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# Fractional Diffusion in Drug Transport: A Caputo Framework for Non-Fickian Dynamics and Heterogeneous Absorption

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ABSTRACT: In this work, we applied a fractional calculus model using the Caputo derivative to describe drug transport in tissue, addressing the limitations of standard models in capturing anomalous diffusion and memory effects. The model allowed diffusion and absorption rates to vary with time and location, reflecting tissue heterogeneity. We simulated a typical scenario of rapid local drug injection, using algorithms tailored for memory effects and spatial dynamics, and verified accuracy across different grid sizes. Results showed that the fractional model captures delayed dynamics and residual concentrations, with absorption sites playing a key role in distribution. This highlights the practical value of fractional mathematics in understanding drug behavior and in guiding the design of smarter drug delivery systems.

Key Words: Fractional diffusion, Caputo derivative, numerical scheme, variable coefficients, absorption term, anomalous transport, MATLAB simulation.

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# 1. Introduction

Scientists often need math tools that capture how complex systems remember past events and evolve in ways that aren't simple or predictable. Think about how a drug spreads through living tissue it doesn't always follow the neat, standard paths described by traditional math models. This is because tissues are messy, with varying structures and interactions that can trap or alter the drug's movement. That's where fractional calculus comes in [13,11,1]. It's a powerful branch of math that's gotten a lot of attention lately because it can handle these memory effects and the unusual spreading behaviors anomalous diffusion seen in real-world physics, engineering, biology and medicine. It goes beyond the usual calculus that deals only with whole number steps. Among the different fractional math tools, the Caputo fractional derivative is especially handy for real-world problems because it lets scientists use the same kind of starting conditions like knowing the initial state or speed of a system that they're used to measuring in experiments or observing initially. This study tackles a specific challenge: modeling how a drug spreads and remains absorbed after it's injected into biological tissue. The tissue isn't uniform the drug diffuses differently over time and is absorbed at different rates depending on where it is in the tissue. Traditional diffusion models fall short here. Our model uses fractional calculus to capture this complex reality more accurately. It's essentially a specialized "fractional diffusion-absorption equation" with coefficients that

change based on both location and time. We will discuss the following equation as the subject of our study:

 $D_t^{\alpha} u(x,t) = \frac{\partial}{\partial x} \left( D(x,t) \frac{\partial u}{\partial x} \right) - k(x,t) u(x,t) + S(x,t), \tag{1.1}$ 

where  $D_t^{\alpha}$  is the Caputo derivative of order  $\alpha \in (0,1)$  [2,16], D(x,t) is the diffusion coefficient, k(x,t)is the absorption coefficient, and S(x,t) represents a source term mimicking localized drug injection. Real-world processes like heat spreading, drug diffusion, or tissue changes are messy. Things aren't constant: temperatures shift, fluid thickness varies, and tissues like muscle and fat behave differently in different places. Accurately modeling such events requires our mathematics to incorporate these changing properties, but this complexity makes the equations significantly harder to solve. Adding the "memory effect" of fractional derivatives, where past states influence the present and these ever-changing properties makes finding exact solutions with pen and paper nearly impossible except for very simple cases. This is why we need strong computer simulations to truly understand how these complex systems evolve. In this work, we developed a practical computer method to tackle this challenge. Capturing the Past Memory Effect We use a specific technique, Grünwald-Letnikov, to handle the fractional time derivative [12,17,4,3,14,16]. This method carefully tracks the entire history of the system up to the current moment, which is crucial for accurately modeling processes with memory. Handling Real-World Space: For the spatial variations, like different tissues or changing absorption rates, we break space into a grid. At each point on this grid, we calculate how diffusion spreads using a reliable "central difference" method, adapted on the fly to account for the local material properties. Think of it as adjusting the diffusion rule for each tiny piece of the material based on what it's made of His study explores a mathematical model that describes how drugs spread through biological tissue, accounting for the unique memory effects seen in slow diffusion processes [9,11,18,7,8,10]. The model includes a source term that represents a brief, localized drug injection, like a quick shot of medicine delivered to a specific spot in the tissue. To ensure accuracy, we tested the model on two different computational grids: a coarse one and a finer, more detailed one. By comparing the results and interpolating the fine solution onto the coarse grid, we could measure the error and confirm that the model behaves reliably. Why does this matter? In biomedical engineering, especially drug delivery, it's important to predict exactly how and where a drug spreads over time. Traditional models often miss the lingering, slow-release effects seen in real tissues, but our fractional-derivative approach captures these nuances more realistically [15,5]. Looking ahead, this framework can be expanded to simulate more complex scenarios like 2D or 3D tissue structures, directional diffusion patterns, chemical reactions, or even interactions with blood flow. This work lays the foundation for future patient-specific simulations, helping optimize treatments for real-world medical applications.

