# MODELLING THE OXYGEN DIFFUSION EQUATION WITHIN THE SCOPE OF FRACTIONAL CALCULUS

## by

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The diffusion of oxygen into human body with simultaneous absorption is an important problem and it is of great importance in medical applications. This problem can be formulated in two stages. At the first stage, the absorption of oxygen at the surface of the medium is constant and an another stage considering the moving boundary problem of oxygen absorbed by the human body. In this paper we obtain analytical solutions for the oxygen diffusion equation considering the Liouville-Caputo, Atangana-Baleanu-Caputo, fractional conformable derivative in the Liouville-Caputo sense, and Atangana-Koca-Caputo fractionalorder derivatives. Numerical simulations were obtained for different values of the fractional order.

Ke ywords: fractional calculus, oxygen diffusion equation, Mittag-Leffler kernel, fractional conformable derivative

## Introduction

Fractional order differential equations as generalizations of classical integerorder differential equations. Recent studies in science and engineering demonstrated that the dynamics of many systems may be described more accurately by means of differential equations of non-integer order. A dynamical process that modelled through fractional order derivatives carries information about its present as well as past states [1-11]. Oxygen diffusion in a sike cell with simultaneous absorption is an important problem and has a wide range of medical applications. The 1-D problem of oxygen diffusion in a medium which simultaneously absorbs the oxygen was originally proposed in [12]. In this paper, the problem is formulated through two different stages. At the first stage, the concentration of oxygen at surface of the medium is maintained constant, whereas at the second stage the medium absorb the available oxygen and the boundary starts to recede towards the sealed surface. Gulkac in [13] considered the homotopy perturbation method for solving the oxygen diffusion problem. Liapis *et al.* in [14] proposed an orthogonal collocation method for solving the PDE of the diffusion of oxygen in absorbing tissue. In [15], the authors applied the Caputo-Fabrizio fractional derivative to the oxygen diffu

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sion equation, the authors obtained the solution using an iterative method. Another interesting applications have been investigated in [16-18].

In this paper we consider the fractional operators of type Liouville-Caputo, Atangana-Baleanu-Caputo, fractional conformable derivative in the LiouvilleCaputo sense and Atangana-Koca-Caputo for obtain analytical solutions for the oxygen diffusion equation [19-23].

The following fractional oxygen diffusion equation [15] is considered:

$$(_{0}\mathcal{D}_{t}^{\alpha}u)(x,t) = \frac{\partial^{2}}{\partial x^{2}}u(x,t) - 1, \ 0 < \alpha \le 1$$

$$\tag{1}$$

with initial and boundary conditions:

$$u(x,0) = \frac{(1-x)^2}{2}, \quad 0 \le x \le 1$$
(2)

$$u_x(0,t) = 0, t \ge 0$$
 (3)

$$u_x(x,t) = 0, \quad x = s(t), \quad t \ge 0, \quad \text{with} \quad s(0) = 1$$
 (4)

In this equation, the fractional operator  $(_0 \mathcal{D}_t^{\alpha} u)(x,t)$  can be of type Liouville-Caputo  $(_0^C \mathcal{D}_t^{\alpha} u)(x,t)$ , fractional conformable of type Liouville-Caputo  $(_0^{C \beta} \mathcal{D}_t^{\alpha} u)(x,t)$ , Atangana-Baleanu-Caputo  $(_0^{ABC} \mathcal{D}_t^{\alpha} u)(x,t)$ , and Atangana-Koca-Caputo  $(_0^{AKC} \mathcal{D}_t^{\alpha} u)(x,t)$ .

#### **Basic tools**

The Liouville-Caputo (C) fractional operator with order  $\alpha$  is defined as [19]:

$${}^{C}_{a}\mathcal{D}^{\alpha}_{t}u(t,x) = \begin{cases} \frac{\mathrm{d}^{n}}{\mathrm{d}t^{n}}u(x,t), & \alpha = n \in \mathbb{N} \\ \frac{1}{\Gamma(n-\alpha)}\int_{a}^{t}(t-z)^{n-\alpha-1}\frac{\partial^{n}}{\partial z^{n}}u(x,z)\mathrm{d}z, & n-1 < \alpha < n \in \mathbb{N} \end{cases}$$
(5)

where  ${}_{0}^{C} \mathcal{D}_{t}^{\alpha}$  is the Liouville-Caputo fractional operator of order  $\alpha$  with respect to t.

