

A GENERALIZED KINETIC MODEL OF THE ADVECTION-DISPERSION PROCESS IN A SORBING MEDIUM

DUMITRU VIERU¹, CONSTANTIN FETECU², NAJMA AHMED³
AND NEHAD ALI SHAH^{4,5,*}

Abstract. A new time-fractional derivative with Mittag-Leffler memory kernel, called the generalized Atangana-Baleanu time-fractional derivative is defined along with the associated integral operator. Some properties of the new operators are proved. The new operator is suitable to generate by particularization the known Atangana-Baleanu, Caputo-Fabrizio and Caputo time-fractional derivatives. A generalized mathematical model of the advection-dispersion process with kinetic adsorption is formulated by considering the constitutive equation of the diffusive flux with the new generalized time-fractional derivative. Analytical solutions of the generalized advection-dispersion equation with kinetic adsorption are determined using the Laplace transform method. The solution corresponding to the ordinary model is compared with solutions corresponding to the four models with fractional derivatives.

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1. INTRODUCTION

The researchers in the agricultural and soil fields, have been interested in the effectiveness of agricultural chemicals, such as fertilizers, pesticides, etc., that are applied to soil for enhancing the crop grows. These concerns, along with possible contamination of groundwater have provided a major impulse to the study of solute transport in soils.

The movement of dissolved substances is significantly influenced by a large number of physical, chemical and microbiological processes. Modeling solute transport requires extensive mathematical and physical knowledge, as well as high-precision experimental procedures.

Transport of a solute (a dissolved substance) depends on the magnitude and direction of the solvent flux (for example, the water flux). The determination of solute concentrations is not always straightforward, particularly if the solute is involved in partitioning between different phases or subject to transformations.

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¹ Department of Theoretical Mechanics, Technical University of Iasi, Iasi, Romania.

² Section of Mathematics, Academy of Romanian Scientists, 050094 Bucharest, Romania.

³ Abdus Salam School of Mathematical Sciences, GC University, Lahore, Pakistan.

⁴ Department of Mechanical Engineering, Sejong University, Seoul, South Korea.

⁵ Department of Mathematics, Lahore Leads University, Lahore, Pakistan.

* Corresponding author: nehadali199@yahoo.com

The standard transport mechanism is mathematically described by the fundamental advection-dispersion equation (convection-dispersion equation). To note that, the traditional advection-dispersion process is not always adequate to describe the solutes transport in soils.

The motion of a solute that undergoes adsorption by the soil requires a modified mathematical model, especially when several solute species are present that may participate in a few different reactions [19]. Wu *et al.* [29] have investigated a nonlinear adsorptive transport model through layered soil and developed an analytical solution to a one-dimensional transport problem. The obtained analytical solution is an exact solution for non-dispersive transport and it becomes an approximate one when the dispersion effects are included. The authors found that the shape and non-linearity of the adsorption isotherm could be a controlling tool on the transport characteristics. Kakur and Van Keer [13] proposed a new numerical algorithm to the mathematical model of convection diffusion and adsorption based on the relaxation method and on the method of characteristics. They proved the convergence of the method and applied it to a one-dimensional problem. Their results could be applied to the model of contaminant transport in porous media with different type of adsorption.

Van Kooten [28] developed a method to find solution of the transport equations for a kinetically adsorbing solute in a porous medium with the velocity field and dispersion coefficients depending on the spatial variables. Using the stochastic nature of the kinetic process of first-order, the author has proceeded to de decoupling of the advection-dispersion equation and the adsorption isotherm process. When the solution for a non-adsorbing solute is given, the proposed method provides an exact solution for the kinetically adsorbing solute. Uffink *et al.* [27] investigated the non-Gaussian spreading of solutes due to advection, dispersion and kinetic sorption (adsorption/desorption). By analyzing the behavior of a single particle and applying a random walk to describe advection/dispersion process plus a Markov chain to describe kinetic sorption, the authors obtained the set of partial differential equations of the model. The authors have shown that two spreading phenomena are active, namely, the Gaussian microdispersive spreading plus the kinetics-induced non-Gaussian spreading. Kurikami *et al.* [16] developed a modified diffusion-sorption-fixation model, based on the advection-dispersion equation and have applied the model to study the vertical migration of radiocesium in soils. The proposed model introduces kinetics for the reversible binding of radiocesium. They have tested the model's results by comparing them results to depth profiles measured in CityplaceFukushima Prefecture, country-regionJapan, since 2011. Their results have shown that the proposed model captures the long tails of the radiocesium distribution at large depths, which are caused by different rates for kinetic sorption and desorption.

Lee *et al.* [18] have investigated how two sorption kinetics of the first-order differ from each other. They compared the sorption parameters of both models estimated from experimental data obtained from the kinetic sorption test, and by simulating the breakthrough curves of a reactive chemical using a solute transport equation coupled with sorption kinetics. Liu *et al.* [21] studied a fractional diffusion equation with variable coefficients by considering a non-local mathematical model based on Caputo time-fractional derivative, respectively on the Riemann-Liouville space-fractional derivatives. Solutions of the studied problem have been determined with the variational iteration method.

An interesting study of the exothermic reactions model with constant heat source in the porous media with strong memory effects was carried out by Kumar *et al.* [14]. The mathematical models used Caputo, Caputo-Fabrizio and Atangana-Baleanu fractional operators to induce memory effects of exothermic reactions.

Kumar *et al.* [15] introduced a new fractional operator based on the Rabotnov fractional-exponential kernels. They provided some properties and applications of these operators.

Povstenko and Kyrlych [24] studied two generalized advection-diffusion equations using mathematical models with space-time-fractional derivatives. Caputo time-fractional derivative and Riesz fractional Laplacian are used in their study. Using the Laplace and Fourier transforms, the authors have determined fundamental solutions to the Cauchy and source problems. Luchko [23] has proved some interesting properties of the fundamental solutions to a multi-dimensional space-time-fractional diffusion-wave equation using the Mellin-Barnes representation of the derived fundamental solutions.

In the present paper, we investigate a generalized mathematical model of the solute transport by considering the mass transport of chemicals in porous media with sorbtion as a part of the dispersion mechanism. In such models, the free phase chemical concentration is related to the sorbed chemical concentration in the medium.

On the other hand, in order to implement the memory effects of the diffusion process, a generalized form of the diffusive flux, based on the generalized Atangana-Baleanu time-fractional derivative is proposed.

First, we introduce the new time-fractional derivative whose kernel is the Mittag-Leffler function with one parameter. This new time-fractional derivative generates by customization three other known fractional derivatives, namely, the Atangana-Baleanu fractional derivative, Caputo-Fabrizio fractional derivative and Caputo fractional derivative. This important property of the new time-fractional derivative makes it possible the comparison between a solute transport based on the mathematical model with derivatives of integer order (the ordinary model) and four other models with different memory kernels. Some basic properties of the generalized time-fractional Atangana-Baleanu derivative are proved.

A mathematical model of the generalized solute transport is developed.

Analytical solutions to the one-dimensional problem are determined using the Laplace transform. Solutions corresponding to the model based on the generalized Atangana-Baleanu fractional derivatives are particularized to obtain solutions for the advection-diffusion equation with the kernel of diffusive flux of Atangana-Baleanu, Caputo-Fabrizio and Caputo type. The solution corresponding to the ordinary advection-diffusion equation has been also obtained as a particular case. An application for the constant concentration on the boundaries is investigated by graphical illustrations. The obtained results lead to the choice of the best model for obtaining the optimal concentrations in a certain practical problem.

2. FORMULATION OF THE PROBLEM

2.1. The ordinary mathematical model

Consider the transport of a chemical species (the solute) in a spatial porous media. The solute transport may be highly affected by interactions between the solute and the solid matrix. At the macroscopic level, the balance equations for the solute species subject to arbitrary reactions are given as [13, 28],

$$\frac{\partial C(X, t)}{\partial t} + \frac{\partial S(X, t)}{\partial t} = -\text{div} \left(\vec{J}_s(X, t) \right) + R(X), X = (x_1, x_2, x_3) \in D \subset \mathbb{R}^3, t \geq 0, \quad (2.1)$$

$$\frac{\partial S(X, t)}{\partial t} = k_1 C(X, t) - k_2 S(X, t), \quad (2.2)$$

$$\vec{J}_s(X, t) = \vec{J}_{adv}(X, t) + \vec{J}_{dif}(X, t), \vec{J}_{adv}(X, t) = \vec{v}(X, t)C(X, t), \vec{J}_{dif}(X, t) = -D(X)\nabla C(X, t), \quad (2.3)$$

where, $C(X, t)$ is the concentration of the solute in the free phase, $S(X, t)$ is the concentration in the adsorbed phase, $\vec{J}_s(X, t)$ is the solute flux density vector, $R(X)$ is the rate of zero-order production at the point X , k_1 is the forward reaction rate, k_2 is the backward reaction rate, $\vec{v}(X, t)$ is the fluid velocity vector, $D(X)$ is the dispersion tensor, $\vec{J}_{adv}(X, t)$ and $\vec{J}_{dif}(X, t)$ are the advective, respectively dispersive components of the solute flux vector, and ∇ is the gradient operator.

In the present article, we consider the one-dimensional problem defined for $x_1 = x \in [0, L]$, $t \geq 0$, $\vec{v}(x, t) = v_0 \vec{e}_x$, $D(x) = D_0$, $v_0 = \text{const.}$, $D_0 = \text{const.}$, $v_0 > 0$, $\vec{e}_x$ being the unit vector in the x -direction.

In this case, the above equations become

$$\frac{\partial C(x, t)}{\partial t} + \frac{\partial S(x, t)}{\partial t} = -\text{div} \left(\vec{J}_{adv}(x, t) \right) - \text{div} \left(\vec{J}_{dif}(x, t) \right) + R(x), x \in [0, L], t \geq 0, \quad (2.4)$$

$$\frac{\partial S(x, t)}{\partial t} = k_1 C(x, t) - k_2 S(x, t), \quad (2.5)$$

$$\vec{J}_{adv} = v_0 C(x, t) \vec{e}_x, \vec{J}_{dif}(x, t) = -D_0 \frac{\partial C(x, t)}{\partial x} \vec{e}_x. \quad (2.6)$$

Introducing the non-dimensional variables

$$\begin{aligned} x^* &= \frac{x}{L}, \quad t^* = \frac{v_0 t}{L}, \quad C^* = \frac{C}{C_0}, \quad S^* = \frac{S}{C_0}, \quad J_{adv}^* = \frac{J_{adv}}{v_0 C_0}, \quad J_{dif}^* = \frac{J_{dif}}{v_0 C_0}, \\ F(x) &= \frac{L}{v_0 C_0} R(Lx^*), \quad k_1^* = \frac{Lk_1}{v_0}, \quad k_2^* = \frac{Lk_2}{v_0}, \end{aligned} \quad (2.7)$$

into equations (2.4)–(2.6) and neglecting the star notation, we obtain the problem written in dimensionless form,

$$\frac{\partial C(x, t)}{\partial t} + \frac{\partial S(x, t)}{\partial t} = -\frac{\partial}{\partial x} (J_{adv}(x, t)) - \frac{\partial}{\partial x} (J_{dif}(x, t)) + F(x), \quad x \in [0, 1], \quad t \geq 0, \quad (2.8)$$

$$\frac{\partial S(x, t)}{\partial t} = k_1 C(x, t) - k_2 S(x, t), \quad (2.9)$$

$$J_{adv}(x, t) = C(x, t), \quad J_{dif}(x, t) = -\frac{D_0}{Lv_0} \frac{\partial C(x, t)}{\partial x}. \quad (2.10)$$

In the following, we aim to develop a mathematical model based on the generalized form of the Atangana-Baleanu time-fractional derivative. This model is suitable for particularizations to describe the memory effects with Caputo kernel, Caputo-Fabrizio kernel, and Atangana-Baleanu kernel. In the next section, we present the basic definitions and properties of the generalized Atangana-Baleanu time-fractional derivatives.