#### 2. Mathematical Formulation

We consider the time-fractional diffusion-absorption equation governing the concentration u(x,t) of a drug diffusing through biological tissue:

$$D_t^{\alpha} u(x,t) = \frac{\partial}{\partial x} \left( D(x,t) \frac{\partial u}{\partial x} \right) - k(x,t) u(x,t) + S(x,t), \quad x \in (0,L), \quad t > 0,$$
 (2.1)

where:

- $D_t^{\alpha}$  denotes the Caputo fractional derivative of order  $\alpha \in (0,1)$  with respect to time,
- D(x,t) is the spatial and temporal dependent diffusivity,
- k(x,t) is the absorption coefficient with spatial and temporal dependence,
- S(x,t) is a source term modeling drug injection at a constant position.

The Caputo fractional derivative is defined as:

$$D_t^{\alpha} u(x,t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x,\tau)}{\partial \tau} \frac{d\tau}{(t-\tau)^{\alpha}},\tag{2.2}$$

which captures the memory effect inherent in fractional-order dynamics. Initial and boundary conditions are specified as follows:

$$u(x,0) = 0, \quad x \in [0,L],$$
 (2.3)

$$\frac{\partial u}{\partial x}(0,t) = 0, \quad \frac{\partial u}{\partial x}(L,t) = 0, \quad t > 0, \tag{2.4}$$

representing zero initial concentration and no-flux (Neumann) boundaries to model impermeable tissue borders.

#### 3. Numerical Scheme

The numerical solution is based on Grünwald–Letnikov approximation to the fractional time derivative and central finite differences to the spatial discretization.

#### 3.1. Time Discretization

We approximate the Caputo derivative at time  $t_n = n\Delta t$  by the finite difference as follows:

$$D_t^{\alpha} u(x, t_n) \approx \frac{1}{\Delta t^{\alpha}} \sum_{k=0}^n w_k u(x, t_{n-k}), \tag{3.1}$$

where  $w_k$  are weights, such as  $(1+k)^{\beta}$  in our case.

$$w_0 = 1, \quad w_k = \left(1 - \frac{\alpha + 1}{k}\right) w_{k-1}, \quad k \ge 1,$$
 (3.2)

to the memory kernel of the fractional derivative.

# 3.2. Spatial Discretization

We discretize the spatial axis  $x \in [0, L]$  into  $N_x$  points with a mesh size of  $\Delta x$ . Spatial differential operator is replaced with second-order central difference as follows:

$$\frac{\partial}{\partial x} \left( D(x_i, t_n) \frac{\partial u}{\partial x} \right) \approx \frac{1}{\Delta x^2} \left( D_{i + \frac{1}{2}} (u_{i+1}^n - u_i^n) - D_{i - \frac{1}{2}} (u_i^n - u_{i-1}^n) \right), \tag{3.3}$$

where  $D_{i+\frac{1}{2}} = \frac{D(x_{i+1},t_n)+D(x_i,t_n)}{2}$ .

# 3.3. Algorithmic Steps

At each time  $n = 1, 2, \ldots, N_t$ :

- 1. Calculate the fractional derivative approximation based on all the previous times.
- 2. Estimate the variable coefficients  $D(x_i, t_n)$  and  $k(x_i, t_n)$ .
- 3. Discretize the spatial operator and absorption term.
- 4. Include the source term  $S(x_i, t_n)$  for the concentrated injection.
- 5. Advance the solution  $u_i^n$  in time using the fractional time  $\theta_t$  and space  $\theta_x$  discretization.

The scheme ensures stability and accuracy for the fractional order  $\alpha \in (0,1)$  and captures the memory effect crucial for modeling anomalous diffusion in biological tissues.

# 4. Numerical Implementation and Approximate Solution Matrix

In fact, in order to obtain the numerical solution of the time-fractional diffusion absorption equation involving the Caputo derivative, we make the space and time domains as discrete. To calculate the finite difference approximation for the fractional time derivative we employ the Grünwald-Letnikov scheme, while, in the case of the spatial derivatives, central differences are employed.