The fractional operator of type Atangana-Baleanu in Liouville-Caputo sense (ABC) of order  $\alpha$  is defined [20]:

$$\left( {}^{ABC}_{a} \mathcal{D}^{(n+\alpha)}_{t} u \right)(x,t) = \frac{1}{g(\alpha)} \int_{a}^{t} E_{\alpha} \left[ -g(\alpha)(t-z)^{\alpha} \right] \frac{\partial^{n+1} u}{\partial z^{n+1}}(x,z) \mathrm{d}z, \ n-1 < \alpha < n \in \mathbb{N}$$
 (6)

where  $n \in \mathbb{N}$  and  $g(\alpha)$  is a normalization function that depend of  $\alpha$ , which satisfies that, g(0) = g(1) = 1.

Let  $0 \le \alpha \le 1$  and  $n \in \mathbb{N}$ , the Laplace transforms of the Liouville-Caputo and Atangana-Baleanu fractional operators are given:

$$\mathcal{L}\left[{}_{0}^{C}\mathcal{D}_{t}^{(n+\alpha)}u(x,t)\right](x,s) = \frac{1}{s^{n-\alpha}}\left\{s^{n}\mathcal{L}\left[u(x,t)\right] - s^{n-1}u(x,0) - \dots - u^{(n-1)}(x,0)\right\}$$
(7)

$$\mathcal{L}\Big[ {}^{ABC}_{0} \mathcal{D}^{(n+\alpha)}_{t} u(x,t) \Big](x,s) = \frac{1}{g(\alpha)} \frac{1}{s^{1-\alpha}} \frac{s^{n+1} \mathcal{L}[u(x,t)] - s^{n} u(x,0) - s^{n-1} \dot{u}(x,0) \dots - u^{(n)}(x,0)}{s + g(\alpha)}$$
(8)

Let  $\operatorname{Re}(\beta) \ge 0$ ,  $n = [\operatorname{Re}(\beta)] + 1$ ,  $f \in C_{\alpha,a}^n([a,b])$ ,  $(f \in C_{\alpha,b}^n([a,b]))$ . Then the left and right fractional conformable derivatives in the Liouville-Caputo sense are given by [21]:

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$${}^{c}{}^{\beta}_{a}\mathcal{D}^{\alpha}_{t}f(t) = \frac{1}{\Gamma(n-\beta)} \int_{a}^{t} \left[ \frac{(t-a)^{\alpha} - (x-a)^{\alpha}}{\alpha} \right]^{n-\beta-1} \frac{{}^{a}\mathcal{D}^{\alpha}_{x}f(x)}{(x-a)^{1-\alpha}} \,\mathrm{d}x = {}^{n-\beta}_{a}I^{\alpha}_{t} \left[ {}^{n}_{a}\mathcal{D}^{\alpha}_{t}f(t) \right] \tag{9}$$

and

$${}^{c}{}^{\beta}_{t}\mathcal{D}^{\alpha}_{b}f(t) = \frac{(-1)^{n}}{\Gamma(n-\beta)} \int_{t}^{b} \left[\frac{(b-t)^{\alpha}-(b-x)^{\alpha}}{\alpha}\right]^{n-\beta-1} \frac{x\mathcal{D}^{\alpha}_{b}f(x)}{(b-x)^{1-\alpha}} \,\mathrm{d}x = {}^{n-\beta}_{t}I^{\alpha}_{b}\left[{}^{n}_{t}\mathcal{D}^{\alpha}_{b}f(t)\right]$$
(10)

Recently Atangana and Koca proposed a new fractional operator called, the Atangana-Koca fractional derivative in Liouville-Caputo sense (AKC) [22, 23]:

$$\binom{AKC}{a}\mathcal{D}_{t}^{\alpha}u(x,t) = \frac{1}{g(\alpha)}\int_{a}^{t}E_{\alpha,\beta}^{\gamma,q}\left[-g(\alpha)(t-z)^{\alpha}\right]\frac{\partial u}{\partial z}(x,z)\mathrm{d}z$$
(11)

where  $g(\alpha)$  is a normalization function as in the previous cases.