2.2. A generalization of the Atangana-Baleanu time-fractional derivative

2.2.1. A summary on the one-parametric Mittag-Leffler function

The special function [8–10, 17, 25]

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}, \quad \alpha \in \mathbb{C}, \quad \operatorname{Re}(\alpha) > 0, \quad z \in \mathbb{C}, \quad (2.11)$$

$\mathbb{C}$ being the set of complex numbers is called the one-parametric Mittag-Leffler function. In the equation (2.11), $\Gamma(\cdot)$ denotes the Euler's integral of second type, namely $\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt$, $\operatorname{Re}(z) > 0$. Some special cases of the function (2.11) are:

$$\text{a).} \quad E_1(z) = \exp(z), \quad E_{1/2}(\pm z^{1/2}) = e^z \left[1 + \operatorname{erf}(\pm z^{1/2}) \right] = e^z \operatorname{erfc}(\pm z^{1/2}), \quad z \in \mathbb{C}, \quad (2.12)$$

where, $\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_0^z \exp(-x^2) dx$, $\operatorname{erfc}(z) = 1 - \operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty \exp(-x^2) dx$ are the error function, respectively the complementary error function.

$$\text{b).} \quad E_2(z^2) = \cosh(z), \quad E_2(-z^2) = \cos(z), \quad E_{2\alpha}(z^2) = \frac{1}{2} [E_\alpha(z) + E_\alpha(-z)]. \quad (2.13)$$

The Mittag-Leffler function defined by (2.11) has the integral representation

$$E_\alpha(z) = \frac{1}{2\pi i} \int_\Omega \frac{x^{\alpha-1} e^x}{x^\alpha - z} dx, \quad \alpha, \quad z \in \mathbb{C}, \quad \operatorname{Re}(\alpha) > 0, \quad (2.14)$$

where the path of integration Ω is a loop starting and ending at $(-\infty)$ and encircling the circular disk $|x| \leq z^{1/\alpha}$ in the positive sense, $-\pi < \arg x < \pi$ on Ω . The integrand has a branch point at $x = 0$. The complex x -plane is cut along the negative axis and in the cut plane the integrand is single-valued, the principal branch of x^α is taken in the cut plane. Using the integral representation (2.14), the following asymptotic expansions of the Mittag-Leffler function at infinity are obtained:

1°. $0 < \alpha < 2$, and β is a real number such that $\frac{\pi\alpha}{2} < \beta < \min(\pi, \pi\alpha)$

$$\begin{aligned} E_\alpha(z) &= \frac{1}{\alpha} z^{\frac{1-\beta}{\alpha}} \exp\left(z^{1/\alpha}\right) - \sum_{k=1}^n \frac{1}{z^k \Gamma(1-\alpha k)} + O\left(\frac{1}{z^{n+2}}\right), \\ n \in \mathbb{N}, |z| \rightarrow \infty, |\arg(z)| &\leq \beta; \\ E_\alpha(z) &= - \sum_{k=1}^n \frac{1}{z^k \Gamma(1-\alpha k)} + O\left(\frac{1}{z^{n+2}}\right), \\ n \in \mathbb{N}, |z| \rightarrow \infty, \beta &\leq |\arg(z)| \leq \pi. \end{aligned} \quad (2.15)$$

$$\begin{aligned} \alpha &\geq 2 \\ \mathbf{2}^\circ. E_\alpha(z) &= \frac{1}{\alpha} \sum_j z^{1/j} \exp\left[z^{1/\alpha} \exp\left(\frac{2j\pi i}{\alpha}\right)\right] - \sum_{k=1}^n \frac{1}{z^k \Gamma(1-\alpha k)} + O\left(\frac{1}{z^{n+1}}\right), \\ |z| \rightarrow \infty, |\arg(z)| &\leq \frac{\alpha\pi}{2}. \end{aligned} \quad (2.16)$$

The first sum in (2.16) is taken over all j such that $|\arg(z) + 2j\pi| \leq \frac{\alpha\pi}{2}$.

For the one-parameter Mittag-Leffler function, the following integral representations are useful [10]:

$$\int_0^\infty e^{-st} t^{m\alpha} E_\alpha^{(m)}(\pm bt^\alpha) dt = \frac{m! s^{\alpha-1}}{(s^\alpha \mp b)^{m+1}}, \quad \operatorname{Re}(s) > 0, \operatorname{Re}(\alpha) > 0, m \in \mathbb{N}, \quad (2.17)$$

$$E_\alpha(-x^\alpha) = \frac{2}{\pi} \sin\left(\frac{\alpha\pi}{2}\right) \int_0^\infty \frac{t^{\alpha-1} \cos(xt)}{1 + 2t^\alpha \cos\left(\frac{\alpha\pi}{2}\right) + t^{2\alpha}} dt, \quad \operatorname{Re}(\alpha) > 0, \quad (2.18)$$

$$E_\alpha(-x) = \frac{1}{\pi} \sin(\alpha\pi) \int_0^\infty \frac{t^{\alpha-1} \exp(-tx^{1/\alpha})}{1 + 2t^\alpha \cos(\alpha\pi) + t^{2\alpha}} dt, \quad \operatorname{Re}(\alpha) > 0, \quad (2.19)$$

$$E_\alpha(-x) = \frac{2x}{\pi} \int_0^\infty \frac{E_{2\alpha}(-t^2)}{x^2 + t^2} dt, \quad 0 \leq \alpha \leq 1. \quad (2.20)$$

Remark 2.1. (The Laplace transform [25] of function $E_\alpha(\pm bt^\alpha)$).

For $m = 0$, equation (2.17) becomes

$$\frac{s^{\alpha-1}}{s^\alpha \mp b} = \int_0^\infty e^{st} E_\alpha(\pm bt^\alpha) dt = L\{E_\alpha(\pm bt^\alpha)\}. \quad (2.21)$$

2.2.2. The generalized Atangana-Baleanu time-fractional derivative

Recently, Caputo fractional derivative [5, 11], Caputo-Fabrizio fractional derivative [6, 7], and Atangana-Baleanu fractional derivative [1, 12] have been introduced and their properties and applications were investigated. We recall the definitions of these fractional derivatives together with some basic properties.

Definition 2.2. (*Caputo kernel*). The function

$$\Phi_0(t, \alpha) = \frac{t^{-\alpha}}{\Gamma(1-\alpha)}, \quad t > 0, \quad \alpha \in [0, 1), \quad (2.22)$$

is called Caputo kernel.

The Laplace transform of Caputo kernel is given by

$$L\{\varphi_0(t, \alpha)\} = \frac{1}{s^{1-\alpha}}. \quad (2.23)$$

Using (2.23), the kernel (2.22) can be defined for $\alpha = 1$, since,

$$\lim_{\alpha \rightarrow 1} L\{\varphi_0(t, \alpha)\} = L\left\{\lim_{\alpha \rightarrow 1} \varphi_0(t, \alpha)\right\} = 1 = L\{\delta(t)\}, \quad (2.24)$$

therefore,

$$\lim_{\alpha \rightarrow 1} \varphi_0(t, \alpha) = \delta(t), \quad (2.25)$$

where $\delta(\cdot)$ is Dirac's distribution.

Definition 2.3. (*Caputo fractional derivative*). If $f \in H^1(0, T)$, $T > 0$, $\alpha \in [0, 1]$, the Caputo fractional derivative of order α of function $f(t)$ is defined as

$$({}^C D_t^\alpha f)(t) = \varphi_0(t, \alpha) * \dot{f}(t) = \int_0^t \varphi_0(t - \tau, \alpha) \dot{f}(\tau) d\tau, \quad (2.26)$$

where $\dot{f}(\tau) = \frac{df(\tau)}{d\tau} \Big|_{t=\tau}$ and “ $*$ ” denotes the convolution product.

Remark 2.4. The following properties are obvious:

$$\begin{aligned} ({}^C D_t^0 f)(t) &= 1 * \dot{f}(t) = \int_0^t \dot{f}(\tau) d\tau = f(t) - f(0), \\ ({}^C D_t^1 f)(t) &= \delta(t) * \dot{f}(t) = \dot{f}(t). \end{aligned} \quad (2.27)$$

Definition 2.5. (*Caputo-Fabrizio kernel*). Function

$$\varphi_1(t, \alpha) = \frac{1}{1-\alpha} \exp\left(\frac{-\alpha t}{1-\alpha}\right), \quad t \geq 0, \quad \alpha \in [0, 1), \quad (2.28)$$

is called Caputo-Fabrizio kernel. The Laplace transform of the Caputo-Fabrizio kernel is given by

$$L\{\varphi_1(t, \alpha)\} = \frac{1}{(1-\alpha)s + \alpha}. \quad (2.29)$$

Using equation (2.29) we extend definition (2.28) for $\alpha = 1$, since

$$\lim_{\alpha \rightarrow 1} L\{\varphi_1(t, \alpha)\} = L\left\{\lim_{\alpha \rightarrow 1} \varphi_1(t, \alpha)\right\} = 1 = L\{\delta(t)\}, \quad (2.30)$$

therefore,

$$\lim_{\alpha \rightarrow 1} \varphi_1(t, \alpha) = \delta(t). \quad (2.31)$$

Definition 2.6. (*Caputo-Fabrizio fractional derivative*). If $f \in H^1(0, T)$, $T > 0$, $\alpha \in [0, 1]$, the Caputo-Fabrizio fractional derivative of order α of function $f(t)$ is defined as

$$({}^{CF}D_t^\alpha f)(t) = \varphi_1(t, \alpha) * \dot{f}(t) = \int_0^t \varphi_1(t - \tau, \alpha) \dot{f}(\tau) d\tau. \quad (2.32)$$

Remark 2.7. The following particular cases are true:

$$\begin{aligned} ({}^{CF}D_t^0 f)(t) &= 1 * \dot{f}(t) = \int_0^t \dot{f}(\tau) d\tau = f(t) - f(0), \\ ({}^{CF}D_t^1 f)(t) &= \delta(t) * \dot{f}(t) = \dot{f}(t). \end{aligned} \quad (2.33)$$

Definition 2.8. (*Atangana-Baleanu kernel*). Function

$$\varphi_2(t, \alpha) = \frac{1}{1 - \alpha} E_\alpha \left(-\frac{\alpha}{1 - \alpha} t^\alpha \right), \quad t \geq 0, \alpha \in (0, 1), \quad (2.34)$$

is called Atangana-Baleanu kernel. Using the property (2.21), we find the Laplace transform of the kernel (2.34) given as

$$L\{\varphi_2(t, \alpha)\} = \frac{s^{\alpha-1}}{(1 - \alpha)s^\alpha + \alpha}. \quad (2.35)$$

Using (2.35), the definition (2.34) is extended for $\alpha \in \{0, 1\}$, namely

$$\begin{aligned} \lim_{\alpha \rightarrow 0} L\{\varphi_2(t, \alpha)\} &= L\left\{\lim_{\alpha \rightarrow 0} \varphi_2(t, \alpha)\right\} = \frac{1}{s} = L\{1\}, \\ \lim_{\alpha \rightarrow 1} L\{\varphi_2(t, \alpha)\} &= L\left\{\lim_{\alpha \rightarrow 1} \varphi_2(t, \alpha)\right\} = 1 = L\{\delta(t)\}, \end{aligned} \quad (2.36)$$

therefore,

$$\lim_{\alpha \rightarrow 0} \varphi_2(t, \alpha) = 1, \quad \lim_{\alpha \rightarrow 1} \varphi_2(t, \alpha) = \delta(t). \quad (2.37)$$

Definition 2.9. (*Atangana-Baleanu fractional derivative in Caputo sense*). If $f \in H^1(0, T)$, $T > 0$, $\alpha \in [0, 1]$, the Atangana-Baleanu fractional derivative in Caputo sense, of order α of the function $f(t)$ is defined as

$$({}^{AB}D_t^\alpha f)(t) = \varphi_2(t, \alpha) * \dot{f}(t) = \int_0^t \varphi_2(t - \tau, \alpha) \dot{f}(\tau) d\tau. \quad (2.38)$$

Remark 2.10. Based on the properties (2.36) and (2.37), we obtain

$$\begin{aligned} ({}^{AB}D_t^0 f)(t) &= 1 * \dot{f}(t) = \int_0^t \dot{f}(\tau) d\tau = f(t) - f(0), \\ ({}^{AB}D_t^1 f)(t) &= \delta(t) * \dot{f}(t) = \dot{f}(t). \end{aligned} \quad (2.39)$$

Remark 2.11. Even if the exponential function is a particular case of the one-parametric Mittag-Leffler function, the Caputo-fabrizio fractional derivative is not a particular case of the Atangana-Baleanu derivative defined above.

In this paper, we will define a generalized Atangana-Baleanu derivative which contains as particular cases Caputo fractional derivative, Caputo-Fabrizio and Atangana-Baleanu fractional derivatives.

Definition 2.12. (*The generalized Atangana-Baleanu kernel*). The function

$$\varphi(t, \alpha, \beta) = \frac{1}{1-\alpha} E_\beta \left(\frac{-\alpha}{1-\alpha} t^\beta \right), \quad t \geq 0, \quad \alpha \in (0, 1), \quad \beta > 0, \quad (2.40)$$

is called the generalized Atangana-Baleanu kernel.

