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Study of transition times in diffusion processes using fractional order derivatives

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- *The paper develops a mathematical model of the diffusion process using Caputo fractional-order derivatives with respect to time. The problem solution was obtained in an analytical form through contour integration methods. An analytical solution provides explicit expressions for the diffusion behavior across the entire time range, including both short- and long-time ranges. The emphasis on analytical solutions arises from the sensitivity of fractional-order models to variations in the derivative order, and the implementation of numerical methods does not always allow for reducing the discretization step. Literature analysis indicates that even slight changes in the fractional derivative order can lead to significant differences in results. Therefore, it is crucial to obtain the results in an analytical form that will allow us to adapt and optimize them in relation to real information about the process being modeled.*

Keywords *- mathematical modeling, fractional calculus, diffusion processes, methods for solving boundary value problems, methods of complex variable function theory.*

Introduction. Partial differential equations of fractional order, being a generalization of integer-order partial derivatives, have not only theoretical interest but also great practical significance. Fractional calculus has found applications in physics [1–8] and mechanics [9–12]. The modeling of multicomponent gas motion in porous media is primarily based on diffusion and filtration processes, which in their classical form are described by partial differential equations. The history of the process plays a significant role. In numerous instances, including gas filtration in underground storage formations and liquids, the history of the process plays a significant role. It is well known that fractional calculus is effectively used for modeling processes of this type. Studies [13–15] have shown that employing time-fractional derivatives provides a much more accurate description of gas extraction and injection processes in underground storage facilities. Modeling such processes typically leads to solving nonlinear differential equations in terms of fractional-order derivatives, or their systems, with variable coefficients (often discontinuous) under conditions of considerable uncertainty [16–18]. The motion of a two-component gas that mixes in a porous medium is a typical convection–diffusion process [13,19].

The purpose of this work is to construct a mathematical model of diffusion based on the application of time-fractional derivatives under conditions of uncertainty. It should be noted that many boundary-value problems involving fractional-order derivatives are solved using the Laplace integral transform and the apparatus of Mittag-Leffler functions [20]. However, when the input data are known with low accuracy, the studied processes are sufficiently slow, and large time intervals are considered, the use of Mittag-Leffler functions becomes problematic due to the rapid accumulation of irrecoverable errors. At the same time, it is known that diffusion coefficients depend on both pressure and temperature. In mathematical modeling of mass transfer processes in gas transportation systems (including modeling the operation of underground gas storage facilities), these parameters are typically known with low precision (usually 3–4 significant digits). One way to overcome these challenges is to construct asymptotic solutions.

The diffusion process without considering the convective component is described by a differential equation [15,19,21].

$$\frac{\partial c}{\partial \tau}=\frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(D\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(D\frac{\partial c}{\partial z}\right), \quad (1)$$

under the given boundary conditions, where the parameter D denotes the mutual diffusion coefficient of substances A and B. A significant number of formulas have been developed for its determination, in particular [21]

$$D_{AB}=\frac{T^{1.5}}{p\left(\sigma_A+\sigma_B\right)^2}\left(\frac{1}{m_A}+\frac{1}{m_B}\right)^{0.5}, \qquad (2)$$

where p,T - pressure and temperature in the system, m_A та m_B - gas masses, σ_A та σ_B - Leonard-Jones potential parameters.

Saxena M. and Saxena S. proposed the following modified Sezeland formula [21] for calculating the mutual diffusion coefficient of gases $D_{AB}\,(cm^2/s)$

$$D_{AB}=\frac{AT^{1.5}\left(\frac{1}{m_A}+\frac{1}{m_B}\right)^{0.5}}{p\left(V_A^{1/3}+V_B^{1/3}\right)\left[1+\left(BT_{AB}/T\right)\right]}, \qquad (3)$$

where V_A, V_B, T_A та T_B - critical volumes (cm^3/mol) and gas temperatures ($^\circ K$), p - pressure in atmosphere, $T_{A,B}=\left(T_AT_B\right)^{0.5}$. For non-polar gases $A=0.022023$ and $B=1.1756$, whereas for systems consisting of a combination of polar and nonpolar gases, $A=0.022023$ and $B=0.90116$.

