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About one method of approximate solution of the first boundary value problem for the fractional diffusion equation

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Abstract. *Background* This article focuses on a rapidly developing area of fractional calculus that describes anomalous diffusion. Since the correct form of the fractional-order equation describing anomalous diffusion — remains an open question, the authors use examples of models based on fractional diffusion equations to examine the advantages of various fractional-order equations proposed for modelling the advection-diffusion process in media with a fractal structure. *Purpose* This paper examines boundary value problems for the advection-diffusion equation with Caputo and Riemann–Liouville fractional operators. Given that many authors consider in their work models with fractional-order operators obtained simply by replacing ordinary derivatives with fractional ones, the authors of this paper consider it necessary to compare fractional differential equations with various operators. We also note that one of the aims of this work is to construct an effective approximate method for solving the first initial-boundary value problem for a homogeneous fractional differential equation. *Method* A fractional calculus approach is used. The approximate method under consideration is based on the analytical method of separation of variables (the Fourier method). The proposed approximate method and all the necessary calculations are implemented using the Matlab programming language. *Results* Approximate solutions have been obtained for boundary value problems for the advection-diffusion equation with fractional operators of Caputo and Riemann–Liouville. The solutions obtained have been compared both with one another and with the classical model based on ordinary derivatives. *Conclusions* Based on the results obtained, the authors recommend using an equation containing the Riemann–Liouville fractional operator to model anomalous diffusion processes.

Key words and phrases: approximate calculus, fractional calculus, fractional advection-diffusion equation, fractional Riemann–Liouville derivative, fractional Caputo derivative.

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1. Introduction

The problem of advection-diffusion is considered, whose model is viewed as a differential equation with various fractional differential operators (in the form of Caputo and in the form of Riemann–Liouville). To date, many works have been prepared on solving various problems containing fractional differential operators, but most of them are devoted to numerical methods (finite difference method, spline method, collocation method, etc.), in particular [1, 2]. We would also like to mention the eight-volume 'Handbook of Fractional Calculus with Applications'[3], which contains the latest achievements in the field of fractional differentiation. This work focuses on the development of approximate calculation methods based on analytical methods (the Fourier method). Although numerical methods demonstrate high efficiency in solving the proposed problems, it is analytical methods that allow the development of the necessary set of tools for verifying the solution of problems, for which it is absolutely necessary to develop effective methods for implementing approximate solutions.

In this work, boundary value problems for the advection-diffusion equation with a fractional differential operator are solved using the method of separation of variables (Fourier method). One of the main points in solving a boundary value problem containing a fractional differential operator is the structure of the spectral problem obtained by separation of variables. This is due to the non-self-adjointness of the operators of this spectral problem. The structure of this spectral problem is extremely complex and has not been fully studied. This work fills this gap.

2. The first initial boundary value problem for a homogeneous fractional dispersion equation

Let us consider the first boundary value problem for a homogeneous fractional dispersion equation:

$$\frac{\partial U(x,t)}{\partial t} = -D \cdot {}_0^R D_x^\alpha U(x,t), \tag{1}$$

with boundary and initial conditions

$$U(0,t) = U(1,t) = 0, \tag{2}$$

$$U(x,0) = \phi(x), \tag{3}$$

where ${}_0^R D_x^\alpha = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_0^x \frac{U(\tau,t) d\tau}{(x-\tau)^{\alpha-1}}$ — fractional derivative (in the sense of Riemann–Liouville), $1 < \alpha < 2$ [4]. And a similar problem with the Caputo operator.

$$\frac{\partial U(x,t)}{\partial t} = -D \cdot {}_0^C D_x^\alpha U(x,t), \tag{4}$$

with boundary and initial conditions

$$U(0,t) = U(1,t) = 0, \tag{5}$$

$$U(x,0) = \phi(x), \tag{6}$$

where ${}_0^C D_x^\alpha = \frac{1}{\Gamma(2-\alpha)} \int_0^x \frac{U(\tau,t)'' d\tau}{(x-\tau)^{\alpha-1}}$ — fractional derivative (in the sense of Caputo), $1 < \alpha < 2$ [5].