The Laplace transform of the kernel (2.40) is given by

$$L\{\varphi(t, \alpha, \beta)\} = \frac{s^{\beta-1}}{(1-\alpha)s^\beta + \alpha}. \quad (2.41)$$

The following properties of the kernel (2.40) are easily deduced:

$$\begin{aligned} \lim_{\alpha \rightarrow 0} L\{\varphi(t, \alpha, \beta)\} &= L\left\{\lim_{\alpha \rightarrow 0} \varphi(t, \alpha, \beta)\right\} = \frac{s^{\beta-1}}{s^\beta} = L\{1\}, \\ \lim_{\alpha \rightarrow 1} L\{\varphi(t, \alpha, \beta)\} &= L\left\{\lim_{\alpha \rightarrow 1} \varphi(t, \alpha, \beta)\right\} = \frac{1}{s^{1-\beta}} = L\left\{\frac{t^{-\beta}}{\Gamma(1-\beta)}\right\} = L\{\varphi_0(t, \beta)\}, \\ \lim_{\beta \rightarrow 0} L\{\varphi(t, \alpha, \beta)\} &= L\left\{\lim_{\beta \rightarrow 0} \varphi(t, \alpha, \beta)\right\} = \frac{1}{s} = L\{1\}, \\ \lim_{\beta \rightarrow 1} L\{\varphi(t, \alpha, \beta)\} &= L\left\{\lim_{\beta \rightarrow 1} \varphi(t, \alpha, \beta)\right\} = \frac{1}{(1-\alpha)s + \alpha} = L\left\{\frac{1}{1-\alpha} e^{\frac{-\alpha t}{1-\alpha}}\right\} = L\{\varphi_1(t, \alpha)\}, \end{aligned} \quad (2.42)$$

therefore,

$$\begin{aligned} \lim_{\alpha \rightarrow 0} \varphi(t, \alpha, \beta) &= \lim_{\beta \rightarrow 0} \varphi(t, \alpha, \beta) = 1, \\ \lim_{\alpha \rightarrow 1} \varphi(t, \alpha, \beta) &= \varphi_0(t, \beta), \\ \lim_{\beta \rightarrow 1} \varphi(t, \alpha, \beta) &= \varphi_1(t, \alpha), \\ \varphi(t, \alpha, \alpha) &= \varphi_2(t, \alpha), \\ \lim_{\alpha \rightarrow 1} \varphi(t, \alpha, \beta) &= \delta(t). \\ \beta &\rightarrow 1 \end{aligned} \quad (2.43)$$

Definition 2.13. (*The generalized Atangana-Baleanu fractional derivative in Caputo sense*). If $f \in H^1(0, T)$, $T > 0$, $\alpha \in [0, 1]$, $\beta \in [0, 1]$, the generalized Atangana-Baleanu fractional derivative in Caputo sense, of order α of the function $f(t)$ is defined as

$$\left({}^{GAB}D_t^{\alpha, \beta} f\right)(t) = \varphi(t, \alpha, \beta) * \dot{f}(t) = \int_0^t \varphi(t-\tau, \alpha, \beta) \dot{f}(\tau) d\tau. \quad (2.44)$$

Remark 2.14. Using equations (2.43) and (2.44), we obtain the following properties of the generalized Atangana-Baleanu time-fractional derivative:

$$\left({}^{GAB}D_t^{0, \beta} f\right)(t) = \left({}^{GAB}D_t^{\alpha, 0} f\right)(t) = 1 * \dot{f}(t) = \int_0^t \dot{f}(\tau) d\tau = f(t) - f(0), \quad (2.45)$$

$$\left({}^{GAB}D_t^{1,1}f\right)(t) = \delta(t) * \dot{f}(t) = \dot{f}(t), \quad (2.46)$$

$$\left({}^{GAB}D_t^{1,\beta}f\right)(t) = \varphi_0(t, \beta) * \dot{f}(t) = \left({}^CD_t^\beta f\right)(t), \quad (2.47)$$

$$\left({}^{GAB}D_t^{\alpha,1}f\right)(t) = \varphi_1(t, \beta) * \dot{f}(t) = \left({}^{CF}D_t^\beta f\right)(t), \quad (2.48)$$

$$\left({}^{GAB}D_t^{\alpha,\alpha}f\right)(t) = \varphi_2(t, \beta) * \dot{f}(t) = \left({}^{AB}D_t^\alpha f\right)(t). \quad (2.49)$$

Associated with the generalized Atangana-Baleanu derivative, we define the following fractional integral operator:

$$\left(J_t^{\alpha,\beta}f\right)(t) = (1 - \alpha)f(t) + \alpha\psi_0(t, \beta) * f(t), \quad \alpha \in [0, 1], \quad \beta \in (0, 1], \quad (2.50)$$

where the kernel $\psi_0(t, \beta)$ is defined as

$$\psi_0(t, \beta) = \frac{t^{\beta-1}}{\Gamma(\beta)}. \quad (2.51)$$

It is observed that $L\{\psi_0(t, \beta)\} = \frac{1}{s^\beta}$, $\lim_{\beta \rightarrow 0} L\{\psi_0(t, \beta)\} = 1 = L\{\delta(t)\}$, therefore,

$$\lim_{\beta \Rightarrow 0} \psi_0(t, \beta) = \delta(t). \quad (2.52)$$

Using the property (2.52), the fractional integral operator can be defined for $\beta = 0$.

Remark 2.15. The fractional integral operator has the following properties:

$$\begin{aligned} \left(J_t^{1,0}f\right)(t) &= \delta(t) * f(t) = f(t), \\ \left(J_t^{1,1}f\right)(t) &= 1 * f(t) = \int_0^t f(\tau) d\tau. \end{aligned} \quad (2.53)$$

Regarding the generalized Atangana-Baleanu derivative and associated fractional integral operator, we prove the proposition

Proposition 2.16. *The following relationships are fulfilled:*

$$\begin{aligned} \left({}^{GAB}D_t^{\alpha,\beta} \left(J_t^{\alpha,\beta}f\right)\right)(t) &= f(t) - (1 - \alpha)f(0)\varphi(t, \alpha, \beta), \\ \left(J_t^{\alpha,\beta} \left({}^{GAB}D_t^{\alpha,\beta}f\right)\right)(t) &= f(t) - f(0). \end{aligned} \quad (2.54)$$

Proof. To demonstrate relations (2.54) we use the Laplace transform. We have

$$\begin{aligned}
L \left\{ \left({}^{GAB}D_t^{\alpha,\beta} \left(J_t^{\alpha,\beta} f \right) \right) (t) \right\} &= \frac{s^{\beta-1} \left[sL \left\{ \left(J_t^{\alpha,\beta} f \right) (t) \right\} - \left(J_t^{\alpha,\beta} f \right) (0) \right]}{(1-\alpha)s^\beta + \alpha} \\
&= \frac{s^{\beta-1}}{(1-\alpha)s^\beta + \alpha} \left[s \left[(1-\alpha)L\{f(t)\} + \alpha s^{-\beta} L\{f(t)\} \right] - (1-\alpha)f(0) \right] \\
&= \frac{\left[(1-\alpha)s^\beta + \alpha \right] L\{f(t)\} - (1-\alpha)s^{\beta-1}f(0)}{(1-\alpha)s^\beta + \alpha} = L\{f(t)\} - \frac{(1-\alpha)s^{\beta-1}f(0)}{(1-\alpha)s^\beta + \alpha} \\
&= L\{f(t)\} - \frac{s^{\beta-1}}{s^\beta + \frac{\alpha}{(1-\alpha)}} f(0) = L \left\{ f(t) - f(0) E_\beta \left(\frac{-\alpha}{1-\alpha} t^\beta \right) \right\}.
\end{aligned} \tag{2.55}$$

Now, applying the inverse Laplace transform the first equality (2.54) is obtained.

For the second relation (2.54), we have

$$\begin{aligned}
L \left\{ \left(J_t^{\alpha,\beta} \left({}^{GAB}D_t^{\alpha,\beta} f \right) \right) (t) \right\} &= [(1-\alpha) + \alpha s^{-\beta}] L \left\{ \left({}^{GAB}D_t^{\alpha,\beta} f \right) (t) \right\} \\
&= \frac{(1-\alpha)s^\beta + \alpha}{s^\beta} \frac{s^{\beta-1} [sL\{f(t)\} - f(0)]}{(1-\alpha)s^\beta + \alpha} = L\{f(t)\} - f(0) \frac{1}{s} = L\{f(t) - f(0)\},
\end{aligned} \tag{2.56}$$

therefore, $\left(J_t^{\alpha,\beta} \left({}^{GAB}D_t^{\alpha,\beta} f \right) \right) (t) = f(t) - f(0)$.

The generalized fractional integral operator (2.50) contains the following particular cases:

$$\begin{aligned}
&\alpha = 1, \beta \in [0, 1], \\
\mathbf{1}^\circ. \quad &\left(J_t^{1,\beta} f \right) (t) = \psi_0(t, \beta) * f(t) = \frac{1}{\Gamma(\beta)} \int_0^t (t-\tau)^{\beta-1} f(\tau) d\tau,
\end{aligned} \tag{2.57}$$

i.e. the well known *Riemann-Liouville fractional integral operator* [3].

$$\begin{aligned}
&\alpha \in [0, 1], \beta = 1, \\
\mathbf{2}^\circ. \quad &\left(J_t^{\alpha,1} f \right) (t) = (1-\alpha)f(t) + \alpha \int_0^t f(\tau) d\tau,
\end{aligned} \tag{2.58}$$

The fractional integral operator associated with Caputo-Fabrizio derivative [2, 4, 22].

$$\begin{aligned}
&\alpha = \beta \in [0, 1], \\
\mathbf{3}^\circ. \quad &\left(J_t^{\alpha,\alpha} f \right) (t) = (1-\alpha)f(t) + \frac{\alpha}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1} f(\tau) d\tau,
\end{aligned} \tag{2.59}$$

is the fractional integral operator associated with Atangana-Baleanu fractional derivative [1].

2.3. The generalized mathematical model with fractional diffusion flux

In the following we will consider a generalized mathematical model based on the new definition of the Atangana-Baleanu fractional derivative, namely, we will consider the non-dimensional diffusive flux having the following definition:

$$J_{dif}(x, t) = -\frac{D_0}{Lv_0} {}^{GAB}D_t^{\alpha,\beta} \left(\frac{\partial C(x, t)}{\partial x} \right), \tag{2.60}$$

where, ${}^{GAB}D_t^{\alpha,\beta}(\cdot)$ is the generalized Atangan-Baleanu time fractional derivative defined by equations (2.40) and (2.44).

In the following we will deal with the dimensionless problem described by equations (2.8), (2.9), (2.10)₁ and (2.60), along with the initial and boundary conditions

$$\begin{aligned} C(x, 0) &= 0, \quad S(x, 0) = 0, \\ C(0, t) &= f_1(t), \quad C(1, t) = f_2(t). \end{aligned} \quad (2.61)$$

In the above relations, $f_i(t)$, $i = 1, 2$ are piecewise continuous functions of exponential order to infinity and $f_i(0) = 0$.

To find analytical or semi-analytical solutions of the problem, the Laplace transform is employed. Applying the Laplace transform [25] to equations (2.8)–(2.10)₁ and (2.60), using the initial conditions (2.61), we obtain the transformed problem

$$p\bar{C}(x, p) + p\bar{S}(x, p) = -\frac{\partial \bar{C}(x, p)}{\partial x} - \frac{\partial}{\partial x} (\bar{J}_{dif}(x, p)) + \frac{1}{p}F(x), \quad x \in [0, 1], \quad (2.62)$$

$$\bar{S}(x, p) = \frac{k_1}{p + k_2} \bar{C}(x, p), \quad (2.63)$$

$$\begin{aligned} \bar{J}_{dif}(x, p) &= -\frac{D_0}{Lv_0} \frac{p^{\beta-1}}{(1-\alpha)p^\beta + \alpha} \left[pL \left\{ \frac{\partial C(x, t)}{\partial x} \right\} - \frac{\partial C(x, t)}{\partial x} \Big|_{t=0} \right] \\ &= -\frac{D_0}{Lv_0} \frac{p^\beta}{(1-\alpha)p^\beta + \alpha} \frac{\partial \bar{C}(x, p)}{\partial x}. \end{aligned} \quad (2.64)$$

where $\bar{\chi}(x, p) = \int_0^\infty \chi(x, t) \exp(-pt) dt$ denotes the Laplace transform of function $\chi(x, t)$.

Replacing (2.63) and (2.64) in equation (2.62) and using the notations $\gamma = \frac{D_0}{Lv_0}$ we obtain the differential equation of concentration as

$$a(p) \frac{\partial^2 \bar{C}(x, p)}{\partial x^2} - \frac{\partial \bar{C}(x, p)}{\partial x} - b(p) \bar{C}(x, p) + \frac{1}{p}F(x) = 0, \quad (2.65)$$

where

$$a(p) = \gamma \frac{p^\beta}{(1-\alpha)p^\beta + \alpha}, \quad b(p) = \frac{p^2 + (k_1 + k_2)p}{p + k_2}. \quad (2.66)$$

Along with the differential equation (2.65), the boundary conditions are

$$\bar{C}(0, p) = \bar{f}_1(p), \quad \bar{C}(1, p) = \bar{f}_2(p). \quad (2.67)$$

Using the transformation

$$\bar{C}(x, p) = \exp\left(\frac{x}{2a(p)}\right) \bar{\varphi}(x, p), \quad (2.68)$$

we obtain for function $\bar{\varphi}(x, p)$ the following differential equation

$$a(p) \frac{\partial^2 \bar{\varphi}(x, p)}{\partial x^2} - c(p) \bar{\varphi}(x, p) + \frac{1}{p} \exp\left(\frac{-x}{2a(p)}\right) F(x) = 0, \quad (2.69)$$

where

$$c(p) = \frac{1 + 4a(p)b(p)}{4a(p)} = \frac{4\gamma p^2 + [(1 - \alpha) + 4\gamma(k_1 + k_2)]p + (1 - \alpha)k_2}{4\gamma(p + k_2)} + \frac{\alpha}{4\gamma p^\beta}. \quad (2.70)$$

The corresponding boundary conditions of the function $\bar{\varphi}(x, p)$ are

$$\bar{\varphi}(0, p) = \bar{f}_1(p), \quad \bar{\varphi}(1, p) = \exp\left(\frac{-1}{2a(p)}\right) \bar{f}_2(p). \quad (2.71)$$

3. TRANSPORT OF CONTAMINANT WITHOUT SPATIAL SOURCE

In this section we will determine the analytical solution of equation (2.69) in the assumption that no contaminant is added to system or extracted from the system, so that $F(x) = 0$. The boundary conditions are $\bar{\varphi}(0, p) = 0, \bar{\varphi}(1, p) = \exp\left(\frac{-1}{2a(p)}\right) \bar{f}_2(p)$.