If the self-diffusion coefficients of gases D_{AA} and D_{BB} are known, then

$$D_{AB}=\sqrt{\frac{m_A+m_B}{2\sqrt{m_Am_B}}}\sqrt{D_{AA}D_{BB}} \;. \qquad (4)$$

1. Definition of fractional derivatives.

The most commonly used fractional derivative operators are the Caputo and Riemann–Liouville operators. In terms of Caputo, the derivative of fractional order is defined as follows [6–12]:

$${}^{c}D_{\tau}^{\alpha}=\frac{{}^{c}\partial^{\alpha}\varphi(\tau)}{\partial\tau^{\alpha}}=\frac{1}{\Gamma(m+1-\alpha)}\int_0^{\tau}\frac{\frac{\partial^{m+1}}{\partial\xi^{m+1}}\varphi(\xi)}{(\tau-\xi)^{\alpha-m}}d\xi \qquad (5)$$

where m=[α] – the integer part of a real number α, and in terms of Riemann-Liouville -

$$D_{\tau}^{\alpha}=\frac{{}^{c}\partial^{\alpha}}{\partial\tau^{\alpha}}\varphi(\tau)=\frac{1}{\Gamma(m+1-\alpha)}\frac{\partial^{m+1}}{\partial\xi^{m+1}}\int_0^{\tau}\frac{\varphi(\xi)}{(\tau-\xi)^{\alpha-m}}d\xi \qquad (6)$$

The following relationship exists between the Caputo and Rimmann-Liouville derivatives [12]

$${}^{C}D_{\tau}^{\alpha}\varphi=D_{\tau}^{\alpha}\varphi-\sum_{k=0}^{m}\frac{\tau^{k-\alpha}}{\Gamma\left(k-\alpha+1\right)}\frac{\partial^k}{\partial\tau^k}\varphi. \qquad (7)$$

2. Problem statement.

Consider a layer of a certain thickness, on the surface of which a gas injection source is evenly distributed. In particular, this may be a stratum of an underground gas storage (UGS), which contains a water layer of thickness l located below the porous medium where natural gas is stored. Depending on pressure and temperature, part of the gas diffuses into the water layer. This raises the problem of estimating the amount of gas that diffuses into the water. In the classical case, such a process is described by a partial differential equation [22,23,24,26]. Since the diffusion coefficient depends on pressure and temperature, both of which vary over time, it is reasonable to generalize the existing model by incorporating the process history. As shown in works [16,13,14,15,18], when mathematically modeling mass transfer processes in porous media, it is advisable to use fractional-order derivatives with respect to time to account for the process history. Considering the above, we will describe diffusion processes using a differential equation with a Caputo fractional derivative with respect to time

$${}^{c}D_{\tau}^{\alpha}=\frac{{}^{c}\partial^{\alpha}c}{\partial t^{\alpha}}=D\frac{\partial^2c}{\partial x^2} \qquad (8)$$

for $0<\alpha<1$. Where t - time, and x - variable coordinate. Let us assume that at the initial moment of time

$$c(x,0) = x_0 + x_l x,$$

at the lower boundary ($x=0$) zero concentration is maintained, and at the top boundary ($x=l$) at the initial moment of time, a concentration equal to d . Under such assumptions

$$c(x,0) = \frac{d}{l}x.$$

In the Laplace-Carson space, the fractional derivative of Caputo has the form [25]

$$L\left({}^{c}D_{\tau}^{\alpha}\right) = L\left(\frac{1}{\Gamma(1-\alpha)}\int_0^{\tau}\frac{f'(\xi)}{(\tau-\xi)^{\alpha}}d\xi\right) = p^{\alpha}\left[F(p) - f(0)\right] \tag{9}$$