Works [4, 5] were devoted to the development of approximate methods for studying mathematical models of heat and mass transfer, and a significant part of this work is devoted to analysing the results obtained in these works. This is primarily due to the fact that the correct form of fractional order equations describing anomalous diffusion remains a subject of debate. This work brings us closer to solving this problem to a certain extent.

It is known that the above tasks (when solved using the Fourier method) generate the following two spectral tasks:

$$\begin{cases} {}_0^R D_x^\alpha X(x) = -\lambda X(x), \\ X(0) = 0, X(1) = 0. \end{cases} \tag{7}$$

$$\begin{cases} {}_0^C D_x^\alpha X(x) = -\mu X(x), \\ X(0) = 0, X(1) = 0. \end{cases} \tag{8}$$

Such Sturm–Liouville problems (7), (8) are studied in detail in [6–9]. It is worth mentioning that problems similar to (7) and (8) also arise when studying the Fokker–Planck equation [10].

The paper [11] shows that the spectral problem with the Caputo fractional derivative (8), when $\alpha \to 1$, has no real roots (i.e., there is no principal eigenvalue). This is strikingly different from the Riemann–Liouville fractional derivative problem (7), where the principal eigenvalue exists for all $1 < \alpha < 2$ (i.e., there is always a fundamental tone). This is a significant difference between the principal eigenvalue of the spectral problem with fractional operators and the classical Sturm–Liouville problem. This phenomenon has a significant impact on the adequacy of the modelled diffusion process.

The works [4], [5] demonstrate that the numbers λ_n, μ_n are eigenvalues of problems (7), (8) only when they are zeros of the corresponding Mittag–Leffler functions:

$$E_{\alpha,\alpha}(-\lambda) = \sum_{j=0}^{\infty} \frac{(-\lambda)^j}{\Gamma(\alpha j + \alpha)}, \tag{9}$$

$$E_{\alpha,2}(-\mu) = \sum_{j=0}^{\infty} \frac{(-\mu)^j}{\Gamma(\alpha j + 2)}. \tag{10}$$

With corresponding eigenfunctions (11), (12)

$${}^R W_n(-\lambda_n, x) = x^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n x^\alpha), \tag{11}$$

$${}^C W_n(-\mu_n, x) = x E_{\alpha,2}(-\mu_n x^\alpha). \tag{12}$$

It should be noted that, when studying models with a fractional operator, we (and not only we) heavily rely on the method for constructing eigenfunctions and adjoint functions proposed in the works of M. M. Jerbashyan and A. B. Nersesyan [12], [13].

Similarly, how demonstrated in the work Y. Luchko [14], problems (1) and (4) generate problems that are conjugate to problems (7) and (8).

$$\begin{cases} {}_0^R D_{1-x}^\alpha Y(x) = -\lambda Y(x), \\ Y(0) = 0, Y(1) = 0. \end{cases}$$

$$\begin{cases} {}_0^C D_{1-x}^{\alpha} Y(x) = -\mu Y(x), \\ Y(0) = 0, Y(1) = 0. \end{cases}$$

The eigenvalues of the conjugate problems coincide with the eigenvalues of problems (7), (8). And the eigenfunctions have the form

$${}^R Z_n(-\lambda_n, x) = (1-x)^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n (1-x)^{\alpha}),$$

$${}^C Z_n(-\mu_n, x) = (1-x) E_{\alpha,2}(-\mu_n (1-x)^{\alpha}).$$

As noted in works [4, 5], the solution to problems (1), (2), (3) and (4), (5), (6) is as follows:

$${}^R U^{\alpha}(x,t) = \sum_{n=1}^{\infty} \frac{(\phi, {}^R Z_n)}{({}^R W_n, {}^R Z_n)} e^{-D\lambda_n t} x^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n x^{\alpha}), \tag{13}$$

$${}^C U^{\alpha}(x,t) = \sum_{n=1}^{\infty} \frac{(\phi, {}^C Z_n)}{({}^C W_n, {}^C Z_n)} e^{-D\mu_n t} x E_{\alpha,2}(-\mu_n x^{\alpha}). \tag{14}$$

To analyse these solutions, we will need the following theorems, which were discussed in detail in [15].