The solution of this problem is given by

$$\begin{aligned} \bar{\varphi}(x, p) &= \exp\left(\frac{-1}{2a(p)}\right) \bar{f}_2(p) \frac{\sinh\left(x\sqrt{\frac{c(p)}{a(p)}}\right)}{\sinh\left(\sqrt{\frac{c(p)}{a(p)}}\right)} \\ &= \left(\frac{c(p)}{pa(p)}\right) \exp\left(\frac{-1}{2a(p)}\right) (p\bar{f}_2(p)) \frac{\sinh\left(x\sqrt{\frac{c(p)}{a(p)}}\right)}{\frac{c(p)}{a(p)} \sinh\left(\sqrt{\frac{c(p)}{a(p)}}\right)}. \end{aligned} \quad (3.1)$$

Replacing (3.1) in equation (2.68), we obtain the following expression of the concentration:

$$\bar{C}(x, p) = (p\bar{f}_2(p)) \left(\frac{c(p)}{pa(p)}\right) \exp\left(\frac{-(1-x)}{2a(p)}\right) \frac{\sinh\left(x\sqrt{\frac{c(p)}{a(p)}}\right)}{\frac{c(p)}{a(p)} \sinh\left(\sqrt{\frac{c(p)}{a(p)}}\right)}. \quad (3.2)$$

To find the solution $C(x, t)$ we need the inverse Laplace transform of the function given by (3.2).

First, we will present the inverse Laplace transforms of some auxiliary functions that will be used further, namely:

1°. **Function** $\bar{\psi}_{\alpha\beta}(p) = \frac{c(p)}{pa(p)}$.

Function $\bar{\psi}_{\alpha\beta}(p)$ can be written in the equivalent form

$$\begin{aligned} \bar{\psi}_{\alpha\beta}(p) &= \frac{c(p)}{pa(p)} = \frac{1 - \alpha}{\gamma} + \frac{(1 - \alpha)^2}{4\gamma^2} \frac{1}{p} + \frac{(1 - \alpha)k_1}{\gamma} \frac{1}{p + k_2} + \frac{\alpha}{\gamma} \frac{1}{p^\beta} \\ &+ \frac{\alpha}{\gamma} \left(\frac{1 - \alpha}{2\gamma} + k_1\right) \frac{1}{p^{1+\beta}} + \frac{\alpha^2}{4\gamma^2} \frac{1}{p^{1+2\beta}} - \frac{\alpha k_1 k_2}{\gamma} \frac{p^{-1-\beta}}{p + k_2}, \quad \alpha, \beta \in [0, 1]. \end{aligned} \quad (3.3)$$

Now, we analyze the following cases:

a). $\alpha = 0, \beta \in [0, 1]$.

In this case, the above function becomes

$$\bar{\psi}_{0\beta}(p) = \frac{1}{\gamma} + \frac{1}{4\gamma^2} \frac{1}{p} + \frac{k_1}{\gamma} \frac{1}{p + k_2}, \quad (3.4)$$

whose inverse Laplace transform is

$$\psi_{0\beta}(t) = \frac{1}{\gamma}\delta(t) + \frac{1}{4\gamma^2} + \frac{k_1}{\gamma}e^{-k_2t}. \quad (3.5)$$

b). $\alpha = 1, \beta \in [0, 1]$.

$$\begin{aligned} \bar{\psi}_{1\beta}(p) &= \frac{1}{\gamma} \frac{1}{p^\beta} + \frac{k_1}{\gamma} \frac{1}{p^{1+\beta}} + \frac{1}{4\gamma^2} \frac{1}{p^{1+2\beta}} - \frac{k_1 k_2}{\gamma} \frac{p^{-1-\beta}}{p+k_2} \\ &= \begin{cases} \bar{\psi}_{10}(p) = \frac{1}{\gamma} + \frac{1}{4\gamma^2} \frac{1}{p} + \frac{k_1}{\gamma} \frac{1}{p+k_2}, \beta = 0, \\ \bar{\psi}_{1\beta}(p) = \frac{1}{\gamma} \frac{1}{p^\beta} + \frac{k_1}{\gamma} \frac{1}{p^{1+\beta}} + \frac{1}{4\gamma^2} \frac{1}{p^{1+2\beta}} - \frac{k_1 k_2}{\gamma} \frac{p^{-1-\beta}}{p+k_2}, \beta \in (0, 1), \\ \bar{\psi}_{11}(p) = \frac{k_1+k_2}{\gamma k_2} \frac{1}{p} + \frac{1}{4\gamma^2} \frac{1}{p^3} - \frac{k_1}{\gamma k_2} \frac{1}{p+k_2}, \beta = 1. \end{cases} \end{aligned} \quad (3.6)$$

The inverse Laplace transforms of functions (3.6) are given by

$$\psi_{1\beta}(t) = \begin{cases} \psi_{10}(t) = \frac{1}{\gamma}\delta(t) + \frac{1}{4\gamma^2} + \frac{k_1}{\gamma}e^{-k_2t}, \beta = 0, \\ \psi_{1\beta}(t) = \frac{1}{\gamma} \frac{t^{\beta-1}}{\Gamma(\beta)} + \frac{k_1}{\gamma} \frac{t^\beta}{\Gamma(\beta+1)} + \frac{1}{4\gamma^2} \frac{t^{2\beta}}{\Gamma(2\beta+1)} - \frac{k_1 k_2 t^{\beta+1}}{\gamma} E_{1,\beta+2}(-k_2 t), \beta \in (0, 1), \\ \psi_{11}(t) = \frac{k_1+k_2}{\gamma k_2} + \frac{t^2}{8\gamma^2} - \frac{k_1}{\gamma k_2} e^{-k_2 t}, \beta = 1. \end{cases} \quad (3.7)$$

c). $\alpha \in (0, 1), \beta = 0$.

$$\bar{\psi}_{\alpha 0}(p) = \frac{1}{\gamma} + \frac{1}{4\gamma^2} \frac{1}{p} + \frac{k_1}{\gamma} \frac{1}{p+k_2}, \quad (3.8)$$

along with the inverse Laplace transform

$$\psi_{\alpha 0}(t) = \frac{1}{\gamma}\delta(t) + \frac{1}{4\gamma^2} + \frac{k_1}{\gamma}e^{-k_2t}, \quad (3.9)$$

d). $\alpha \in (0, 1), \beta = 1$.

$$\begin{aligned} \bar{\psi}_{\alpha 1}(p) &= \frac{1-\alpha}{\gamma} + \left(\frac{4\alpha\gamma(k_1+k_2) + (1-\alpha)^2 k_2}{4\gamma^2 k_2} \right) \frac{1}{p} \\ &\quad + \frac{\alpha(1-\alpha)}{2\gamma^2} \frac{1}{p^2} + \frac{\alpha^2}{4\gamma^2} \frac{1}{p^3} + \frac{k_1[(1-\alpha)k_2 - \alpha]}{\gamma k_2} \frac{1}{p+k_2}, \end{aligned} \quad (3.10)$$

$$\begin{aligned} \psi_{\alpha 1}(t) &= \frac{1-\alpha}{\gamma}\delta(t) + \left(\frac{4\alpha\gamma(k_1+k_2) + (1-\alpha)^2 k_2}{4\gamma^2 k_2} \right) \\ &\quad + \frac{\alpha(1-\alpha)}{2\gamma^2} t + \frac{\alpha^2}{8\gamma^2} t^2 + \frac{k_1[(1-\alpha)k_2 - \alpha]}{\gamma k_2} e^{-k_2 t}. \end{aligned} \quad (3.11)$$

e). $\alpha \in (0, 1)$, $\beta \in (0, 1)$.

$$\begin{aligned} \bar{\psi}_{\alpha\beta}(p) &= \frac{1-\alpha}{\gamma} + \frac{(1-\alpha)^2}{4\gamma^2} \frac{1}{p} + \frac{(1-\alpha)k_1}{\gamma} \frac{1}{p+k_2} + \frac{\alpha}{\gamma} \frac{1}{p^\beta} \\ &+ \frac{\alpha}{\gamma} \left(\frac{1-\alpha}{2\gamma} + k_1 \right) \frac{1}{p^{1+\beta}} + \frac{\alpha^2}{4\gamma^2} \frac{1}{p^{1+2\beta}} - \frac{\alpha k_1 k_2}{\gamma} \frac{p^{-1-\beta}}{p+k_2}. \end{aligned} \quad (3.12)$$

The inverse Laplace transform of function (3.12) is given by

$$\begin{aligned} \psi_{\alpha\beta}(t) &= \frac{1-\alpha}{\gamma} \delta(t) + \frac{(1-\alpha)^2}{4\gamma^2} + \frac{(1-\alpha)k_1}{\gamma} e^{-k_2 t} + \frac{\alpha}{\gamma} \frac{t^{\beta-1}}{\Gamma(\beta)} \\ &+ \frac{\alpha}{\gamma} \left(\frac{1-\alpha}{2\gamma} + k_1 \right) \frac{t^\beta}{\Gamma(1+\beta)} + \frac{\alpha^2}{4\gamma^2} \frac{t^{2\beta}}{\Gamma(1+2\beta)} - \frac{\alpha k_1 k_2}{\gamma} t^{\beta+1} E_{1,\beta+2}(-k_2 t). \end{aligned} \quad (3.13)$$

2°. **Function** $\bar{\vartheta}_{\alpha\beta}(p, u) = \exp\left(-u \frac{c(p)}{a(p)}\right)$, $u > 0$, written in the suitable form as

$$\begin{aligned} \bar{\vartheta}_{\alpha\beta}(p, u) &= \bar{\Theta}_\alpha(p, u) \bar{\Omega}_{\alpha\beta}(p, u), \\ \bar{\Theta}_\alpha(p, u) &= \exp\left(-\frac{1-\alpha}{\gamma} \left(\frac{1-\alpha}{4\gamma} + k_1\right) u\right) \exp\left(-\frac{1-\alpha}{\gamma} up\right) \exp\left(\frac{(1-\alpha)k_1 k_2}{\gamma} \frac{u}{p+k_2}\right), \\ \bar{\Omega}_{\alpha\beta}(p, u) &= \exp\left(-\frac{\alpha u}{\gamma} p^{1-\beta}\right) \exp\left(-\frac{\alpha u}{\gamma} \left(\frac{1-\alpha}{2\gamma} + k_1\right) p^{-\beta}\right) \exp\left(-\frac{\alpha^2 u}{4\gamma^2} p^{-2\beta}\right) \exp\left(\frac{\alpha k_1 k_2 u}{\gamma} \frac{p^{-\beta}}{p+k_2}\right). \end{aligned} \quad (3.14)$$

As in the previous case, we analyze the following situations:

a). $\alpha = 0$, $\beta \in [0, 1]$.

$$\begin{aligned} \bar{\vartheta}_{0\beta}(p, u) &= \bar{\Theta}_0(p, u) \bar{\Omega}_{0\beta}(p, u) = \exp\left(-\frac{u}{\gamma} \left(\frac{1}{4\gamma} + k_1\right)\right) \exp\left(-\frac{up}{\gamma}\right) \exp\left(\frac{k_1 k_2}{\gamma} \frac{u}{p+k_2}\right) \\ &= \exp\left(-\frac{u}{\gamma} \left(\frac{1}{4\gamma} + k_1\right)\right) \left\{ \exp\left(-\frac{up}{\gamma}\right) \left[\exp\left(\frac{k_1 k_2}{\gamma} \frac{u}{p+k_2}\right) - 1 \right] + \exp\left(-\frac{up}{\gamma}\right) \right\}, \end{aligned} \quad (3.15)$$

whose the inverse Laplace transform is

$$\begin{aligned} \vartheta_{0\beta}(t, u) &= \Theta_0(t, u) \Omega_{0\beta}(t, u) \\ &= \exp\left(-\frac{u}{\gamma} \left(\frac{1}{4\gamma} + k_1\right)\right) \sqrt{\frac{k_1 k_2 u}{\gamma t - u}} I_1\left(\frac{2}{\gamma} \sqrt{k_1 k_2 u(\gamma t - u)}\right) \exp\left(-\frac{k_2(\gamma t - u)}{\gamma}\right) \\ &+ \delta\left(t - \frac{u}{\gamma}\right) \exp\left(-\frac{u}{\gamma} \left(\frac{1}{4\gamma} + k_1\right)\right). \end{aligned} \quad (3.16)$$

b). $\alpha = 1$, $\beta \in [0, 1]$.