Then, in Laplace-Carson transform, equation (8) will have the form

$$p^{\alpha}\left[\bar{c} - c(x,0)\right] = D\frac{\partial^2\bar{c}}{\partial x^2}, \tag{10}$$

where p is the transform parameter, and $\bar{c}(x,p)$ is the original Laplace-Carson transform. If we introduce the notation

$$p_1 = p^{\alpha}/D,\quad c_{11} = p^{\alpha}c(x,0)/D,$$

then in Laplace-Carson transform, equation (10) will be

$$\bar{c}'' - p_1\bar{c} = -c_{11}. \tag{11}$$

Characteristic equation corresponding to the homogeneous differential equation (11)

$$z^2 - p_1 = 0$$

has the following roots

$$z_{12} = \pm\sqrt{\frac{p^{\alpha}}{D}}.$$

The general solution of the homogeneous differential equation (11) will be

$$\bar{c}_c(x,p) = Ae^{z_1x} + Be^{z_2x}.$$

With this initial distribution, the partial solution will have the form

$$\bar{c}_h(x,p) = \frac{d}{l}x.$$

Thus, the general solution will have the form

$$\bar{c}_z(x,p) = Ae^{z_1x} + Be^{z_2x} + \frac{d}{l}x. \tag{12}$$

As noted, at the lower boundary the concentration is maintained at zero, and at the top boundary we accept that it is

$$c(l,t) = d + c_{0l}\left(1 - e^{-\zeta t}\right) \tag{13}$$

where ζ parameter characterizes the rate at which the concentration reaches a steady state, and c_{0l} - some coefficient, which is defined as the difference between the maximum concentration value and its initial value at the upper limit. The Laplace-Carson transform of this boundary condition (13) will be

$$\bar{c}(l,p) = d + c_{0l}\left(1 - \frac{p}{p+\zeta}\right). \tag{14}$$

Taking into account the above, to determine the constants in the general solution (12), we obtain the following system

$$A + B = 0,\qquad Ae^{z_1l} + Be^{z_2l} = \bar{c}_{\alpha},$$

where

$$\bar{c}_{\alpha} = 2d + c_{0l}\left(1 - \frac{p}{p+\zeta}\right), \tag{15}$$

and the solution of which is

$$A=\frac{\overline{c}_\alpha}{e^{z_1 l}-e^{z_2 l}}, \quad B=-\frac{\overline{c}_\alpha}{e^{z_1 l}-e^{z_2 l}}.$$

After substituting the parameters A and B into equation (12), a general solution is obtained

$$\overline{c}_z(x,p)=\frac{\overline{c}_\alpha}{e^{z_1 l}-e^{z_2 l}}\left(e^{z_1 x}-e^{z_2 x}\right)+\frac{d}{l}x,$$

or

$$\overline{c}_z(x,p)=\overline{c}_\alpha\frac{sh\left(x\sqrt{p^\alpha/D}\right)}{sh\left(l\sqrt{p^\alpha/D}\right)}+\frac{d}{l}x. \quad (16)$$

The last formula is a solution to the problem formulated above in the Laplace-Carson transform. To find the final solution, it is necessary to move from the Laplace-Carson transform to the original. Several ways can be used for this.

- Apply numerical methods.
- Apply contour integration methods in the complex domain, which ultimately bring into numerical calculations of the corresponding integrals.
- Apply approximate methods known in the literature.

Works [13,14,18] show that mathematical models of processes using fractional derivatives are sensitive to the order of the fractional derivative. Therefore, the application of numerical methods is often problematic. Moreover, in the mathematical modeling of many physical processes, the most informative time intervals are typically the start-up (transient) and steady-state regimes, corresponding to small and large times, respectively. In this regard, we will proceed to finding the asymptotics of the desired solution for large and small times.

Equality (16) will be written using the Dirichlet series in the form

$$\overline{c}_z(x,p)=\overline{c}_\alpha\left(e^{-z_1(l-x)}-e^{-z_1(l+x)}\right)\times\sum_{j=0}^{\infty}(-1)^j e^{-2jz_1 l}+\frac{dx}{l}. \quad (17)$$

3. **As follows from equality (17), to find the original $c(x,t)$, it is necessary to know the original of the Laplace-Carson transform**

$$G(\beta,w,p)=p^{-\beta/2}e^{-wp^{\alpha/2}}, \quad (18)$$

which is not listed in the existing tables of correspondence between originals and Laplace-Carson transforms.