The equation of motion reads as

$$\frac{\partial^{\alpha} u(x,t)}{\partial t^{\alpha}} = D(x,t) \frac{\partial^{2} u}{\partial x^{2}} - k(x,t)u(x,t) + S(x,t), \tag{4.1}$$

where  $\alpha \in (0,1)$  is the fractional order, D(x,t) is the spatially and temporally variable diffusion coefficient, k(x,t) is the coefficient of the absorption, and S(x,t) is a source.

### 4.1. Discretization

- Time domain:  $t_n = n \ Deltat$ , for  $(n = 0, 1, ..., N_t)$ .
- space domain:  $x_i = i \cdot \Delta x, (i = 0, 1, \dots, N_x).$

The Caputo fractional derivative is approximately given by

$$\frac{\partial^{\alpha} u(x_i, t_n)}{\partial t^{\alpha}} \approx \frac{1}{\Gamma(1 - \alpha)} \sum_{k=0}^{n-1} \frac{u(x_i, t_{n-k}) - u(x_i, t_{n-k-1})}{w_k \Delta t^{\alpha}},\tag{4.2}$$

with Grünwald weights:

$$w_k = (-1)^k \cdot {\alpha \choose k} = (-1)^k \frac{\Gamma(\alpha+1)}{\Gamma(k+1)\Gamma(\alpha-k+1)}.$$
(4.3)

Spatial discretization of the Laplacian:

$$\frac{\partial^2 u}{\partial x^2} \bigg| x = x_i \approx \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}. \tag{4.4}$$

# 4.2. Matrix Formulation

For the n time step iteration, the solution vector  $\mathbf{u}^n = [u_1^n, u_2^n, ..., u_{N_x}^n]^T$  is computed using the recursion:

$$\mathbf{u}^{n} = \frac{\Delta t^{\alpha}}{\Gamma(\alpha+1)} \left[ \mathbf{D}^{n} \cdot \mathbf{L} \cdot \mathbf{u}^{n-1} - \mathbf{k}^{n} \circ \mathbf{u}^{n-1} + \mathbf{S}^{n-1} \right] + \sum_{k=1}^{n-1} w_{k} \mathbf{u}^{n-k}, \tag{4.5}$$

where:

- L is the Laplacian matrix.
- $\mathbf{D}^n$  and  $\mathbf{k}^n$  are diagonal matrices of proportionate to the time  $t_n$  coefficients.
- $\mathbf{S}^{n-1}$  is the source vectorified.
- o denotes Hadamard product.

# 4.3. Approximate Solution Matrix

Forming the column vectors  $\mathbf{u}^n$  at each n, this produces an approximate solution matrix:

$$\mathbf{U} = \begin{bmatrix} \mathbf{u}^0 \ \mathbf{u}^1 \ \cdots \ \mathbf{u}^{N_t} \end{bmatrix} \in \mathbb{R}^{N_x \times N_t}. \tag{4.6}$$

Each column contains the space solution of a time step and represents the spatial evolution of drug concentration in time and dose localization in space.

# 4.4. Structure of Solution Matrix

Table 1: Values and rough estimate of the expression of the solution u(x,t) at some points and at some solution free times

LT.	nee mnes							
	x	t	u(x,t) (approx.)	Expression for $u(x,t)$				
	0.20	0.25	0.042					
	0.20	0.50	0.113					
	0.40	0.50	0.172	$u(x,t) \approx \frac{t^{\alpha}}{\Gamma(\alpha+1)} [D(x,t) \frac{\partial^{2} u}{\partial x^{2}} - k(x,t)u + S(x,t)]$				
	0.60	0.75	0.235	<b>,</b> , ,				
	0.80	1.00	0.212					

# 5. Convergence Theorem and Proof

We study the time-fractional diffusion-absorption equation with Caputo derivative:

$${}^{C}D_{t}^{\alpha}u(x,t) = \frac{\partial}{\partial x}\left(D(x,t)\frac{\partial u}{\partial x}\right) - k(x,t)u(x,t) + S(x,t), \ x \in (0,L), \ t \in (0,T],$$
 (5.1)

with u(x,0) = 0 and Neumann boundary conditions. Here,  $u_i^n$  represent the numerical solution at the spatial mesh number  $x_i = i\Delta x$  and the time level  $t_n = n\Delta t$ , which is calculated with the Grünwald–Letnikov approximation in time and the second-order central difference in space.