In this case, we analyze the following situations:

b1). $\alpha = 1$, $\beta = 0$.

$$\bar{\vartheta}_{10}(p, u) = e^{-\frac{1+4\gamma k_1}{4\gamma^2} u} e^{-\frac{u}{\gamma} p} e^{\frac{k_1 k_2 u}{\gamma} \frac{1}{p+k_2}} = e^{-\frac{1+4\gamma k_1}{4\gamma^2} u} \left\{ e^{-\frac{u}{\gamma} p} \left[e^{\frac{k_1 k_2 u}{\gamma} \frac{1}{p+k_2}} - 1 \right] + e^{-\frac{u}{\gamma} p} \right\}, \quad (3.17)$$

$$\begin{aligned} \vartheta_{10}(t, u) = & \exp\left(-\frac{u}{\gamma}\left(\frac{1}{4\gamma} + k_1\right)\right) \sqrt{\frac{k_1 k_2 u}{\gamma t - u}} I_1\left(\frac{2}{\gamma} \sqrt{k_1 k_2 u(\gamma t - u)}\right) \exp\left(-\frac{k_2(\gamma t - u)}{\gamma}\right) \\ & + \delta\left(t - \frac{u}{\gamma}\right) \exp\left(-\frac{u}{\gamma}\left(\frac{1}{4\gamma} + k_1\right)\right). \end{aligned} \quad (3.18)$$

b2). $\alpha = 1, \beta = 1$.

$$\begin{aligned} \bar{\vartheta}_{11}(p, u) &= e^{-\frac{u}{\gamma}} e^{-\frac{u}{4\gamma^2 p^2}} e^{-\frac{k_1 u}{\gamma} \frac{1}{p+k_2}} = e^{-\frac{u}{\gamma}} e^{-\frac{u}{4\gamma^2 p^2}} \left\{1 - \left[1 - e^{-\frac{k_1 u}{\gamma} \frac{1}{p+k_2}}\right]\right\} = \bar{h}_{11}(p, u) - \bar{h}_{11}(p, u) \bar{g}_{11}(p, u), \\ \bar{h}_{11}(p, u) &= e^{-\frac{u}{\gamma}} e^{-\frac{u}{4\gamma^2 p^2}} = e^{-\frac{u}{\gamma}} \left(1 + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-u}{4\gamma^2}\right)^k \frac{1}{p^{2k}}\right), \quad \bar{g}_{11}(p, u) = 1 - e^{-\frac{k_1 u}{\gamma} \frac{1}{p+k_2}}, \end{aligned} \quad (3.19)$$

whose Laplace transform is

$$\begin{aligned} \vartheta_{11}(t, u) &= h_{11}(t, u) - h_{11}(t, u) * g_{11}(t, u), \\ h_{11}(t, u) &= e^{-\frac{u}{\gamma}} \left(\delta(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-u}{4\gamma^2}\right)^k \frac{t^{2k-1}}{(2k-1)!}\right), \quad g_{11}(t, u) = \sqrt{\frac{k_1 u}{\gamma t}} J_1\left(2\sqrt{\frac{k_1 u}{\gamma} t}\right) e^{-k_2 t}. \end{aligned} \quad (3.20)$$

b3). $\alpha = 1, \beta \in (0, 1)$.

$$\begin{aligned} \bar{\vartheta}_{1\beta}(p, u) &= \bar{\chi}_{1\beta}(p, u) \bar{\chi}_{2\beta}(p, u) \bar{\chi}_{3\beta}(p, u), \quad \bar{\chi}_{1\beta}(p, u) = \exp\left(\frac{-u}{\gamma} p^{1-\beta}\right), \\ \bar{\chi}_{2\beta}(p, u) &= \exp\left(\frac{-u}{4\gamma^2} \frac{1 + 4\gamma k_1 p^\beta}{p^{2\beta}}\right), \quad \bar{\chi}_{3\beta}(p, u) = \exp\left(\frac{k_1 k_2 u}{\gamma} \frac{p^{-\beta}}{p + k_2}\right). \end{aligned} \quad (3.21)$$

For the inverse Laplace transforms of function (3.21) we have:

Since $\beta \in (0, 1)$, therefore $1 - \beta \in (0, 1)$, the function $\bar{\chi}_{1\beta}(p, u)$ is the Laplace transform of the Wright function $\chi_{1\beta}(t, u) = t^{-1} \Phi\left(0, \beta - 1, -\frac{u}{\gamma} t^{\beta-1}\right)$, [26].

Functions $\bar{\chi}_{2\beta}, \bar{\chi}_{3\beta}$ can be written in the equivalent forms

$$\begin{aligned} \bar{\chi}_{2\beta}(p, u) &= 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-u}{4\gamma^2}\right)^k \frac{(1 + 4\gamma k_1 p^\beta)^k}{p^{2\beta k}} = 1 + \sum_{k=1}^{\infty} \sum_{l=0}^k \frac{(4\gamma k_1)^l}{l!(k-l)!} \left(\frac{-u}{4\gamma^2}\right)^k \frac{1}{p^{\beta(2k-l)}}, \\ \bar{\chi}_{3\beta}(p, u) &= 1 + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{k_1 k_2 u}{\gamma}\right)^k \frac{p^{-\beta k}}{(p + k_2)^k}. \end{aligned} \quad (3.22)$$

The inverse Laplace transforms of functions $\bar{\chi}_{2\beta}, \bar{\chi}_{3\beta}, \bar{\vartheta}_{1\beta}$ are given by

$$\begin{aligned} \chi_{2\beta}(t, u) &= \delta(t) + \sum_{k=1}^{\infty} \sum_{l=0}^k \frac{(4\gamma k_1)^l}{l!(k-l)!} \left(\frac{-u}{4\gamma^2}\right)^k \frac{t^{\beta(2k-l)-1}}{\Gamma(\beta(2k-l))}, \\ \chi_{3\beta}(t, u) &= \delta(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{k_1 k_2 u}{\gamma}\right)^k G_{1-\beta k, k}(t, -k_2), \\ \vartheta_{1\beta}(t, u) &= \chi_{1\beta}(t, u) * \chi_{2\beta}(t, u) * \chi_{3\beta}(t, u), \end{aligned} \quad (3.23)$$

where $G_{a,b,c}(\cdot)$ denotes the generalized Lorenzo-Hartley function [20].

c). $\alpha \in (0, 1), \beta = 0$.

In this case we obtain

$$\bar{\vartheta}_{\alpha 0}(p, u) = \bar{\vartheta}_{10}(p, u), \quad (3.24)$$

therefore,

$$\vartheta_{\alpha 0}(t, u) = \vartheta_{10}(t, u). \quad (3.25)$$

d). $\alpha \in (0, 1)$, $\beta = 1$.

$$\begin{aligned} \bar{\vartheta}_{\alpha 1}(p, u) &= \exp\left(\frac{-u[(1-\alpha)^2 + 4\gamma k_1(1-\alpha) + 4\alpha\gamma]}{4\gamma^2}\right) \exp\left(\frac{-(1-\alpha)up}{\gamma}\right) \\ &\times \exp\left(\frac{-\alpha u[2(1-\alpha)p + \alpha]}{4\gamma^2 p^2}\right) \exp\left(\frac{k_1 u[(1-\alpha)k_2 - \alpha]}{\gamma} \frac{1}{p + k_2}\right). \end{aligned} \quad (3.26)$$

To determine the inverse Laplace transform of the function (3.26) we use relationships

$$\begin{aligned} w_{\alpha 1}(t, u) &= L^{-1} \left\{ \exp\left(\frac{-(1-\alpha)up}{\gamma}\right) \exp\left(\frac{-\alpha u[2(1-\alpha)p + \alpha]}{4\gamma^2 p^2}\right) \right\} \\ &= \delta(t - (1-\alpha)/\gamma) * L^{-1} \left\{ \exp\left(\frac{-\alpha u[2(1-\alpha)p + \alpha]}{4\gamma^2 p^2}\right) \right\} \\ &= \delta(t - (1-\alpha)/\gamma) * L^{-1} \left\{ 1 + \sum_{k=1}^{\infty} \sum_{l=0}^k \frac{1}{l!(k-l)!} \left(\frac{-\alpha^2 u}{4\gamma^2}\right)^k \left(\frac{2(1-\alpha)}{\alpha}\right)^l \frac{1}{p^{2k-l}} \right\} \\ &= \delta(t - (1-\alpha)/\gamma) * \left\{ \delta(t) + \sum_{k=1}^{\infty} \sum_{l=0}^k \frac{1}{l!(k-l)!} \left(\frac{-\alpha^2 u}{4\gamma^2}\right)^k \left(\frac{2(1-\alpha)}{\alpha}\right)^l \frac{t^{2k-l-1}}{(2k-l-1)!} \right\} \\ &= \delta(t - (1-\alpha)/\gamma) + \sum_{k=1}^{\infty} \sum_{l=0}^k \frac{1}{l!(k-l)!} \left(\frac{-\alpha^2 u}{4\gamma^2}\right)^k \left(\frac{2(1-\alpha)}{\alpha}\right)^l \frac{(t - (1-\alpha)/\gamma)^{2k-l-1}}{(2k-l-1)!}. \end{aligned} \quad (3.27)$$

$$\begin{aligned} w_{\alpha 2}(t, u) &= L^{-1} \left\{ \left(\frac{k_1 u[(1-\alpha)k_2 - \alpha]}{\gamma} \frac{1}{p + k_2} \right) \right\} \\ &= \delta(t) + \sqrt{\frac{k_1 u[(1-\alpha)k_2 - \alpha]}{\gamma t}} I_1 \left(2\sqrt{\frac{k_1 u[(1-\alpha)k_2 - \alpha]}{\gamma}} t \right) \exp(-k_2 t). \end{aligned} \quad (3.28)$$

Now, the inverse Laplace of the function (3.26) is given by

$$\vartheta_{\alpha 1}(t, u) = \exp\left(\frac{-u[(1-\alpha)^2 + 4\gamma k_1(1-\alpha) + 4\alpha\gamma]}{4\gamma^2}\right) w_{\alpha 1}(t, u) * w_{\alpha 2}(t, u). \quad (3.29)$$

e). $\alpha \in (0, 1)$, $\beta \in (0, 1)$.

In this case, we have

$$\bar{\Theta}_{\alpha}(p, u) = \exp\left(-\frac{(1-\alpha)u}{\gamma} \left(\frac{1-\alpha}{4\gamma} + k_1\right)\right) \exp\left(-\frac{(1-\alpha)up}{\gamma}\right) \left\{ \left[\exp\left(\frac{(1-\alpha)k_1 k_2 u}{\gamma(p + k_2)}\right) - 1 \right] + 1 \right\}, \quad (3.30)$$

whose inverse Laplace transform is

$$\begin{aligned} \Theta_\alpha(t, u) = & \exp\left(-\frac{(1-\alpha)u}{\gamma} \left(\frac{1-\alpha}{4\gamma} + k_1\right)\right) \left\{ \delta\left(t - \frac{(1-\alpha)u}{\gamma}\right) \right. \\ & \left. + \sqrt{\frac{(1-\alpha)k_1k_2u}{\gamma t - (1-\alpha)u}} I_1\left(\frac{2}{\gamma} \sqrt{(1-\alpha)k_1k_2u[\gamma t - (1-\alpha)u]}\right) \exp\left(\frac{-k_2(\gamma t - (1-\alpha)u)}{\gamma}\right) \right\}. \end{aligned} \quad (3.31)$$

$$\begin{aligned} \bar{\Omega}_{\alpha\beta}(p, u) = & \exp\left(-\frac{\alpha u}{\gamma} p\right) \exp\left(-\frac{\varepsilon_0 u}{p^\beta}\right) \exp\left(-\frac{\varepsilon_1 u}{p^{2\beta}}\right) \exp\left(\varepsilon_2 u \frac{p^{-\beta}}{p + k_2}\right) \\ = & \exp\left(-\frac{\alpha u}{\gamma} p\right) \left[1 + \sum_{k=1}^{\infty} \frac{(-\varepsilon_0 u)^k}{k! p^{\beta k}}\right] \left[1 + \sum_{k=1}^{\infty} \frac{(-\varepsilon_1 u)^k}{k! p^{2\beta k}}\right] \left[1 + \sum_{k=1}^{\infty} \frac{(\varepsilon_2 u)^k}{k!} \frac{p^{-\beta k}}{(p + k_2)^k}\right], \end{aligned} \quad (3.32)$$

respectively,

$$\begin{aligned} \Omega_{\alpha\beta}(t, u) = & \delta\left(t - \frac{\alpha u}{\gamma}\right) * \left[\delta(t) + \sum_{k=1}^{\infty} \frac{(-\varepsilon_0 u)^k t^{\beta k - 1}}{k! \Gamma(\beta k)}\right] * \left[\delta(t) + \sum_{k=1}^{\infty} \frac{(-\varepsilon_1 u)^k t^{2\beta k - 1}}{k! \Gamma(2\beta k)}\right] \\ & * \left[\delta(t) + \sum_{k=1}^{\infty} \frac{(\varepsilon_2 u)^k}{k!} G_{1, -\beta k, k}(t, -k_2)\right], \end{aligned} \quad (3.33)$$

where $\varepsilon_0 = \frac{\alpha}{\gamma} \left(1 + k_1 + \frac{1-\alpha}{2\gamma}\right)$, $\varepsilon_1 = \frac{\alpha^2}{4\gamma^2}$, $\varepsilon_2 = \frac{\alpha k_1 k_2}{\gamma}$.