The function $G(\beta,w,p)$ is unambiguous and analytical on a space p with a section along the negative real axis (Fig. 1). At the top section l_1 we have $p=\rho e^{\pi i}$ та $p^\alpha=\rho^\alpha e^{\alpha\pi i}$, and at the lower - $p=\rho e^{-\pi i}$ та $p^\alpha=\rho^\alpha e^{-\alpha\pi i}$. Since point $p=0$ is a branching point, we will calculate the original $g(\beta,w,t)$ using formula [25]

$$g(\beta,w,t)=-\frac{1}{2\pi i}\int_\gamma e^{pt}p^{-\beta/2}e^{-wp^{\alpha/2}}dp, \quad (19)$$

where the integration is performed counterclockwise (Fig.1), and $\int_\gamma=\int_{l_2}+\int_{c_0}+\int_{l_1}$.

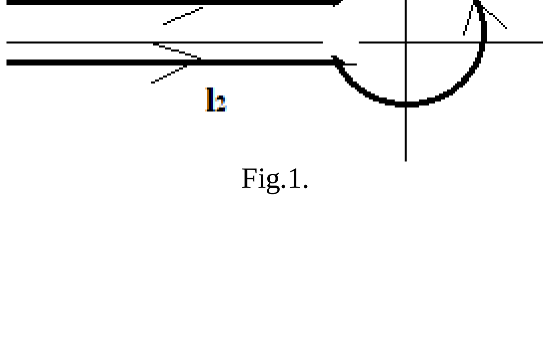

Fig.1.

Let us find the value of the integral along each of the contours, in particular along the contour c_0. Let's assign $p = re^{i\varphi}$. We will obtain

$$\left|\int_{c_0} e^{pt}\frac{e^{-wp^{\alpha/2}}}{p^{\beta/2}}dp\right| \le \int_{c_0}\left|e^{pt}\right|\left|\frac{e^{-wp^{\alpha/2}}}{p^{\beta/2}}\right||dp| = \int_{-\pi}^{\pi} e^{rt\cos\varphi}\frac{e^{-wr^{\alpha/2}\cos\frac{\alpha\varphi}{2}}}{r^{\beta/2}}rd\varphi \le 2\pi r^{1-\beta/2}e^{rt} \to 0 .$$

Under the condition $1-\beta/2>0 \Rightarrow \beta<2$. Since the integral over the circle is zero, then from formula (19)

$$g(\beta,w,t) = \int_{l_1} e^{pt}\frac{e^{-wp^{\alpha/2}}}{p^{\beta/2}}dp + \int_{l_2} e^{pt}\frac{e^{-wp^{\alpha/2}}}{p^{\beta/2}}dp = \int_0^\infty e^{-\rho t}\frac{e^{w(-1)^{\alpha/2}\rho^{\alpha/2}} + e^{-w(-1)^{\alpha/2}\rho^{\alpha/2}}}{(-1)^{\beta/2}\rho^{\beta/2}}d\rho. \tag{20}$$

In formula (20), we will make a replacement $\rho t = u^2$. Then $\rho = u^2/t$, $d\rho = 2udu/dt$, and

$$g(\beta,w,t) = \frac{2}{(-1)^{\beta/2}t^{1-\beta/2}} \times \left[\int_0^\infty \exp\left(-u^2 + w_1u^\alpha\right)u^{1-\beta}du + \int_0^\infty \exp\left(-u^2 - w_1u^\alpha\right)u^{1-\beta}du\right]. \tag{21}$$

where it is indicated

$$w_1 = \frac{w(-1)^{\alpha/2}}{t^{\alpha/2}} .$$

4. Let's figure out the behavior of the original $g(\beta,w,t)$ for $t\to\infty$.

1. Obviously, for $t\to\infty$ is satisfied $|w_1| = \to 0$. To simplify the notation, we find the asymptotics for large times of the integral

$$g_1(\beta,w,t) = \frac{2}{(-1)^{\beta/2}t^{1-\beta/2}}\int_0^\infty \mathrm{e}^{-u^2+w_1u^\alpha}u^{1-\beta}du = \frac{2}{(-1)^{\beta/2}t^{1-\beta/2}}\int_0^\infty e^{-u^2}u^{1-\beta}\left(1 + w_1u^\alpha + \frac{1}{2}w_1^2u^{2\alpha}\right)du. \tag{22}$$