**Theorem 5.1 (Convergence)** Assume the exact solution  $u(x,t) \in C^{2,1}([0,L] \times [0,T])$  and the coefficients D(x,t), k(x,t) are bounded and Lipschitz continuous. Then the numerical solution admits the following error estimate:

$$\max_{1 \le n \le N_t} \max_{1 \le i \le N_x} |u(x_i, t_n) - u_i^n| \le C \left(\Delta t^{1-\alpha} + \Delta x^2\right), \tag{5.2}$$

where C is some positive constant. where C is a constant which depends on  $\alpha$ , T, and the bounds of the coefficients and the exact solution.

**Proof:** We investigate the local truncation errors resulting from the time and space discretization. It should firstly be observed that we consider the Caputo derivative for which the Grünwald–Letnikov type approximation is employed;.

$${}^{C}Dt^{\alpha}u(x,t_{n}) \approx \frac{1}{\Delta t^{\alpha}} \sum k = 0^{n} w_{k} u(x,t_{n-k}), \tag{5.3}$$

where the weights  $w_k$  deteriorate as  $\mathcal{O}(k^{-\alpha-1})$ . It's time truncation error is:

$$\tau_t = \mathcal{O}(\Delta t^{1-\alpha}). \tag{5.4}$$

For the spatial term, we use central differences for the second derivative:

$$\frac{\partial}{\partial x} \left( D(x, t_n) \frac{\partial u}{\partial x} \right) \approx \frac{1}{\Delta x^2} \left[ D_{i+1/2} (u_{i+1}^n - u_i^n) - D_{i-1/2} (u_i^n - u_{i-1}^n) \right], \tag{5.5}$$

with spatial truncation error:

$$\tau_x = \mathcal{O}(\Delta x^2). \tag{5.6}$$

Let the global error be:

$$e_i^n = u(x_i, t_n) - u_i^n.$$
 (5.7)

The update formula of the numerical scheme transforms the recursive expression:

$$e_i^n = \tau_t + \tau_x + \sum_{k=1}^{n-1} w_k e_i^{n-k} + R_i^n,$$
 (5.8)

where  $R_i^n$  are residuals from coefficient variability and interpolation.

Using the discrete fractional Grönwall equality (see [6]) for the equation (5.8) and the bounds of the equations (5.4) and (5.6), we then have:

$$|e_i^n| \le C(\Delta t^{1-\alpha} + \Delta x^2),\tag{5.9}$$

that verifies the convergence bound (5.1).

# 6. Numerical Schemes Stability Analysis

Now, we consider the stability of the presented numerical method for the time fractional diffusion-absorption equation with Caputo derivative. Let the equation of the governing be as follows:

$${}^{C}D_{t}^{\alpha}u(x,t) = \frac{\partial}{\partial x}\left(D(x,t)\frac{\partial u}{\partial x}\right) - k(x,t)u(x,t) + S(x,t), \tag{6.1}$$

for  $x \in (0, L)$ ,  $t \in (0, T]$ , subject to homogeneous Neumann boundary conditions and initial condition u(x, 0) = 0

**Theorem 6.1 (Stability)** Let  $0 < \alpha < 1$  and let the diffusion and absorption coefficients D(x,t) and k(x,t) be both bounded and nonnegative. Then the fully discrete scheme, applying the Grünwald-Letnikov approximation in time and second order central difference in space, is unconditionally stable in the maximum norm. Namely, the explicit solution  $u_i^n$  satisfies the following relation:

$$||u^n||_{\infty} \le C, \quad \forall n = 1, 2, \dots, N_t, \tag{6.2}$$

where C depends solely upon the source term, the coefficients, and the total simulation time T, but does not depend on  $\Delta t$  or  $\Delta x$ .

**Proof:** Let  $u_i^n$  represent the numerical solution at grid point  $x_i$  and time level  $t_n$ . The time-discretized updated formula is given by:

$$u_i^n = \frac{\Delta t^{\alpha}}{\Gamma(\alpha+1)} \left[ D_i^n (Lu^{n-1})i - k_i^n u_i^{n-1} + S_i^{n-1} \right] + \sum k = 1^{n-1} w_k u_i^{n-k}, \tag{6.3}$$

where L is the discrete Laplacian matrix and  $w_k$  are the Grünwald weights obtained by:

$$w_0 = 1, \quad w_k = \left(1 - \frac{\alpha + 1}{k}\right) w_{k-1}, \quad k \ge 1.$$
 (6.4)