3°. Function

$$\begin{aligned} \bar{\zeta}_{\alpha\beta}(x, p) = & \exp\left(\frac{-(1-x)}{2a(p)}\right) = \exp\left(-\frac{(1-\alpha)(1-x)}{2\gamma}\right) \exp\left(\frac{-\alpha(1-x)}{2\gamma p^\beta}\right) \\ = & \begin{cases} \exp\left(-\frac{1-x}{2\gamma}\right), \beta = 0, \alpha \in [0, 1], \\ \exp\left(-\frac{(1-\alpha)(1-x)}{2\gamma}\right) \left(1 + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-\alpha(1-x)}{2\gamma}\right)^k \frac{1}{p^{\beta k}}\right), \beta \in (0, 1), \alpha \in [0, 1], \\ \exp\left(-\frac{(1-\alpha)(1-x)}{2\gamma}\right) \exp\left(\frac{-\alpha}{2\gamma p}\right) = \exp\left(\frac{1-\alpha}{2\gamma}\right) \left[1 - \left(1 - \exp\left(\frac{-\alpha(1-x)}{2\gamma p}\right)\right)\right], \beta = 1, \alpha \in [0, 1], \end{cases} \end{aligned} \quad (3.34)$$

whose inverse Laplace transform is given by

$$\zeta_{\alpha\beta}(x, t) = \begin{cases} \exp\left(-\frac{1-x}{2\gamma}\right) \delta(t), \beta = 0, \alpha \in [0, 1], \\ \exp\left(-\frac{(1-\alpha)(1-x)}{2\gamma}\right) \left(\delta(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-\alpha(1-x)}{2\gamma}\right)^k \frac{t^{\beta k - 1}}{\Gamma(\beta k)}\right), \beta \in (0, 1), \alpha \in [0, 1], \\ \exp\left(-\frac{(1-\alpha)(1-x)}{2\gamma}\right) \left(\delta(t) - \sqrt{\frac{\alpha(1-x)}{2\gamma t}} J_1\left(2\sqrt{\frac{\alpha(1-x)t}{2\gamma}}\right)\right), \beta = 1, \alpha \in [0, 1]. \end{cases} \quad (3.35)$$

4°. **Function**

$$\bar{\Phi}_{\alpha\beta}(x, p) = \frac{\sinh\left(x\sqrt{\frac{c(p)}{a(p)}}\right)}{\frac{c(p)}{a(p)} \sinh\left(\sqrt{\frac{c(p)}{a(p)}}\right)}. \quad (3.36)$$

Considering the auxiliary functions

$$\begin{aligned} \bar{\Psi}(x, p) &= \frac{\sinh(x\sqrt{p})}{p \sinh(\sqrt{p})} = \frac{e^{x\sqrt{p}} - e^{-x\sqrt{p}}}{p(e^{\sqrt{p}} - e^{-\sqrt{p}})} = \frac{e^{-(1-x)\sqrt{p}} - e^{-(1+x)\sqrt{p}}}{p(1 - e^{-2\sqrt{p}})} \\ &= \frac{e^{-(1-x)\sqrt{p}} - e^{-(1+x)\sqrt{p}}}{p} \sum_{k=0}^{\infty} e^{-2k\sqrt{p}} = \sum_{k=0}^{\infty} \left(\frac{e^{-(2k+1-x)\sqrt{p}}}{p} - \frac{e^{-(2k+1+x)\sqrt{p}}}{p} \right), \end{aligned} \quad (3.37)$$

$$\omega_{\alpha\beta} = \frac{c(p)}{a(p)}, \quad (3.38)$$

function $\bar{\Phi}_{\alpha\beta}$ given by equation (3.36) is written as

$$\bar{\Phi}_{\alpha\beta}(x, p) = \Psi[x, \omega_{\alpha\beta}(p)]. \quad (3.39)$$

The inverse Laplace of function (3.39) is

$$\Phi_{\alpha\beta}(x, t) = \int_0^{\infty} \Psi(x, u) L^{-1}\{\exp(-u\omega_{\alpha\beta}(p))\} du = \int_0^{\infty} \Psi(x, u) \vartheta_{\alpha\beta}(t, u) du, \quad (3.40)$$

where, $\vartheta_{\alpha\beta}(t, u)$ has been analyzed in the paragraph 20, and $\Psi(x, t)$ is the inverse Laplace transform of function (3.37), namely,

$$\Psi(x, t) = \sum_{k=0}^{\infty} \left(\operatorname{erfc}\left(\frac{2k+1-x}{2\sqrt{t}}\right) - \operatorname{erfc}\left(\frac{2k+1+x}{2\sqrt{t}}\right) \right), \quad (3.41)$$

$\operatorname{erfc}(\cdot)$ denotes the complementary error function defined as $\operatorname{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^{\infty} \exp(-x^2) dx$.

Now, applying the inverse Laplace transform to the function (3.2) and using the results presented in paragraph 2.2, we obtain the following final results:

1). The solution corresponding to the generalized Atangana-Baleanu fractional derivative ($\alpha \in (0, 1)$, $\beta \in (0, 1)$).

$$C(x, t) = f_2'(t) * \psi_{\alpha\beta}(t) * \zeta_{\alpha\beta}(x, t) * \bar{\Phi}_{\alpha\beta}(x, t), \quad (3.42)$$

where functions $\psi_{\alpha\beta}(t)$, $\zeta_{\alpha\beta}(x, t)$, $\bar{\Phi}_{\alpha\beta}(x, t)$ are given by (3.13), (3.35) and (3.40), respectively.

2). The solution corresponding to Atangana-Baleanu fractional derivative ($\alpha = \beta \in (0, 1)$).

The concentration $C(x, t)$ is given by

$$C(x, t) = f_2'(t) * \psi_{\alpha\alpha}(t) * \zeta_{\alpha\alpha}(x, t) * \bar{\Phi}_{\alpha\alpha}(x, t), \quad (3.43)$$

where,

$$\begin{aligned} \psi_{\alpha\alpha}(t) = & \frac{1-\alpha}{\gamma} \delta(t) + \frac{(1-\alpha)^2}{4\gamma^2} + \frac{(1-\alpha)k_1}{\gamma} e^{-k_2 t} + \frac{\alpha t^{\alpha-1}}{\gamma \Gamma(\alpha)} \\ & + \frac{(1-\alpha) + 2\gamma k_1}{2\gamma^2} \frac{t^\alpha}{\Gamma(\alpha)} + \frac{\alpha}{8\gamma^2} \frac{t^{2\alpha}}{\Gamma(2\alpha)} - \frac{\alpha k_1 k_2}{\gamma} t^{\alpha+1} E_{1,\alpha+2}(-k_2 t), \end{aligned} \quad (3.44)$$

$$\zeta_{\alpha\alpha}(x, t) = \exp\left(\frac{-(1-\alpha)(1-x)}{2\gamma}\right) \left[\delta(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-\alpha(1-x)}{2\gamma}\right)^k \frac{t^{2\alpha-1}}{\Gamma(\alpha k)} \right], \quad (3.45)$$

$$\Phi_{\alpha\alpha}(x, t) = \int_0^\infty \Psi(x, u) \vartheta_{\alpha\alpha}(t, u) du, \quad (3.46)$$

$$\vartheta_{\alpha\alpha}(t, u) = \Theta_\alpha(t, u) * \Omega_{\alpha\alpha}(t, u), \quad (3.47)$$

where $\Theta_\alpha(t, u)$, $\Omega_{\alpha\alpha}(t, u)$ are given by (3.31) and (3.32), respectively.

3). The solution corresponding to Caputo-Fabrizio fractional derivative ($\alpha \in (0, 1)$, $\beta = 1$).

In this case, the solutions is

$$C(x, t) = f'_2(t) * \psi_{\alpha 1}(t) * \zeta_{\alpha 1}(x, t) * \Phi_{\alpha 1}(x, t), \quad (3.48)$$

where,

$$\begin{aligned} \psi_{\alpha 1}(t) = & \frac{1-\alpha}{\gamma} \delta(t) + \frac{(1-\alpha)^2 + 4\alpha\gamma}{4\gamma^2} + \frac{(1-\alpha)k_1}{\gamma} e^{-k_2 t} \\ & + \frac{\alpha [(1-\alpha) + 2\gamma k_1] t}{2\gamma^2} + \frac{\alpha^2 t^2}{8\gamma^2} - \frac{\alpha k_1 k_2}{\gamma} t^2 E_{1,3}(-k_2 t), \end{aligned} \quad (3.49)$$

$$\zeta_{\alpha 1}(x, t) = \exp\left(\frac{-(1-\alpha)(1-x)}{2\gamma}\right) \left[\delta(t) - \sqrt{\frac{\alpha(1-x)}{2\gamma t}} J_1\left(2\sqrt{\frac{\alpha(1-x)t}{2\gamma}}\right) \right], \quad (3.50)$$

$$\Phi_{\alpha 1}(x, t) = \int_0^\infty \Psi(x, u) \vartheta_{\alpha 1}(t, u) du, \quad (3.51)$$

and $\vartheta_{\alpha 1}(t, u)$ is given by equation (3.29).

4). The solution corresponding to Caputo fractional derivative ($\alpha = 1$, $\beta \in (0, 1)$).

The solution of solute concentration in the case of time-fractional Caputo derivative is given by

$$C(x, t) = f'_2(t) * \psi_{1\beta}(t) * \zeta_{1\beta}(x, t) * \Phi_{1\beta}(x, t), \quad (3.52)$$

where,

$$\psi_{1\beta}(t) = \frac{1}{\gamma} \frac{t^{\beta-1}}{\Gamma(\beta)} + \frac{k_1}{\gamma} \frac{t^\beta}{\Gamma(\beta+1)} + \frac{1}{4\gamma^2} \frac{t^{2\beta}}{\Gamma(1+2\beta)} - \frac{k_1 k_2}{\gamma} t^{\beta+1} E_{1,\beta+2}(-k_2 t), \quad (3.53)$$

$$\zeta_{1\beta}(x, t) = \delta(t) + \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{-(1-x)}{2\gamma}\right)^k \frac{t^{k\beta-1}}{\Gamma(\beta k)}, \quad (3.54)$$

$$\Phi_{1\beta}(x, t) = \int_0^\infty \Psi(x, u) \vartheta_{1\beta}(t, u) du, \quad (3.55)$$

where, $\vartheta_{1\beta}(t, u)$ is given by equation (3.23).

5). The solution corresponding to the derivative of order one (the ordinary model) ($\alpha = 0, \beta \in (0, 1)$).

The solution for this particular case is

$$C(x, t) = f_2'(t) * \psi_{0\beta}(t) * \zeta_{0\beta}(x, t) * \Phi_{0\beta}(x, t), \quad (3.56)$$

where,

$$\psi_{0\beta}(t) = \frac{1}{\gamma} \delta(t) + \frac{1}{4\gamma^2} + \frac{k_1}{\gamma} e^{-k_2 t}, \quad (3.57)$$

$$\zeta_{0\beta}(x, t) = e^{-\frac{1-x}{2\gamma}} \delta(t), \quad (3.58)$$

$$\Phi_{0\beta}(x, t) = \int_0^\infty \Psi(x, u) \vartheta_{0\beta}(t, u) du, \quad (3.59)$$

with

$$\begin{aligned} \vartheta_{0\beta}(t, u) &= \Theta_0(t, u) * \Omega_{0\beta}(t, u) \\ &= e^{\frac{-u}{\gamma}(\frac{1}{4\gamma} + k_1)} \left[\delta\left(t - \frac{u}{\gamma}\right) + \sqrt{\frac{k_1 k_2 u}{\gamma t - u}} I_1\left(\frac{2}{\gamma} \sqrt{k_1 k_2 u(\gamma t - u)}\right) \exp\left(\frac{-k_2(\gamma t - u)}{\gamma}\right) \right] * \delta(t) \\ &= e^{\frac{-u}{\gamma}(\frac{1}{4\gamma} + k_1)} \left[\delta\left(t - \frac{u}{\gamma}\right) + \sqrt{\frac{k_1 k_2 u}{\gamma t - u}} I_1\left(\frac{2}{\gamma} \sqrt{k_1 k_2 u(\gamma t - u)}\right) \exp\left(\frac{-k_2(\gamma t - u)}{\gamma}\right) \right]. \end{aligned} \quad (3.60)$$

In this case, the convolution $H_{0\beta}(x, t) = \psi_{0\beta}(t) * \zeta_{0\beta}(x, t) * \Phi_{0\beta}(x, t)$ can be written in the simpler form

$$\begin{aligned} H_{0\beta}(x, t) &= \psi_{0\beta}(t) * \zeta_{0\beta}(x, t) * \Phi_{0\beta}(x, t) = e^{\frac{1-x}{\gamma}} \left[\frac{1}{\gamma} \delta(t) + \frac{1}{4\gamma^2} + \frac{k_1}{\gamma} e^{-k_2 t} \right] * \Phi_{0\beta}(x, t) \\ &= \frac{1}{\gamma} e^{\frac{1-x}{\gamma}} \Phi_{0\beta}(x, t) + e^{\frac{1-x}{\gamma}} \int_0^t \left(\frac{1}{4\gamma^2} + \frac{k_1}{\gamma} e^{-k_2(t-\tau)} \right) \Phi_{0\beta}(x, \tau) d\tau, \end{aligned} \quad (3.61)$$

where,

$$\begin{aligned} \Phi_{0\beta}(x, t) &= \Psi(x, \gamma t) \exp\left(\frac{-(1+4\gamma k_1)t}{4\gamma}\right) \\ &+ \int_0^\infty \Psi(x, u) \sqrt{\frac{k_1 k_2 u}{\gamma t - u}} \exp\left[-k_2 t - \left(\frac{1}{4\gamma^2} + \frac{k_1 - k_2}{\gamma}\right) u\right] I_1\left(\frac{2}{\gamma} \sqrt{k_1 k_2 u(\gamma t - u)}\right) du. \end{aligned} \quad (3.62)$$

The solute concentration corresponding to the ordinary process is given by

$$C(x, t) = f_2'(t) * H_{0\beta}(x, t). \quad (3.63)$$

It is important to note that, for $f_2(t) = \frac{1}{2}\text{sign}(t)(1 + \text{sign}(t)) = \begin{cases} 0, & t \leq 0, \\ 1, & t > 0, \end{cases}$ with $f_2'(t) = \delta(t)$, the solution (3.63) becomes

$$C(x, t) = H_{0\beta}(x, t), \quad (3.64)$$

which is equivalent with results obtained by Kooten [28].