Similarly, the formula is obtained

$$g_2(\beta,w,t) = \frac{2}{(-1)^{\beta/2}t^{1-\beta/2}}\int_0^\infty \mathrm{e}^{-u^2+w_1u^\alpha}u^{1-\beta}du = \frac{2}{(-1)^{\beta/2}t^{1-\beta/2}}\int_0^\infty e^{-u^2}u^{1-\beta}\left(1 - w_1u^\alpha + \frac{1}{2}w_1^2u^{2\alpha}\right)du. \tag{23}$$

Since, according to (21)-(23)

$$g(\beta,w,p) = g_1(\beta,w,p) + g_2(\beta,w,p),$$

then

$$g(\beta,w,t) = \frac{4}{(-1)^{\beta/2}t^{1-\beta/2}} \times \int_0^\infty e^{-u^2}u^{1-\beta}\left(1 + \frac{1}{2}w_1^2u^{2\alpha}\right)du. \tag{24}$$

Under the following conditions $[\mathrm{Re}\,\alpha, \mathrm{Re}\,p > 0]$, or $[\mathrm{Re}\,p = \mathrm{Re}\,q = 0,\ \mathrm{Im}\,p \ne 0]$, or $[0 < Re\alpha < 2,\ \mathrm{Re}\,p = \mathrm{Re}\,q = 0,\ \mathrm{Im}\,p \ne 0]$ the following equality is valid [27]

$$\int_0^\infty x^{\alpha-1}e^{-px^2-qx}dx = \frac{\Gamma(\alpha)}{(2p)^{\alpha/2}}e^{q^2/(8p)}D_{-\alpha}\left(\frac{q}{\sqrt{2p}}\right).$$

In the last formula, $D_v(z)$ is the function of a parabolic cylinder [27,28,29]. If $p=1,\ q=0$, then

$$\int_0^\infty x^{\mu-1}e^{-x^2}dx = \Gamma(\mu)2^{-\mu/2}D_{-\mu}(0).$$

Since

$$D_{-\mu}(0) = 2^{-\mu/2}\frac{\sqrt{\pi}}{\Gamma((\mu+1)/2)},$$

then

$$\int_0^\infty x^{\mu-1}e^{-x^2}dx = 2^{-\mu}\frac{\sqrt{\pi}\Gamma(\mu)}{\Gamma((\mu+1)/2)} = \Omega(-\mu).$$

Thus, from (24) for large values of time, we obtain the following behavior of the original

$$g(\beta,w,t) = \frac{4}{(-1)^{\beta/2}t^{1-\beta/2}}\times\left[\Omega(\beta-2)+\frac{1}{2}w_1^2\Omega(\beta-2\alpha-2)\right]. \quad (25)$$

2. At the extreme right singular point, an asymptotic expansion occurs

$$sh\left(x\sqrt{p^\alpha/D}\right) = x\sqrt{p^\alpha/D}+\frac{1}{6}\left(x\sqrt{p^\alpha/D}\right)^3$$

Then

$$\frac{sh\left(x\sqrt{p^\alpha/D}\right)}{sh\left(l\sqrt{p^\alpha/D}\right)} \approx \frac{x+\frac{1}{6}x^3\frac{p^\alpha}{D}}{l+\frac{1}{6}l^3\frac{p^\alpha}{D}} = \frac{x}{l}\frac{1+\frac{1}{6}x^2\frac{p^\alpha}{D}}{1+\frac{1}{6}l^2\frac{p^\alpha}{D}} \approx \frac{x}{l}\left(1-\frac{1}{6}\left(l^2-x^2\right)\frac{p^\alpha}{D}\right)$$

and in the vicinity of a special point

$$\frac{1}{p}\bar{c}_z(x,p) = \frac{x}{l}\left\{\frac{d+c_{0l}}{p}-\frac{c_{0l}}{\zeta}+\frac{c_{0l}}{\zeta^2}p-\frac{l^2-x^2}{6}\left(d+c_{0l}\right)\frac{p^{\alpha-1}}{D}+\frac{c_{0l}}{6}\left(l^2-x^2\right)\frac{p^\alpha}{\zeta D}+\frac{p^{2\alpha-1}d}{6D}\left(l^2-x^2\right)\right\}$$