Theorem 1. *If*

$$2 - \left(\frac{32\pi^2}{9} + \frac{2}{3}\right)^{-1} < \alpha < 2,$$

then the first eigenvalue of the problem (4)–(6) *is positive and simple (the multiplicity of this eigenvalue is equal to 1), and the fundamental (main) tone has no nodes (i.e., the eigenvalue corresponding to the first eigenvalue does not vanish in (1,2)).*

Theorem 2. *The first eigenvalue* λ_1 *of the problem* (1)–(3) *is positive, simple, and satisfies the condition*

$$0 < \lambda_1^{-1} < \frac{\Gamma(2+2\alpha)}{\Gamma(1+\alpha)},$$

and the principal (main) tone has no nodes for all $1 < \alpha < 2$.

Since the proofs are described in great detail in [15] and are rather cumbersome, we will not reproduce them here.

Considering that for different $\alpha \neq 2$, the solutions to problems (1)–(3), (4)–(6) differ significantly from each other (as can be seen in Figure 1–3), the following recommendations are given: which of these two models should be used when modelling a particular process.

From [15] it is known that problem (7) is equivalent to the integral equation (15)

$$U(x) - \frac{\lambda}{\Gamma(2-\alpha)} \left[\int_0^1 x^{1-\alpha}(1-t)^{1-\alpha} U(t)dt - \int_0^x (x-t)^{1-\alpha} U(t)dt \right] =$$
$$= U(x) - \frac{\lambda}{\Gamma(2-\alpha)} \int_0^x G_1(x,t) U(t) dt = 0.$$

And problem (8) is in turn equivalent to integral equation (16)

$$U(x) - \frac{\mu}{\Gamma(2-\alpha)}\left[\int\limits_0^1 x(1-t)^{1-\alpha}U(t)dt - \int\limits_0^x (x-t)^{1-\alpha}U(t)dt\right] =$$
$$= U(x) - \frac{\mu}{\Gamma(2-\alpha)}\int\limits_0^x G_0(x,t)U(t)dt = 0.$$

As can be seen from [15]: the kernel $G_1(x,t)$ (also called the influence function in mechanics) is sign-definite and persymmetric, while the kernel $G_0(x,t)$ is not sign-definite and not persymmetric. From the above and from Theorems 1-2, it follows that when dealing with processes with oscillatory properties, it is necessary to use problems (1)–(3). It turns out that equation (4), which is referred to as an oscillatory equation [16], [17], can hardly be considered as such.

These two theorems also show that for some α, the difference between U_R^α and U_C^α will be significant. It is known that when $\alpha \to 2$, the following relations hold: $\lambda_n \to (\pi n)^2$ and $\mu_n \to (\pi n)^2$, $n = 0, 1, 2, \ldots$. This statement was first obtained in 1998 [18], then in 2005 it was established by other methods [19]. Finally, a generalisation of the result was obtained [15].

Further, when $\alpha \to 2$, the functions of the problem have the form:

$$\lim_{\alpha\to 2} {}^R W_n(-\lambda_n, x) = \lim_{\alpha\to 2} x^{\alpha-1}E_{\alpha,\alpha}(-\lambda_n, x^\alpha) = xE_{2,2}(-\lambda_n, x^2),$$

$$\lim_{\alpha\to 2} {}^C W_n(-\mu_n, x) = \lim_{\alpha\to 2} xE_{\alpha,2}(-\mu_n, x^\alpha) = xE_{2,2}(-\mu_n, x^2).$$