Let  $0 < \alpha \le 1$ , the Laplace transform of the Atangana-Koca fractional-order derivative is given:

$$\mathcal{L}\left\{{}^{AKC}_{0}\mathcal{D}^{\alpha}_{t}u(x,t)\right\}(x,s) = \frac{1}{g(\alpha)\left[1-g(\alpha)\right]^{q}}\left\{s^{-n\alpha}\mathcal{L}\left[u(x,t)\right] - s^{-n\alpha-1}u(x,0)\right\}$$
(12)

Given a function  $u(x) \in L_1(\mathbb{R})$ , the Fourier transform is given:

$$\hat{u}(k) = \left(\mathcal{F}_{x}u(x)\right)(k) \coloneqq \int_{-\infty}^{\infty} e^{ikx} u(x) dx$$
(13)

and the inverse Fourier transform of u(x) is given:

$$\mathcal{F}_{k}^{-1}\big(\mathcal{F}_{x}u(k)\big)(x) \coloneqq \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} \big(\mathcal{F}_{x}u(x)\big)(k) \mathrm{d}k \tag{14}$$

## Fractional oxygen diffusion equations

In this paper, we consider the oxygen diffusion eq. (1) involving fractional operators of type Liouville-Caputo, fractional conformable derivative in Liouville-Caputo sense, Atangana-Baleanu-Caputo and Atangana-Koca-Caputo.

*Liouville-Caputo sense.* We have the following oxygen diffusion equation:

$$\binom{C}{0} \mathcal{D}_t^{\alpha} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t) - 1, \ 0 < \alpha \le 1$$
(15)

with initial and boundary conditions:

$$u(x,0) = \frac{(1-x)^2}{2}, \quad 0 \le x \le 1$$
(16)

$$u_x(0,t) = 0, \quad t \ge 0$$
 (17)

$$u_x(x,t) = 0, \quad x = s(t), \quad t \ge 0 \quad \text{with} \quad s(0) = 1$$
 (18)

Solution. Applying the Laplace transform to eq. (15) and taking the conditions (16)-(18) we get:

$$s^{\alpha} (\mathcal{L}_{t} u)(x,s) - s^{\alpha - 1} \frac{(1 - x)^{2}}{2} = \frac{\partial^{2}}{\partial x^{2}} (\mathcal{L}_{t} u)(x,s) - \frac{1}{s}$$
(19)

Applying the Fourier transform we have:

$$\hat{u}(k,s) = \pi \left[ \delta(k) + 2i\delta'(k) - \delta''(k) \right] \frac{s^{\alpha - 1}}{s^{\alpha} + k^2} - \frac{2\pi\delta(k)}{s(s^{\alpha} + k^2)}$$
(20)

Now, applying the inverse Laplace and inverse Fourier transform to eq. (20) we have:

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \pi \left[ \delta(k) + 2i\delta'(k) - \delta''(k) \right] E_{\alpha} \left( -k^2 t^{\alpha} \right) e^{-ikx} dk - \frac{1}{2\pi} \int_{-\infty}^{\infty} 2\pi \delta(k) t^{\alpha} E_{\alpha,\alpha+1} \left( -k^2 t^{\alpha} \right) e^{-ikx} dk$$
(21)

where

$$\delta(k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dx$$
 (22)

Atangana-Baleanu-Caputo sense. We have the following oxygen diffusion equation:

$$\binom{ABC}{0} D_t^{\alpha} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t) - 1, \ 0 < \alpha \le 1$$
(23)

with initial and boundary conditions:

$$u(x,0) = \frac{(1-x)^2}{2}, \quad 0 \le x \le 1$$
(24)

$$u_x(0,t), \quad t \ge 0 \tag{25}$$

$$u_x(x,t) = 0, \quad x = s(t), \quad t \ge 0, \quad \text{with} \quad s(0) = 1$$
 (26)

Solution. Applying the Laplace transform to eq. (23) and taking the conditions (24)-(26) we get:

$$\frac{1}{1-\alpha} \frac{s^{\alpha} (\mathcal{L}_{t}u)(x,s) - s^{\alpha-1} \frac{(1-x)^{2}}{2}}{s + \frac{\alpha}{1-\alpha}} = \frac{\partial^{2}}{\partial x^{2}} (\mathcal{L}_{t}u)(x,s) - \frac{1}{s}$$
(27)

Applying the Fourier transform to eq. (27) and simplifying, we have the following relation forb  $\hat{u}(k,s)$ :

$$\hat{u}(k,s) = \frac{\pi \left[\delta(k) + 2i\delta'(k) - \delta''(k)\right]s^{\alpha - 1}}{s^{\alpha} + k^{2}\left(1 - \alpha\right)\left(s^{\alpha} + \frac{\alpha}{1 - \alpha}\right)} - \frac{2\pi\delta(k)(1 - \alpha)s^{-1}\left(s^{\alpha} + \frac{\alpha}{1 - \alpha}\right)}{s^{\alpha} + k^{2}\left(1 - \alpha\right)\left(s^{\alpha} + \frac{\alpha}{1 - \alpha}\right)}$$
(28)