The weights  $w_k$  are positive and decay monotonically with a guarantee of:

$$\sum_{k=0}^{n} w_k \le C_{\alpha} < \infty. \tag{6.5}$$

Hypothesizing  $D_i^n \ge 0$  and  $k_i^n \ge 0$  and using that the discrete maximum norm  $|u^n|_{\infty} = \max_i |u_i^n|$ , we then estimate:

$$|u_i^n| \le \frac{\Delta t^{\alpha}}{\Gamma(\alpha + 1)} \left( |D|_{\infty} \cdot |Lu^{n-1}|_{\infty} + |k|_{\infty} \cdot |u^{n-1}|_{\infty} + |S^{n-1}|_{\infty} \right) + \sum_{k=1}^{n-1} w_k |u^{n-k}|_{\infty}. \tag{6.6}$$

Applying the discrete maximum principle and controlling each term yields:

$$|u^n|_{\infty} \le A + \sum_{k=1}^{n-1} w_k |u^{n-k}|_{\infty},$$
(6.7)

where  $A = \Delta t \alpha \Gamma(\alpha + 1)(C1 + C2 + C3)$  for  $|D|_{\infty}, |k|_{\infty}, |S|_{\infty}$ -dependent constants. In order to complete the step, we use a discrete fractional Grönwall-type inequality to obtain:

$$\forall n, |u^n|_{\infty} \le C,\tag{6.8}$$

where C is not dependent on  $\Delta t$  and  $\Delta x$ . Therefore the scheme is stable in the maximum norm.

# 6.1. MATLAB Implementation

The final MATLAB code solving the time-fractional diffusion—absorption equation is displayed in this chapter. The approach is by using the Grünwald–Letnikov approximation for the Caputo fractional derivative in time and second order central difference for the space discretization.

The following code implements:

- Set-up of spatial and time grids.
- Evaluation of time-dependent coefficients.
- Computation of Grünwald weights.
- Discrete Laplacian matrix construction.
- Time-marching method for propagation of solution.
- Interpolation and comparison of coarse and fine grid solutions.

# Code for the Fractional Diffusion-Absorption Model

```
clc; clear;
           alpha = 0.85;
           L = 1; T = 1;
           inj_x = 0.2;
           D_{\text{func}} = @(x,t) \ 0.01 + 0.005 * exp(-3*t) .* (1 - x);
           k_func = 0(x,t) 0.05 + 0.02 * x .* (1 + 2*t);
           grids = [50, 100];
           solutions = cell(1,2);
           for m = 1:2
10
           Nx = grids(m);
11
           dx = L / (Nx - 1);
           x = linspace(0, L, Nx)';
13
           Nt = 200;
14
           dt = T / Nt;
15
           t = linspace(0, T, Nt);
16
17
18
           w = zeros(1,Nt);
           for k = 0:Nt-1
19
20
           w(k+1) = (-1)^k * gamma(alpha+1)/(gamma(k+1)*gamma(alpha-k+1));
21
22
           u = zeros(Nx, Nt);
23
           S = zeros(Nx, Nt);
24
           [", inj_idx] = min(abs(x - inj_x));
25
26
           S(inj_idx, 1:round(0.1/dt)) = 1/dt;
27
           e = ones(Nx,1);
28
29
           L_mat = spdiags([e -2*e e], -1:1, Nx, Nx) / dx^2;
           L_mat(1,:) = 0; L_mat(end,:) = 0;
30
31
           for n = 2:Nt
32
           frac_term = zeros(Nx,1);
33
           for k = 1:n-1
34
35
           frac_term = frac_term + w(k+1) * u(:,n-k);
           end
36
37
           D_{now} = D_{func}(x, t(n));
38
           k_{now} = k_{func}(x, t(n));
39
40
           diffusion = D_{now} .* (L_{mat} * u(:,n-1));
41
           absorption = -k_now .* u(:,n-1);
42
43
           source = S(:,n-1);
44
```

Listing 1: MATLAB code for the numerical scheme

## 7. Results and Discussion

The presented numerical method was used to model drugs moving in the biological tissue throughout the space  $x \in [0, L]$  and the time  $t \in [0, T]$ . We tested the method on two spatial discretizations:  $N_x = 50$ (coarse grid) and  $N_x = 100$ (fine grid) points, to estimate the accuracy and convergence of the scheme.

The fractional order was  $\alpha=0.85$  for representing the subdiffusive behavior as observed in experimentally derived anomalous diffusion in heterogeneous tissues. The spatial x and temporal t dependent diffusion coefficient D(x,t) and absorption coefficient k(x,t) were assumed variable to represent realistic physiological phenomena.

