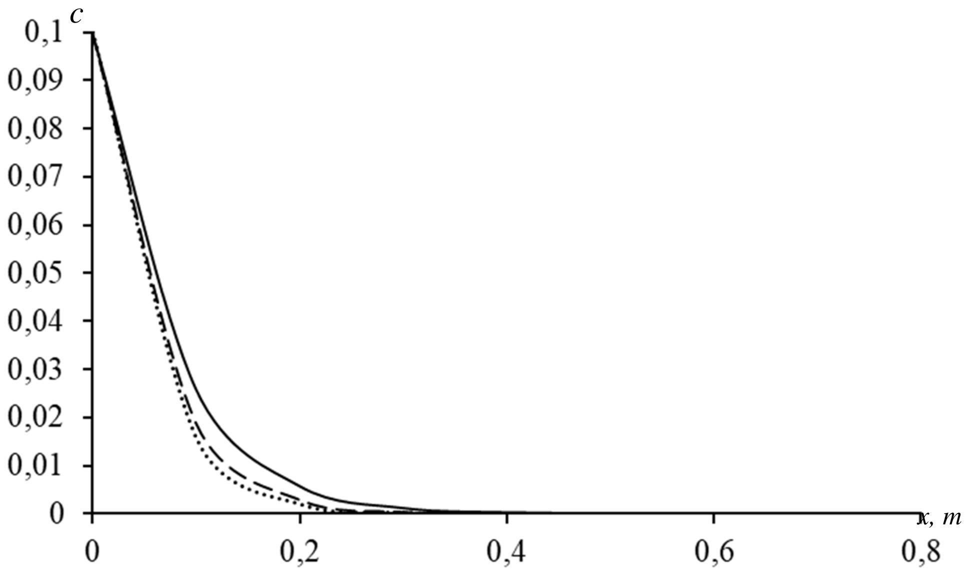
$r_1 = 0.6$, $r_2 = 0.5$ $r_1 = 1.0$, $r_2 = 0.8$ $r_1 = 1.5$, $r_2 = 1.0$

FIGURE. 3. Concentration profiles: $\gamma = 2$, $\alpha = 0.9$, $\beta_1 = 0.8$, $\beta_2 = 0.7$, $t = 3600s$



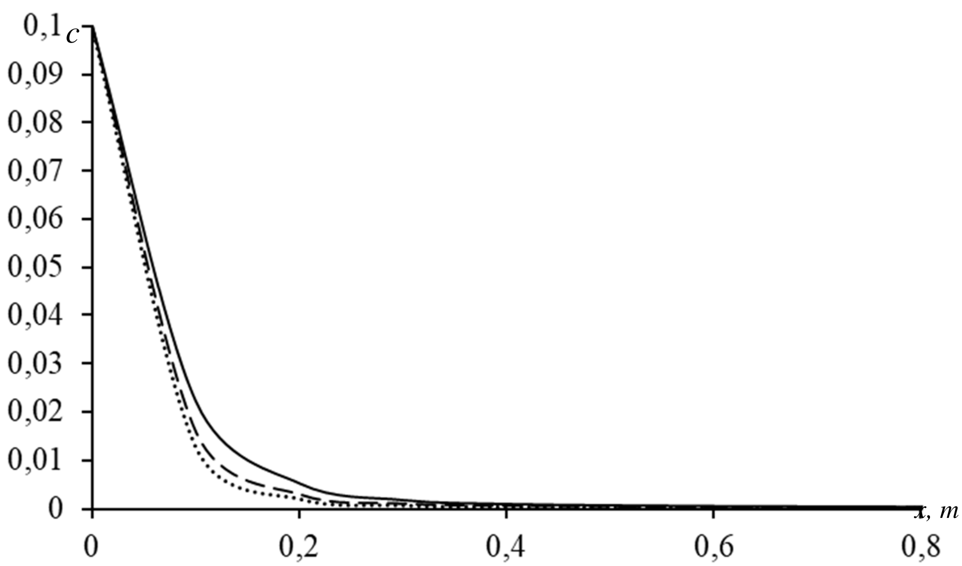
$r_1 = 0.6$, $r_2 = 0.5$ $r_1 = 1.0$, $r_2 = 0.8$ $r_1 = 1.5$, $r_2 = 1.0$

FIGURE. 4. Concentration profiles: $\gamma = 1.9$, $\alpha = 0.9$, $\beta_1 = 0.8$, $\beta_2 = 0.7$



$r_1 = 0.6$, $r_2 = 0.5$ $r_1 = 1.0$, $r_2 = 0.8$ $r_1 = 1.5$, $r_2 = 1.0$

FIGURE. 5. Concentration profiles: $\gamma = 2$, $\alpha = 0.9$, $\beta_1 = 0.7$, $\beta_2 = 0.5$



$r_1 = 0.6$, $r_2 = 0.5$ $r_1 = 1.0$, $r_2 = 0.8$ $r_1 = 1.5$, $r_2 = 1.0$

FIGURE. 6. Concentration profiles: $\gamma = 1.9$, $\alpha = 0.9$, $\beta_1 = 0.7$, $\beta_2 = 0.5$

CONCLUSION

In this paper considers the numerical solution of the multi-term time fractional diffusion equations in a finite region. The problem is numerically solved. The analysis of the obtained results shows that the use of differential equations with multi-term time fractional derivatives for modeling anomalous diffusion processes allows us to describe the effects of delayed development of concentration profiles. Taking into account the multi-term of the diffusion equation in comparison with the single-term equation leads to a slower diffusion of the substance concentration in the medium. It is shown that an increase in the value of constant coefficients (r_1 and r_2) at local fractional time derivatives contributes to the strengthening of the process of slowing down the propagation of concentration profiles. Similar strengthening of the lagging effects also results in decreasing orders of these local time derivatives.

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