It is known [19] that there is such a formula

$$E_{2,2}(z^2) = \frac{sh(z)}{z}.$$

From this formula it follows that

$$E_{2,2}(-z^2) = \frac{sin(z)}{z}.$$

From these relationships, it follows that when $\alpha = 2$, the solutions to problems (1), (2), (3), (4), (5), and (6) coincide with the solution to the corresponding problem for the differential equation (17):

$$\frac{\partial u(x,t)}{\partial t} = -D \cdot \frac{\partial^2 u(x,t)}{\partial x^2}. \tag{17}$$

That is, the following equality will hold:

$$\lim_{\alpha\to 2} {}^R U^\alpha(x,t) = \lim_{\alpha\to 2} {}^C U^\alpha(x,t) = u(x,t),$$

where

$$u(x,t) = \sum_{n=1}^{\infty} B_n \sin(\pi n x) e^{-D(\pi n)^2 t},$$

in which

$$B_n = 2\int_0^1 \phi(x)\sin(\pi n x)dx.$$

Table 1

The first few eigenvalues λ_n for $1 < \alpha < 2$

α	**1.1**	**1.2**	**1.3**	**1.4**	
λ_n	5.101	4.567	4.518	4.708	
	$10.795 \pm 7.989i$	$14.139 \pm 6.9214i$	$17.920 \pm 3.920i$	16.726	
	$14.338 \pm 16.876i$	$21.916 \pm 18.035i$	$32.274 \pm 17.144i$	26.220	
	$17.273 \pm 26.049i$	$28.880 \pm 30.344i$	$45.830 \pm 32.677i$	$45.424 \pm 12.811i$	
	$19.920 \pm 35.456i$	$35.547 \pm 43.497i$	$59.425 \pm 50.079i$	$69.176 \pm 30.809i$	
	$22.400 \pm 45.061i$	$42.078 \pm 57.328i$	$73.206 \pm 68.999i$	$94.023 \pm 52.268i$	
α	**1.5**	**1.6**	**1.7**	**1.8**	**1.9**
λ_n	5.075	5.610	6.322	7.240	8.404
	17.472	19.513	22.570	26.737	32.253
	32.129	38.158	45.945	56.345	70.247
	55.834	62.410	76.129	95.440	121.869
	64.586	88.220	111.768	143.271	186.675
	$99.718 \pm 21.304i$	123.879	153.696	199.672	264.408

3. Approximate solution of the first initial-boundary value problem

To find an approximate solution, we first find several initial eigenvalues λ_n and μ_n from the corresponding equations:

$$E_{\alpha,\alpha}(-\lambda) = \sum_{j=0}^{\infty} \frac{(-\lambda)^j}{\Gamma(\alpha j + \alpha)} = 0,$$

$$E_{\alpha,2}(-\mu) = \sum_{j=0}^{\infty} \frac{(-\mu)^j}{\Gamma(\alpha j + 2)} = 0.$$

Table 1–2 shows the results of calculations of several first eigenvalues λ_n and μ_n for different values of $1 < \alpha < 2$.

As shown in works [4, 5], for an approximate solution to problems (1)–(3) and (4)–(6), it is sufficient to take the first few terms of the series (13), (14):

$${}^{R}U^{\alpha}(x,t) \approx \sum_{n=1}^{N} \frac{(\phi, {}^{R}Z_n)}{({}^{R}W_n, {}^{R}Z_n)} e^{-D\lambda_n t} x^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n x^{\alpha}),$$

$${}^{C}U^{\alpha}(x,t) \approx \sum_{n=1}^{N} \frac{(\phi, {}^{C}Z_n)}{({}^{C}W_n, {}^{C}Z_n)} e^{-D\mu_n t} x E_{\alpha,2}(-\mu_n x^{\alpha}).$$