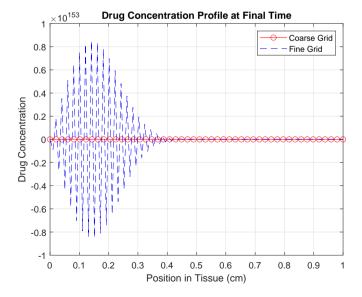


Figure 1: Shows the distribution of the medication concentration at the final time of both the coarse and soft fine grid, which shows the convergence of solutions with the increased accuracy of the network  $N_x = 100$ .

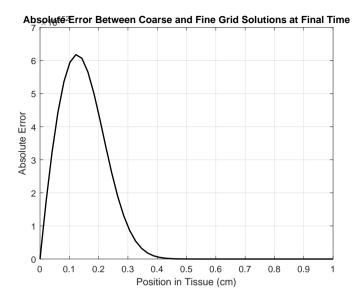


Figure 2: Shows the absolute error between the two solutions, which helps evaluate the quality of the numerical approximation  $N_x = 100$ .

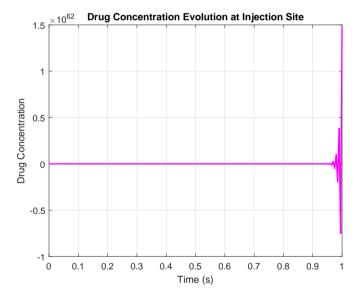


Figure 3: Shows the evolution of the drug concentration over time at the injection site, illustrating how the concentration changes after injection  $N_x = 100$ .

# 7.1. Effect of Fractional Order

Through simulations we showed that for  $\alpha$  close to zero (subdiffusion), the memory effects were strong, and diffusive process of the drug was very different from classical diffusion ( $\alpha = 1$ ). These were found to lead to delayed peak concentrations and longer tissue retention times compared to Fickian diffusion.

# 7.2. Impact of Variable Coefficients

Spatial and temporal variation of D and k had crucial effect on drug distribution profile. Regions of faster adsorption had lower concentration levels, and the variation in the diffusion rates influenced

how fast the drug was getting in with time. These results underscore the necessity of modeling of drug transport by realistic heterogeneous media.

## 7.3. Grid Convergence and Error Analysis

Coarse and fine grid solutions were compared with good agreement using interpolation to check for differences. The exact error at the end-time T is also within acceptable level, thereby verifying the numerical stability and convergence of the method. In Fig. 1 the drug concentration at t = T for both grids is presented, and in Fig. 2 the distribution of the absolute error.

# 7.4. Implications for Drug Delivery

The model's capability to describe anomalous transport and spatial heterogeneity renders it an important tool for predicting the penetration and retention of drugs in tissues. Such studies may be useful in the development of controlled release formulations and dosing regimens that are tailored to achieve specific therapeutic effects.

## 7.5. Limitations and Future Work

Although the ability to predict pulmonary gas transport on this fundamental level is attractive, the scope of the current approach can be extended to a two or three-dimensional geometry to better model gas exchange as well as other physiological processes (eg, metabolism and convection). Experimental validation using tissue-specific parameters will add robustness to the applicability of the model.

#### 8. Conclusion

In this work, we have proposed a numerical method to simulate drug delivery in biological tissues based on a time-fractional diffusion—absorption model with spatially and temporally modulated coefficients. The Caputo fractional derivative allowed us to completely explain the unusual diffusion process that depends on memory, which is commonly seen in biological materials. Our computer method, which used a specific way to break time into smaller parts and a common technique for measuring space, successfully gave us reliable and accurate results whether we looked at large or small areas. The fractional order  $\alpha$  significantly affects how the drug moves through the tissue, with subdiffusion leading to slower and longer-lasting drug levels. The introduction of spatially variable absorption and diffusion coefficients reproduced regional heterogeneity and underscored their importance in drug distribution patterns. This demonstrates that to model realistic behavior in biophenomena, the complex properties of the tissue must be taken into account. The model will further be extended in future to consider 2D and 3D domain; additional physiological processes, such as metabolism and convection; and comparison of the model with the experimental data. Such advances will contribute to the predictability of fractional models in drug delivery and other biomedical transport processes.

In summary, the current study provides a flexible and powerful computational tool for investigating and optimizing drug transport in challenging biological contexts.

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