Using Tauber-type theorems [30] leads to the following formula for finding the asymptotic behavior of the original for large times

$$c_z(x,t) = \frac{x}{l}\left\{d+c_{0l}-\frac{l^2-x^2}{6D}\left(d+c_{0l}\right)\frac{t^{-\alpha}}{\Gamma(1-\alpha)}+\frac{c_{0l}}{6\zeta D}\left(l^2-x^2\right)\frac{t^{-\alpha-1}}{\Gamma(-\alpha)}+\frac{d\left(l^2-x^2\right)}{6D}\frac{t^{-2\alpha}}{\Gamma(1-2\alpha)}\right\}$$

5. Let's figure out asymptotic behavior $g(\beta,w,t)$ for small time values.

Let's find out the asymptotics of the integral

$$I_1(\beta,w,t) = \int_0^\infty \exp\left(-u^2+w_1u^\alpha\right)u^{1-\beta}du \quad (26)$$

For small time values. Function

$$f(u) = u^2 - w_1u^\alpha$$

has an extremum at the point

$$u_0 = \left[\frac{\alpha w(-1)^{\alpha/2}}{2t^{\alpha/2}}\right]^{\frac{1}{2-\alpha}}.$$

At the point of extremum

$$f(u_0) = -u_0^2\frac{2-\alpha}{\alpha}, \quad f''(u_0) = 2(2-\alpha)$$

And the following formulas are valid

$$u^{1-\beta} = u_0^{1-\beta}+(1-\beta)u_0^{-\beta},$$

$$f(u) = f(u_0)+f''(u_0)(u-u_0)^2.$$

Using the above formulas, we can rewrite formula (26) in the following way

$$I_1(\beta,w,t) = e^{-f(u_0)}\left[u_0^{1-\beta}\int_0^\infty \exp\left(-f''(u_0)(u-u_0)^2\right)du+(1-\beta)u_0^{-\beta}\int_0^\infty \exp\left(-f''(u_0)(u-u_0)^2\right)(u-u_0)du\right],$$

where from

$$I_1(\beta,w,t) = e^{-f(u_0)}\left[\beta u_0^{1-\beta}\int_0^\infty e^{-f''(u_0)(u-u_0)^2}du+(1-\beta)u_0^{-\beta}\int_0^\infty e^{-f''(u_0)(u-u_0)^2}udu\right]. \quad (27)$$

Under the conditions $\left[\operatorname{Re} p>0\right]$, or $\left[\operatorname{Re} p=0,\ \operatorname{Im} p\neq 0,\ \operatorname{Re} q\geq 0\right]$ the following equality is valid [27,28]

$$\int_0^\infty e^{-px^2-qx}dx=\frac{1}{2}\sqrt{\frac{\pi}{p}}e^{\left(q^2/(4p)\right)}erfc\left(\frac{q}{2\sqrt{p}}\right),$$

and under the conditions $\left[\operatorname{Re} p>0\right]$, or $\left[\operatorname{Re} p=0,\ \operatorname{Re} q>0\right]$ the following equality is valid [27,28]

$$\int_0^\infty x^n e^{-px^2-qx}dx=\frac{(-1)^n}{2}\sqrt{\frac{\pi}{p}}\frac{\partial^n}{\partial q^n}\left[e^{\frac{q^2}{4p}}erfc\left(\frac{q}{2\sqrt{p}}\right)\right].$$

Here $erfc(x)=1-erf(x)$, where $erf(x)$ - is the probability integral [18, 27, 29]. Taking into account the latest formulas, from (27) we obtain

$$I_1(\beta,w,t)=\frac{1}{2}u_0^{-\beta}\exp\left[-f(u_0)-f''(u_0)u_0^2\right]\times\sqrt{\frac{\pi}{f''(u_0)}}\Big\{\beta u_0\exp\left(u_0^2 f''(u_0)\right)erfc\left(u_0\sqrt{f''(u_0)}\right)-$$
$$\left.-(1-\beta)\frac{\partial}{\partial q}e^{\frac{q^2}{4f''(u_0)}}erfc\left(\frac{q}{2\sqrt{f''(u_0)}}\right)_{q=2u_0 f''(u_0)}\right\} \qquad (28)$$