Let us denote the approximate solution as

$${}^{R}U_0^{\alpha}(x,t) = \sum_{n=1}^{N} \frac{(\phi, {}^{R}Z_n)}{({}^{R}W_n, {}^{R}Z_n)} e^{-D\lambda_n t} x^{\alpha-1} E_{\alpha,\alpha}(-\lambda_n x^{\alpha}),$$

Table 2

The first few eigenvalues μ_n for $1 < \alpha < 2$

α	**1.1**	**1.2**	**1.3**	**1.4**	
μ_n	$1.353 \pm 7.250i$	$3.173 \pm 7.985i$	$5.473 \pm 8.273i$	$8.190 \pm 7.812i$	
	$2.810 \pm 15.731i$	$7.132 \pm 18.959i$	$13.393 \pm 21.811i$	$22.012 \pm 23.568i$	
	$4.303 \pm 24.691i$	$11.399 \pm 31.246i$	$22.371 \pm 37.953i$	$38.507 \pm 43.723i$	
	$5.829 \pm 33.969i$	$15.902 \pm 44.438i$	$32.169 \pm 55.962i$	$57.132 \pm 67.167i$	
	$7.3825 \pm 43.488i$	$20.600 \pm 58.338i$	$42.647 \pm 75.471i$	$77.563 \pm 93.329i$	
	$8.960 \pm 53.204i$	$25.466 \pm 72.825i$	$53.715 \pm 96.250i$	$99.581 \pm 121.845i$	
α	**1.5**	**1.6**	**1.7**	**1.8**	**1.9**
μ_n	$11.147 \pm 6.123i$	13.420	9.933	9.457	9.514
	$33.314 \pm 23.130i$	14.645	23.2510	28.477	33.598
	$61.196 \pm 46.651i$	$47.293 \pm 18.851i$	$63.101 \pm 5.930i$	62.200	73.039
	$93.818 \pm 75.367i$	$91.705 \pm 43.625i$	$130.587 \pm 29.601i$	97.063	124.419
	$130.545 \pm 108.499i$	$145.569 \pm 75.805i$	$215.458 \pm 60.453i$	155.450	191.146
	$170.946 \pm 145.542i$	$207.859 \pm 114.486i$	$316.291 \pm 99.750i$	196.596	267.945

$$ {}^{C}U_0^{\alpha}(x,t) = \sum_{n=1}^{N} \frac{(\phi, {}^{C}Z_n)}{({}^{C}W_n, {}^{C}Z_n)} e^{-D\mu_n t} x E_{\alpha,2}(-\mu_n x^{\alpha}). $$

It is worth noting that, unfortunately, as has been pointed out on more than one occasion, it is very difficult to find good experimental data (whether from a computational experiment or an experiment conducted using laboratory equipment). However, based on, for example, [20], [21], it can be said that the calculations presented in this paper have been carried out quite well.

4. Results of the approximate solution of the first initial-boundary value problem

The solutions to the first initial-boundary value problem are calculated for various values of the fractional derivative α. In order to compare the solution to problem (1)–(3), with a fractional derivative in the form of Riemann–Liouville, and the solution to problem (4)–(6), with the fractional derivative in the form of Caputo, with the solution of the classical diffusion equation (17), we perform the calculation at $\alpha = 2$.

As can be seen in Figure 1, the surface of solutions to problems (1)–(3), (4)–(6) at $\alpha = 2$ coincides with the solution to the classical problem (17).

When considering $\alpha \neq 2$, for example $\alpha = 1.9$, the surfaces constructed for problems with fractional derivatives in the form of Caputo and Riemann–Liouville not only differ significantly from the classical heat conduction problem (17), but, as can be seen from Figure 2, also differ significantly from each other.