To determine the concentration in the adsorbed phase $S(x, t)$, we apply the inverse Laplace transform to equation (2.63) and obtain

$$S(x, t) = k_1 \int_0^t e^{-k_2(t-\tau)} C(x, \tau) d\tau. \quad (3.65)$$

4. APPLICATION OF THE KINETIC MODEL

In this section we will present the results corresponding to the boundary conditions $f_1(t) = 0, f_2(t) = H(t) = \frac{1}{2}\text{sign}(t)(1 + \text{sign}(t)) = \begin{cases} 0, & t \leq 0, \\ 1, & t > 0. \end{cases}$

The above boundary conditions show that in the spatial position $x = 0$ the concentrations are kept at zero value, while in the spatial position $x = 1$ solute concentrations are kept at the constant value $C(1, t) = 1, t > 0$.

To make a comparison between the values of the free phase concentration $C(x, t)$ corresponding to the four models with memory and the ordinary model, we use Mathcad software and determine the numerical values of the concentration for the following values of non-dimensional diffusion coefficient $\gamma = 0.1$ and reaction rates $k_1 = 0.1, k_2 = 0.01$. Numerical results are presented in graphical illustrations given by Figures 1–5. In these figures are presented 2D and 3D representations of functions $C(x, t)$ and $S(x, t)$ for different values of the fractional parameters α and β .

In Figure 1 are presented profiles of the solute concentration $C(x, t)$ corresponding to the models with generalized Atangana-Baleanu derivative, Atangana-Baleanu and the derivative of integer order. It is observed in Figure 1 that the lowest concentration is obtained for the ordinary diffusive process. Generally, the model based on the Atangana-Baleanu derivative leads to a smaller concentration than the model with generalized Atangana-Baleanu memory kernel. However, there are values of the fractional parameter for which the model with generalized Atangana-Baleanu derivative leads to smaller values than the Atangana-Baleanu model. These changing behaviors of the solute concentration are generated by the generalized diffusive flux because different memory kernels lead to different dumping of the concentration gradient, therefore to a different diffusion process.

Figures 2 and 3 show profiles of solute concentration $C(x, t)$ for three mathematical models namely, models based on the generalized Atangana-Baleanu derivative, Caputo-Fabrizio derivative and the derivative of integer order into Figure 2, respectively models with generalized Atangana-Baleanu kernel, Caputo kernel and the ordinary model. It can be seen from these figures that the solute concentration is maximum for the models with Caputo-Fabrizio or Caputo kernel. The smallest concentration is obtained in the ordinary diffusive process.

In Figure 4 are drawn the profiles of the concentration $C(x, t)$ corresponding to the diffusion with the generalized damping Atangana-Baleanu for variable values of the fractional parameters α and β . It is observed that the maximum values are reached when the two parameters approach simultaneously to the value 1. The results of these investigations can provide the optimal choice of the mathematical model for which the concentration of the solute is maximum / minimum depending on the requirements of the studied problem.

Figure 5 shows the comparison of the solute concentration profiles in the adsorbed phase $S(x, t)$ for different mathematical models of the generalized diffusion flow. First, it is observed that the values of the concentration $S(x, t)$ are much lower compared to the values of the concentration $C(x, t)$. As in the case of the concentration $C(x, t)$, the maximum values are obtained in the case of Caputo or Caputo-Fabrizio type memory kernels.

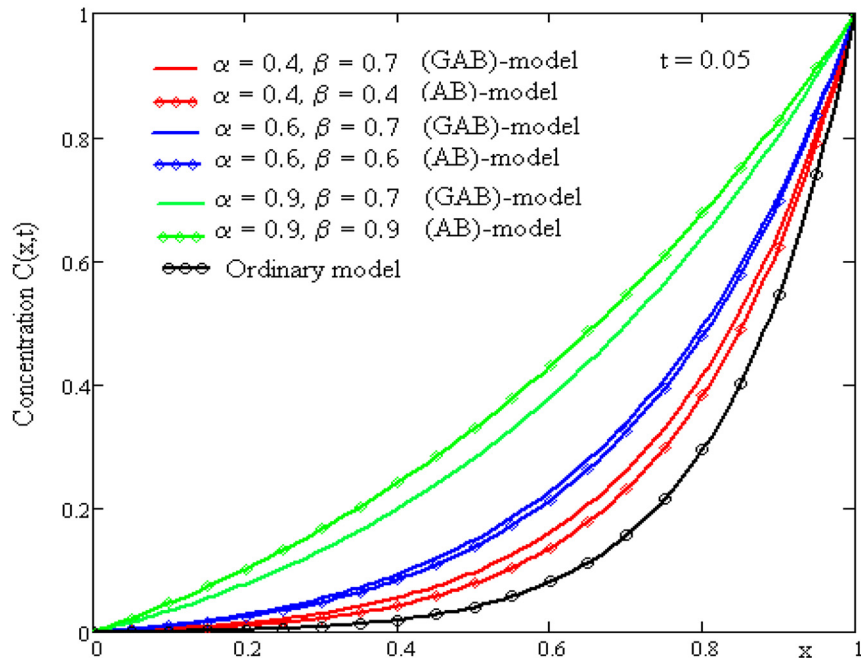
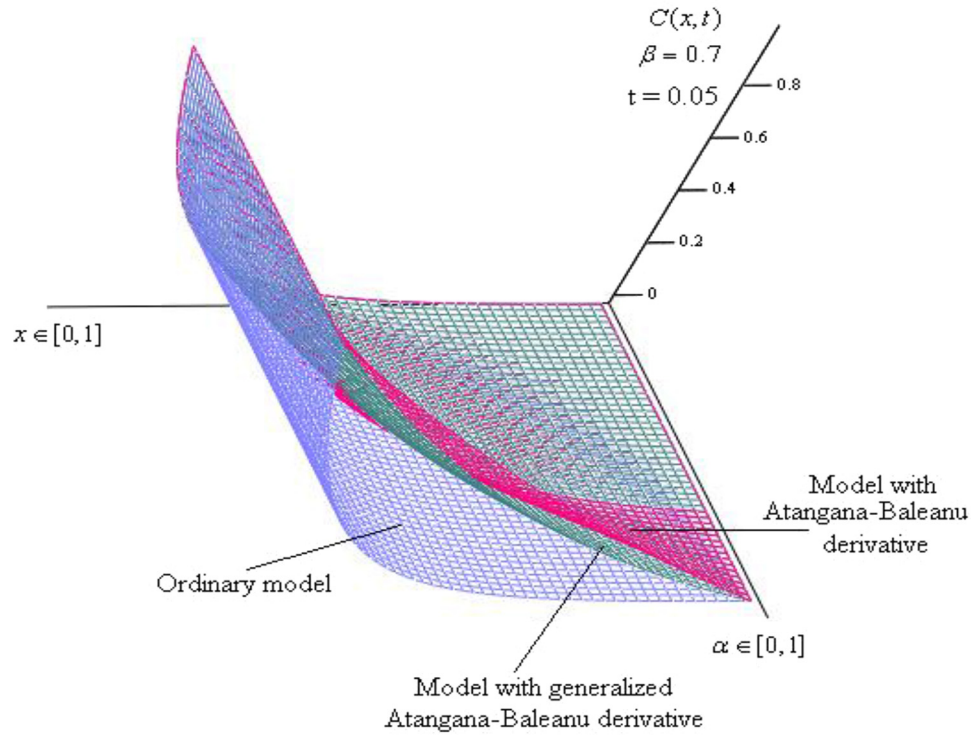


FIGURE 1. Comparison between the three models: generalized Atangana-Baleanu (GAB), Atangana-Baleanu (AB) derivative and ordinary model.

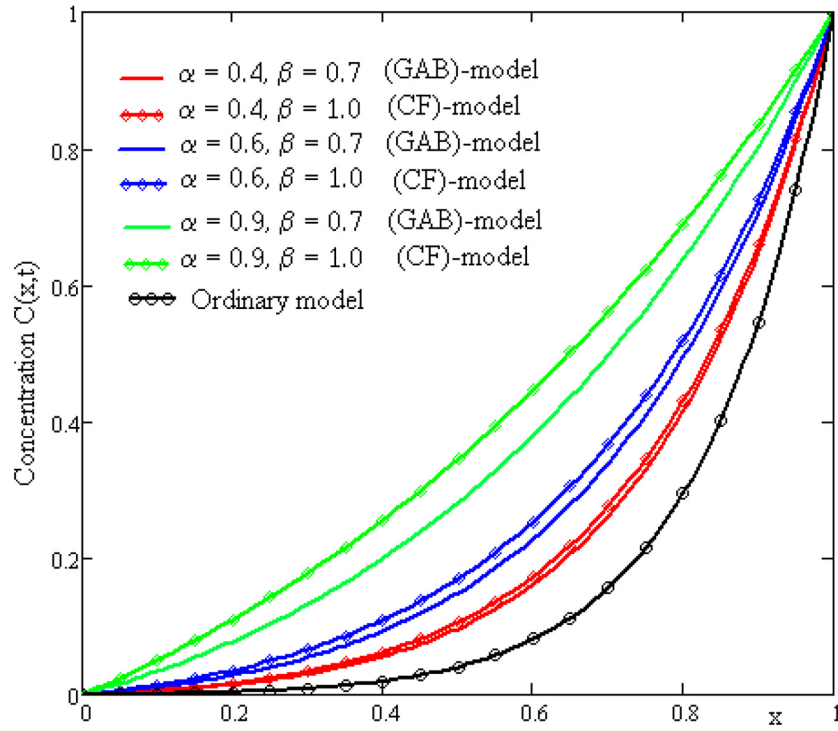
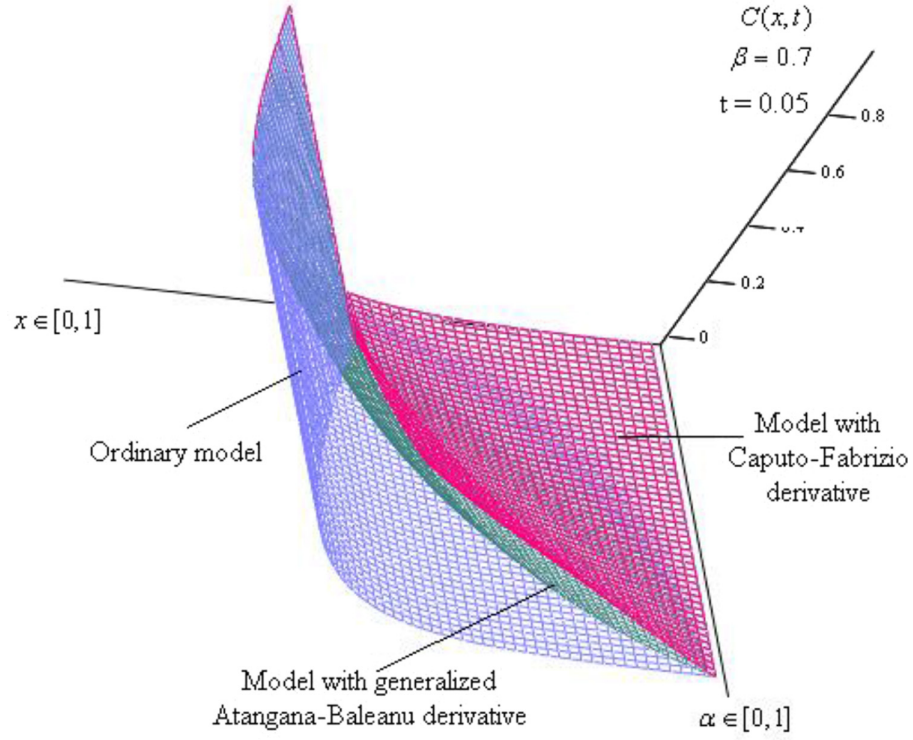


FIGURE 2. Comparison between the three models: generalized Atangana-Baleanu (GAB), Caputo-Fabrizio (CF) derivative and ordinary model.