The asymptotics of the integral

$$I_2(\beta,w,t)=\int_0^\infty \exp\left(-u^2-w_1u^\alpha\right)u^{1-\beta}du$$

is obtained from the asymptotics of the integral I_1 by replacing w with $-w$, therefore

$$I_2(\beta,w,t)=I_1(\beta,-w,t).$$

Thus, for small times from formula (21) we obtain

$$g(\beta,w,t)=\frac{2\left[I_1(\beta,w,t)+I_1(\beta,-w,t)\right]}{(-1)^{\beta/2}t^{1-\beta/2}}.$$

6. Solution of the formulated problem.

With formula (21), we can now find the solution to the formulated problem. To do this, formula (21) should be applied to each term of the Dirichlet series (17), using the convolution theorem [25]

$$F(p)G(p)\to\frac{d}{dt}\int_0^t f(t-\tau)g(\tau)d\tau .$$

It should be emphasized that, in modeling many physical processes, it is essential to obtain accurate and reliable solutions within the most informative space–time zones. Quite often, these zones correspond to start-up (transient) regimes associated with small times or steady-state regimes, particularly when constructing balance-based mathematical models. In such cases, it is sufficient to have a solution of the boundary-value problem for small or large times. If we limit computation to the first term of the series expansion (17)

$$\bar{c}_z(x,p)\approx\bar{c}_\alpha\exp\left[-(l-x)\sqrt{\frac{p^\alpha}{D}}\right]+\frac{d}{l}x,$$

then the behavior of the original over time in the border zones $c(x,t)$ can be calculated in several ways. One of them is to use the original convolution theorem. Another way could be the following. Since the original is known

$$c_\alpha(t)=d+c_{0l}\left(1-e^{-\zeta t}\right)-\frac{d}{\Gamma(1-\alpha)t^\alpha},$$

then it is easy to determine the behavior of this original for small and large times. Next, we apply the principle that the asymptotic of a product equals the product of the asymptotics of each factor [30].

Discussion and conclusions. The paper presents a mathematical model of diffusion taking into account the Caputo fractional derivative with respect to time. The choice of the fractional derivative with

respect to time is justified by the fact that the diffusion process, like filtration processes, currently depends on the behavior of these processes in previous periods. Since the fractional derivative parameter significantly influences the modeling results, the Laplace–Carson integral transform is used extensively in constructing the mathematical model of the diffusion process. This yields a solution in the transform domain, which must then be inverted to obtain the original function. Existing tables of correspondences between originals and transform values practically lack formulas that allow one to define the original based on the obtained transformant-based solutions using fractional-order derivatives. Applying the generalized Efros theorem [25] involves significant computational complexity and does not always yield results that satisfy accuracy requirements or technological constraints. Therefore, the paper derives an analytical expression that enables the identification of originals for transformants with an exponential form. It is worth highlighting that such a form is characteristic of solutions to boundary-value problems that describe diffusion and filtration processes, thermoelasticity processes, and so on.
It should be noted that the application of fractional calculus to the mathematical modeling of processes is associated with several unresolved issues: the problem of choosing the appropriate form of fractional calculus, the criterion for selecting the order of the fractional derivative is unknown; methods for solving relevant boundary-value problems that would yield results with guaranteed reliability and accuracy have not been developed, etc.

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Дослідження перехідних часів в процесах дифузії з використанням похідних дробового порядку

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В роботі побудована математична модель процесу дифузії з використанням похідних дробового порядку Капутто за часом. Розв΄язок задачі отримано в аналітичному вигляді з використання методів контурного інтегрування. В аналітичному вигляді знайдено поведінку процесу дифузії як для всього діапазону часів, так і для великих та малих часів. Необхідність отримання розв΄язку в аналітичному вигляді пояснюється тим, що математичні моделі процесів з використання похідних дробових порядків є досить чутливими до зміни порядку похідної, а застосування числових методів не завжди дозволяють зменшувати крок дискретизації. Разом з тим, з аналізу літературних джерел слідує, що невелика зміна порядку дробової похідної може привести до суттєво відмінних результатів. Тому важливе значення має отримання результату в аналітичній формі. Це дозволить адаптувати та оптимізувати отриманий результат стосовно реальної інформації про процес, який моделюється.

Keywords — *математичне моделювання, дробове числення, процеси дифузії, методи розв΄язування крайових задач, методи теорії функції комплексної змінної.*

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