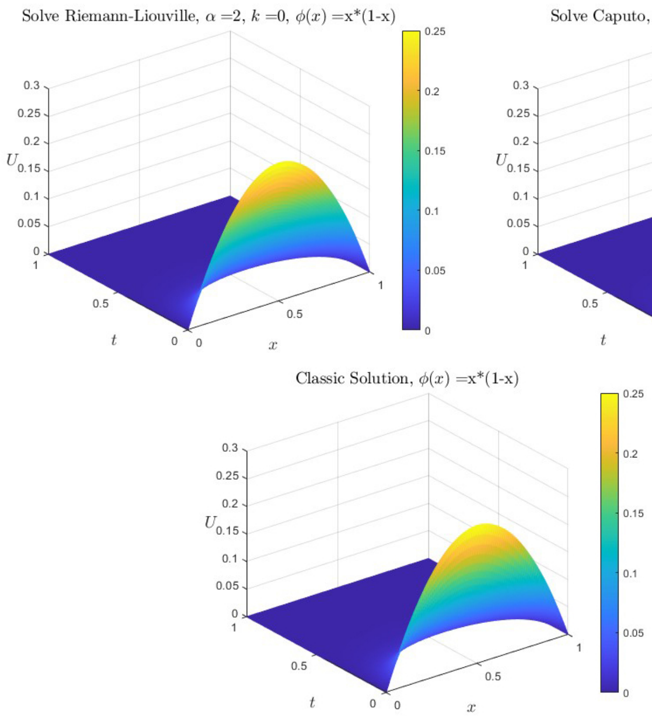

Figure 1. An approximate solution to the classical diffusion problem and problems with derivatives in the sense of Caputo and Riemann–Liouville for $\alpha = 2$

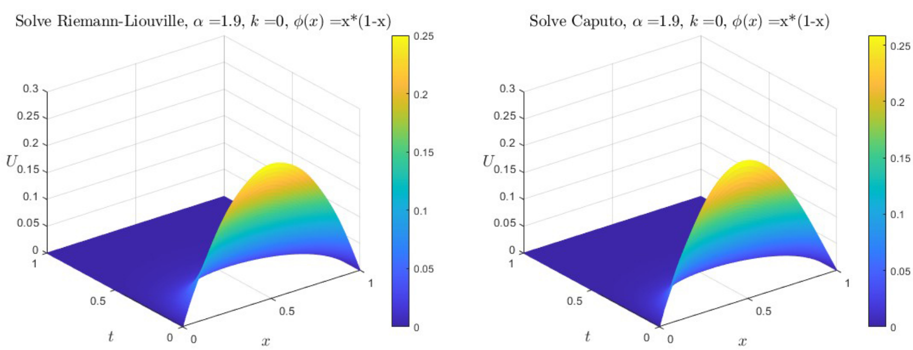

Figure 2. Approximate solution of the boundary value problem with operators in the sense of Caputo and Riemann–Liouville for $\alpha = 1.9$

As noted by the authors earlier, these differences arise due to the significant difference in the generated spectral problems (7), (8), which generate completely different structures of eigenvalues ((9), (10)) and eigenfunctions ((11), (12)).

When $\alpha \to 1$, the differences become more noticeable (Figure 3).

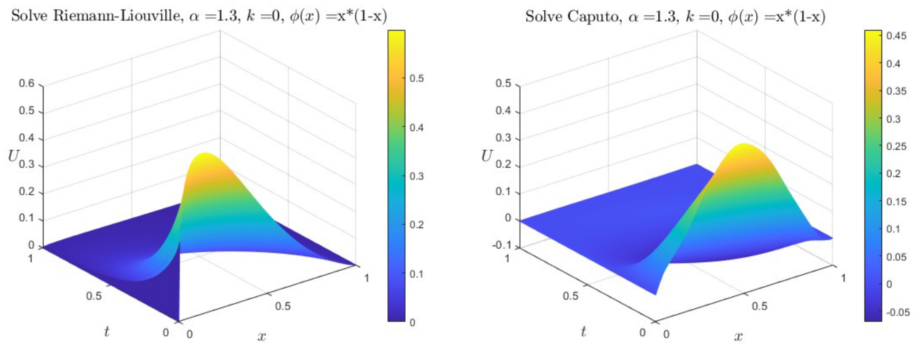

Figure 3. Approximate solution of the boundary value problem with operators in the sense of Caputo and Riemann–Liouville for $\alpha = 1.3$