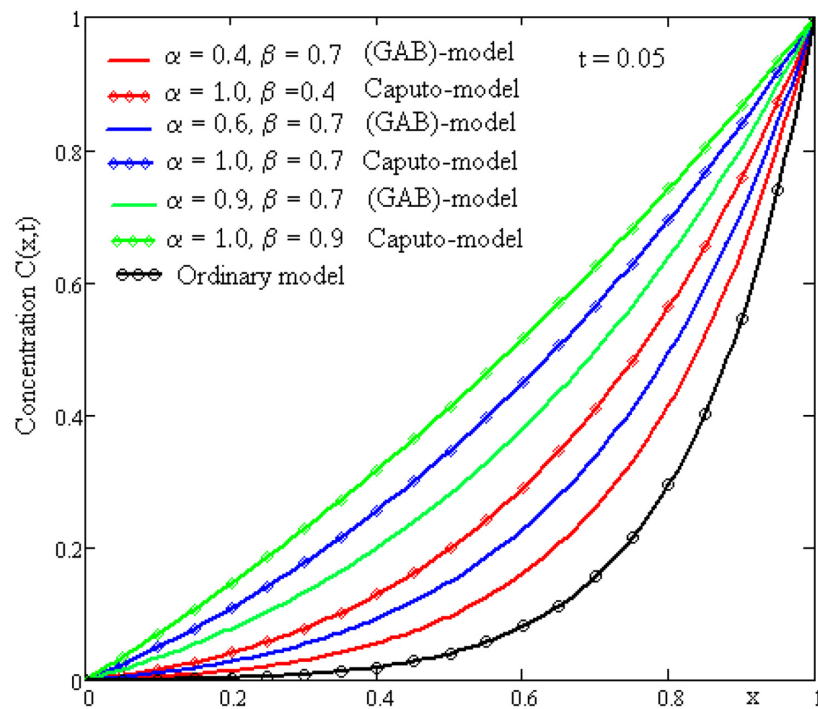
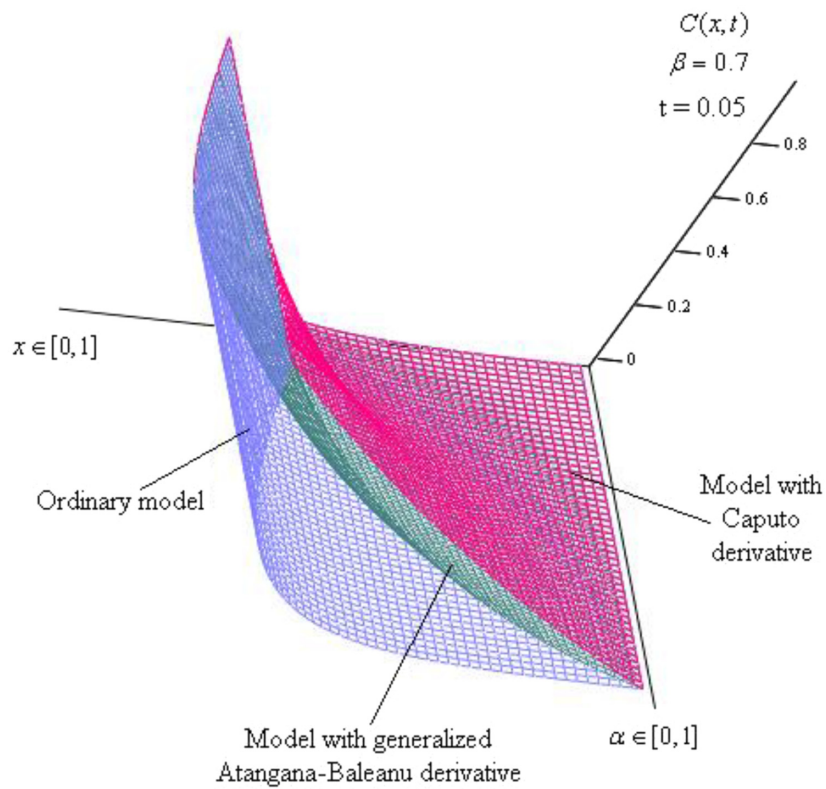


FIGURE 3. Comparison between the three models: generalized Atangana-Baleanu (GAB), Caputo derivative and ordinary model.

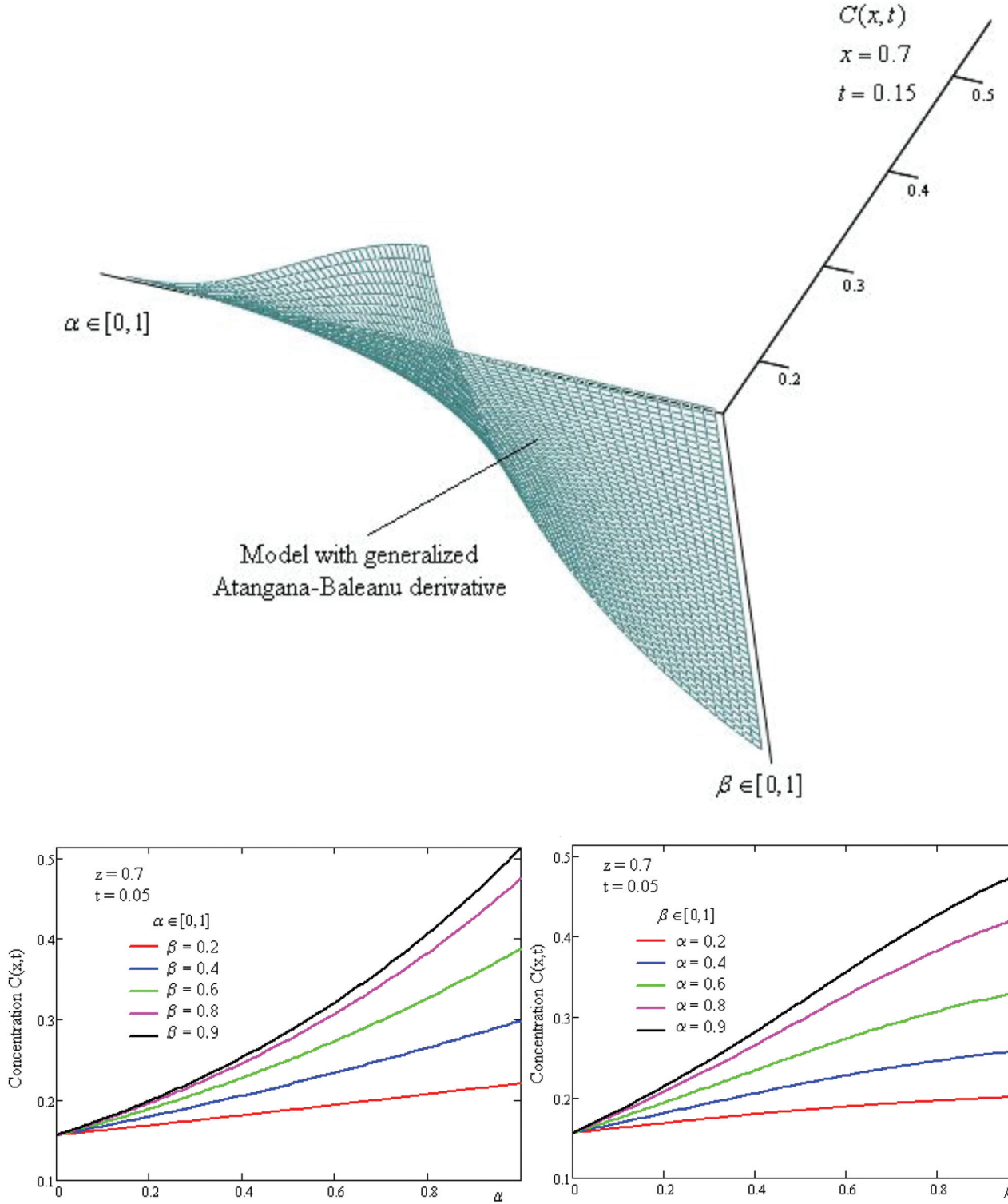


FIGURE 4. The profiles of the concentration $C(x,t)$ with the generalized Atangana-Baleanu derivative for different values of the fractional parameters α and β .

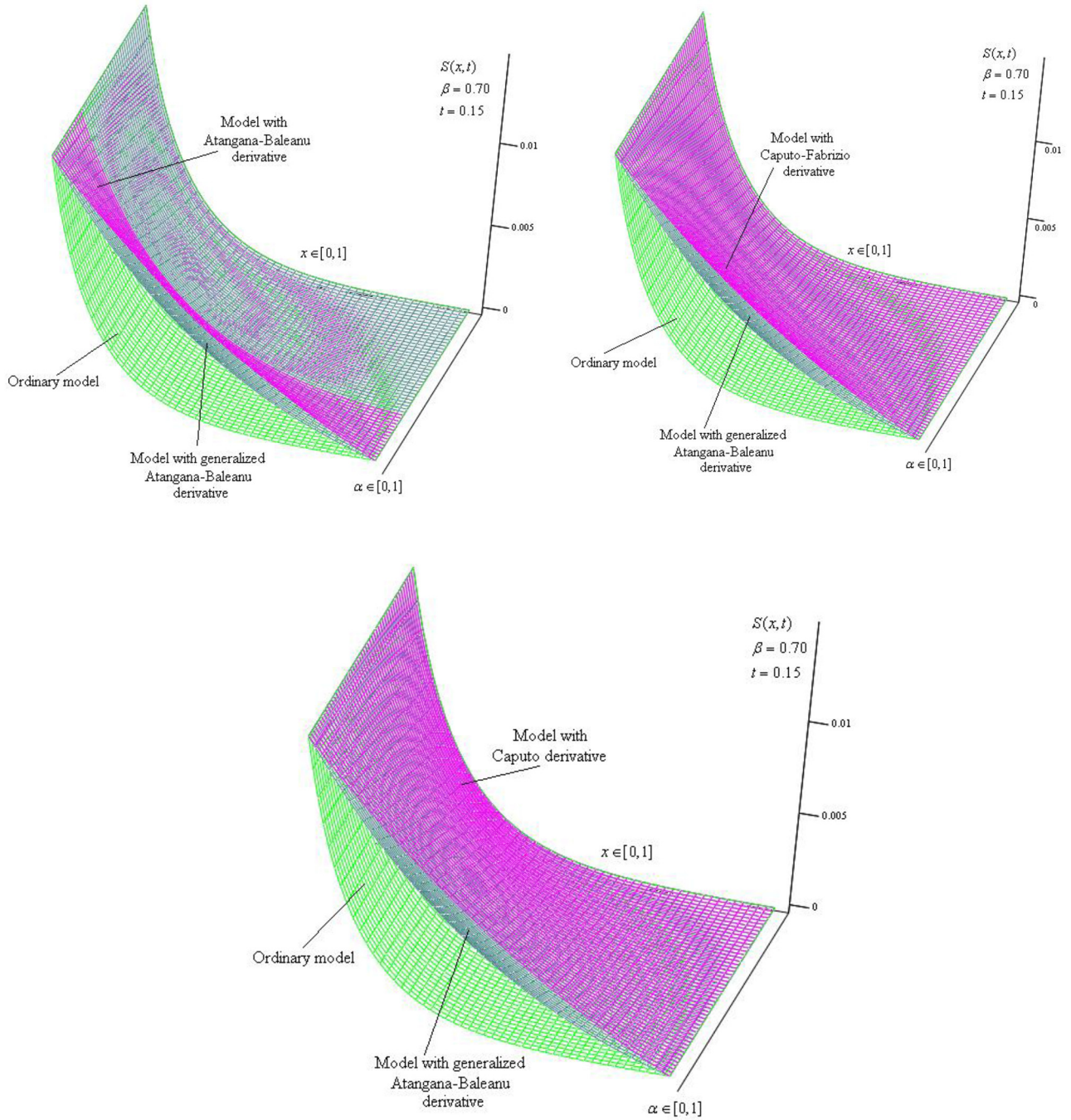


FIGURE 5. The profiles of concentration $S(x, t)$ for different memory kernels.

5. CONCLUSIONS

A generalized mathematical model of the solute transport by considering the mass transport of chemicals in porous media with sorption as a part of the dispersion mechanism has been investigated.

The memory effects of the diffusion process have been considered in the mathematical model introducing a new form of the diffusive flux based on the generalized Atangana-Baleanu time-fractional derivative.

The new time-fractional derivative/integral operators with Mittag-Leffler function as kernel have been presented together with their properties. The new time-fractional derivative generates by customization three other known fractional derivatives, namely, the Atangana-Baleanu fractional derivative, Caputo-Fabrizio fractional derivative and Caputo fractional derivative. This important property of the new time-fractional derivative makes it possible the comparison between a solute transport based on the mathematical model with derivatives of integer order (the ordinary model) and four other models with different memory kernels.

A mathematical model of the generalized solute transport based on the new Atangana-Baleanu derivative has been formulated and studied. Analytical solutions to the one-dimensional problem are determined using the Laplace transform.

Solutions corresponding to the generalized model are particularized to obtain solutions for the advection-diffusion equation with the kernel of diffusive flux of Atangana-Baleanu, Caputo-Fabrizio and Caputo type. The solution corresponding to the ordinary advection-diffusion equation has been also obtained as a particular case. An application for the constant concentration on the boundaries is investigated by graphical illustrations.

The obtained results lead to the choice of the best model for obtaining the optimal concentrations in a certain practical problem.

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