Applying the inverse Laplace and Fourier transform to the eq. (28) we get:

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\pi \left[\delta(k) + 2i\delta'(k) - \delta''(k)\right]}{1 + k^2(1 - \alpha)} E_{\alpha} \left[ -\frac{\alpha k^2 t^{\alpha}}{1 + k^2(1 - \alpha)} \right] e^{-ikx} dk - \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{2\pi(1 - \alpha)\delta(k)}{1 + k^2(1 - \alpha)} \left\{ E_{\alpha} \left[ -\frac{\alpha k^2 t^{\alpha}}{1 + k^2(1 - \alpha)} \right] + \frac{\alpha}{1 - \alpha} t^{\alpha} E_{\alpha,\alpha+1} \left[ -\frac{\alpha k^2 t^{\alpha}}{1 + k^2(1 - \alpha)} \right] \right\} e^{-ikx} dk$$
(29)

*Fractional conformable derivative in the Liouville-Caputo sense.* We have the following oxygen diffusion equation:

$$\binom{c\ \beta}{0} D_t^{\alpha} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t) - 1, \ 0 < \alpha \le 1$$
(30)

with initial and boundary conditions:

$$u(x,0) = \frac{(1-x)^2}{2}, \quad 0 \le x \le 1$$
(31)

$$u_x(0,t) = 0, \quad t \ge 0$$
 (32)

$$u_x(x,t) = 0, \quad x = s(t), \quad t \ge 0, \quad \text{with} \quad s(0) = 1$$
 (33)

Solution. Applying the Laplace transform to eq. (30) and taking the conditions (31)-(33) we get:

$$\frac{\Gamma(1-\alpha\beta)}{\alpha^{-\beta}\Gamma(1-\beta)} \left[ s^{\alpha\beta} \left( \mathcal{L}_{t}u \right)(x,s) - s^{\alpha\beta-1} \frac{(1-x)^{2}}{2} \right] = \frac{\partial^{2}}{\partial x^{2}} \left( \mathcal{L}_{t}u \right)(x,s) - \frac{1}{s}$$
(34)

Applying the Fourier transform to eq. (34) and simplifying, we have:

$$\hat{u}(k,s) = \pi \Big[ \delta(k) + 2i\delta'(k) - \delta''(k) \Big] \frac{s^{\alpha\beta-1}}{s^{\alpha\beta} + k^2} \frac{\Gamma(1-\beta)}{\alpha^{\beta}\Gamma(1-\alpha\beta)} - \frac{\Gamma(1-\beta)2\pi\delta(k)}{\alpha^{\beta}\Gamma(1-\alpha\beta)} \frac{s^{\alpha\beta-(\alpha\beta+1)}}{s^{\alpha\beta} + k^2} \frac{\Gamma(1-\beta)}{\alpha^{\beta}\Gamma(1-\alpha\beta)}$$
(35)

Now applying the inverse Laplace and inverse Fourier transform to eq. (35) we have:

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \pi \left[ \delta(k) + 2i\delta'(k) - \delta''(k) \right] E_{\alpha\beta,1} \left[ -\frac{\Gamma(1-\beta)k^2}{\alpha^{\beta}\Gamma(1-\alpha\beta)} t^{\alpha\beta} \right] e^{-ikx} dk + \frac{\Gamma(1-\beta)}{\alpha^{\beta}\Gamma(1-\alpha\beta)} \frac{1}{2\pi} \int_{-\infty}^{\infty} 2\pi \delta(k) t^{\alpha\beta} E_{\alpha\beta,\alpha\beta+1} \left[ -\frac{\Gamma(1-\beta)k^2}{\alpha^{\beta}\Gamma(1-\alpha\beta)} t^{\alpha\beta} \right] e^{-ikx} dk$$
(36)

In the case when  $\alpha = 1$  the expression (36) matches the solution obtained in the eq. (21) in the Liouville-Caputo sense.