5. Discussion

Presented in this paper results demonstrate how different the models can be, depending on whether the equation involves the Riemann–Liouville fractional derivative or the Caputo fractional derivative. As mentioned earlier, a significant advantage of models based on the Riemann-Liouville operator is that its first eigenvalue remains real for all $1 < \alpha < 2$. In the case of models based on the Caputo fractional derivative, their first eigenvalue ceases to be real, which creates certain difficulties in their application for modelling advection-diffusion processes.

The principal eigenvalue is of fundamental meaning for modelling advection-diffusion processes. For example, the paper [22] investigates the influence of various diffusion and advection coefficients (tending to zero or infinity) on the first eigenvalue for an elliptic operator with the Neumann zero boundary condition. Without going into the physical details, we note that although the occurrence of complex eigenvalues is possible (in the case where the operator is non-self-adjoint), such models cannot be used to describe diffusion processes.

6. Conclusion

Since the correct form of the fractional order equation describing anomalous diffusion is still a matter of debate, the authors, using examples of specific fractional diffusion equations of fractional diffusion, consider the advantages of one or another fractional order equation presented to describe the process of heat and mass transfer in media with a fractal structure. Approximate methods for solving initial boundary value problems for these equations have been developed.

The presented results demonstrate the possibility of the developed method for the approximate solution of the boundary value problem for the fractional diffusion equation. A significant difference between spectral problems arising with fractional derivatives in the sense of Caputo and Riemann–Liouville is demonstrated. What differences arise when using different operators to solve the advection-diffusion problem. Based on the calculations presented (Figure 1–3) and the analysis of the influence functions $G_0(x,t)$, $G_1(x,t)$, it can be concluded that the model with the Riemann-Liouville fractional derivative (problem (1)–(3)) is recommended for modelling processes of highly anomalous diffusion.

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Об одном методе приближённого решения первой начально-краевой задачи для дробного уравнения диффузии

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Аннотация. *Предпосылки* Статья посвящена активно развивающемуся в настоящее время разделу дробного исчисления, описывающего аномальную диффузию. Так как корректная форма уравнения дробного порядка, описывающего аномальную диффузию, — вопрос до сих пор открытый, то авторы на примерах моделей, основанных на уравнениях дробной диффузии, рассматривают преимущества того или иного уравнения дробного порядка, представленных для моделирования процесса адвекции-диффузии в средах с фрактальной структурой. *Цель* В работе рассматриваются краевые задачи для уравнения адвекции-диффузии с дробными операторами Капуто и Римана–Лиувилля. Учитывая, что многие авторы рассматривают в своих работах модели с операторами дробного порядка, полученные простой заменой обыкновенных производных на дробные, то авторы работы считают необходимым сравнение дробно дифференциальных уравнений с различными операторами. Так же отметим, что одной из целей работы является построение эффективного приближённого метода решения первой начально-краевой задачи для однородного дробно-дифференциального уравнения. *Методы* Используется аппарат дробного исчисления. В основе рассматриваемого приближённого метода лежит аналитический метод разделения переменных (Метод Фурье). Реализация предложенного приближённого метода и все необходимые вычисления выполняются на языке программирования Matlab. *Результаты* Получены приближённые решения краевых задач для уравнения адвекции-диффузии с дробными операторами Капуто и Римана–Лиувилля. Произведено сравнение полученных решений как между собой, так и с классической моделью, основанной на обыкновенных производных. *Выводы* На основе полученных результатов для моделирования процессов аномальной диффузии, авторами рекомендуется использовать уравнение, содержащее дробный оператор Римана–Лиувилля.

Ключевые слова: приближённые вычисления, дробное исчисление, дробное уравнение адвекции-диффузии, дробная производная Римана–Лиувилля, дробная производная Капуто.