*Fractional Atangana-Koca derivative in the Liouville-Caputo sense*. We have the following oxygen diffusion equation:

$$\binom{AKC}{0} D_t^{\alpha} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t) - 1, \quad 0 < \alpha \le 1$$
(37)

with initial and boundary conditions:

$$u(x,0) = \frac{(1-x)^2}{2}, \quad 0 \le x \le 1$$
(38)

$$u_x(0,t) = 0, \quad t \ge 0$$
 (39)

$$u_x(x,t) = 0, \quad x = s(t), \quad t \ge 0, \quad \text{with} \quad s(0) = 1$$
 (40)

*Solution.* Applying the Laplace transform to eq. (37) and taking the conditions (38)-(40) we get:

$$\frac{1}{b}\left\{s^{-n\alpha}\mathcal{L}\left[u(x,t)\right] - s^{-n\alpha-1}\frac{(1-x)^2}{2}\right\} = \frac{\partial^2}{\partial x^2}(\mathcal{L}_t u)(x,s) - \frac{1}{s}$$
(41)

where  $b = g(\alpha)(1-g(\alpha))^{\alpha}$ .

Applying the Fourier transform to eq. (41) and simplifying, we have:

$$\hat{u}(k,s) = \pi \left[\delta(k) + 2i\delta'(k) - \delta''(k)\right] \frac{s^{-n\alpha-1}}{s^{-n\alpha} + bk^2} - 2\pi b\delta(k) \frac{s^{-1}}{s^{-n\alpha} + bk^2}$$
(42)

Now applying the inverse Laplace and inverse Fourier transform to eq. (42) we have:

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\pi}{bk^2} \left[ \delta(k) + 2i\delta'(k) - \delta''(k) \right] t^{n\alpha} E_{n\alpha,n\alpha+1} \left( -\frac{t^{n\alpha}}{bk^2} \right) e^{-ikx} dk - \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{2\pi\delta(k)}{k^2} E_{n\alpha} \left( -\frac{t^{n\alpha}}{bk^2} \right) e^{-ikxt} dk$$
(43)

The figs. 1(a)-1(d) shows numerical simulations of the eqs. (21), (29), (36), and (43) for  $\alpha = 0.9$  and  $\alpha = 0.9 - \beta = 0.94$  for the fractional conformable derivative in the Liouville-Caputo sense. The figs. 2(a)-2(d) shows numerical simulations of the eqs. (21), (29), (36), and (43) for  $\alpha = 0.8$  and  $\alpha = 0.8 - \beta = 0.83$  for the fractional conformable derivative in the Liouville-Caputo sense.

#### Conclusion

Fractional-order derivatives of type Liouville-Caputo, Atangana-Baleanu-Caputo, fractional conformable derivative in the Liouville-Caputo sense and Atangana-Koca-Caputo were used in this work to model the oxygen diffusion equation. Analytical solutions were obtained by using the Laplace and Fourier transforms. The Liouville-Caputo fractional-order derivative is based in the powerlaw, the Atangana-Baleanu-Caputo and the Atangana-Koca-Caputo fractional-order derivatives are based in the Mittag-Leffler Kernel. The Mittag-Leffler kernel is a combination of both exponential and power-law memory and can be used as waiting time distribution as well as first passage time distributions for renewal process. This kernel appears naturally in several physical problems as generalized exponential decay and as power-law asymptotic for a very large time. The fractional conformable derivative in the Liouville-Caputo sense have properties similar to the Newton's derivative and the standard fractional integrals

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Figure 1. Numerical solutions of eqs. (21), (29), (36), and (43); (a) eq. (21), (b) eq. (29), (c) eq. (36), and (d) eq. (43), we consider  $\alpha = 0.9$  for the cases (a), (b), (d) and for (c), we consider  $\alpha = 0.9 - \beta = 0.94$  for the fractional conformable derivative in the Liouville-Caputo sense



Figure 2. Numerical solutions of eqs. (21), (29), (36), and (43); (a) eq. (21), (b) eq. (29), (c) eq. (36), and (d) eq. (43), we consider  $\alpha = 0.9$  for the cases (a), (b), (d), and for (c), we consider  $\alpha = 0.9 - \beta = 0.94$  for the fractional conformable derivative in the Liouville-Caputo sense

and derivatives. Due to this operator depend on two fractional parameters  $\alpha$  and  $\beta$ , we obtain a better detection of the memory. The solutions obtained with these fractional derivatives has not been achieved before in the literature. Finally, we observe novel behaviors that cannot be obtained with standard models.

## Nomenclature

u(x, t) - concentration of oxygen t -time, [s] x -space, [m]

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## **Conflicts of interest**

The authors declare no conflict of interest.

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