A MULTI-SCALE ARTIFICIAL INTELLIGENCE FRACTAL CONVECTION DIFFUSION IN A POROUS NANOFIBER MEMBRANE

by

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This paper examines the fascinating phenomenon of fractal convection-diffusion in a porous nanofiber membrane. A multi-scale artificial intelligence model has been developed, in which the temporal Caputo fractional derivative, the spatial Riesz fractional derivative, and the traditional derivative for the convection process have been employed. The convection-diffusion process exerts a significant influence on the permeability of the nanofiber membrane. This paper examines the influence of the convection process on the permeability of the membrane. The findings indicate that when the fluid velocity is minimal, the diffusion process assumes control. However, when a certain threshold is reached, the convection process assumes dominance, accelerating the permeability process. The direction of the fractal convection-diffusion process is predominantly influenced by the direction of the fluid-flow.

Key words: *fractal convection diffusion, fractional derivative, numerical method, convection-diffusion process, nanofiber membrane*

Introduction

The convection-diffusion process in a porous medium is a pervasive phenomenon across a multitude of scientific and engineering disciplines. A substantial body of literature has concentrated on the topic of permeability, with notable advancements being made. For example, Miao *et al.* [1] elucidated the transport mechanism of two-phase flow through porous fractured media. Liu *et al.* [2] conducted an investigation into the primary factors influencing coal seam permeability. Xiao *et al.* [3] made an intriguing discovery regarding oxygen diffusion in porous media. In a further contribution to this field of study, Liu *et al.* [4] examined the process of gas migration through a porous medium. Su *et al.* [5] provided a detailed explanation of the mechanism governing oil-water relative permeabilities in a low-permeability reservoir. A plethora of models have emerged, including the fractal permeability model [6], the fractal model for gas diffusivity in porous media [7], the anomalous diffusion model [8], the time fractional diffusion model [9], and the fractal diffusion model for isotropic media [10]. Currently, fractal diffusion is employed extensively in modern science and technology, spanning applications in electrochemistry [11-14] and microelectromechanical (MEMS) sensors [15-18]. A multi-scale artificial intelligence (AI) diffusion model [10] incorporating the convection effect through a nanofiber membrane can be expressed as [19]:

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$$ {}_0^C\mathrm{D}_T^{\alpha} C + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D_c\left[\frac{\partial^{1+\beta} C}{\partial |x|^{1+\beta}} + \frac{\partial^{1+\gamma} C}{\partial |y|^{1+\gamma}}\right] + f, \quad (x,y)\in\Omega, \quad 0<t\le T \tag{1} $$

with the following boundary and initial conditions:

$$ C = 0, (x,y)\in\partial\Omega, \quad 0<t\le T \tag{2} $$

$$ C = 0, (x,y)\in\Omega, \quad t=0 \tag{3} $$

where C is the concentration, D_c – the diffusion coefficient, u and v are the fluid velocities along x- and y-directions, and f – the source term.

In this AI model, the Caputo fractional derivative and Riesz space fractional derivative are adopted, which are defined, respectively, [19]:

$$ {}_0^C\mathrm{D}_t^{\alpha} u(t) = \frac{1}{\Gamma(m-\alpha)}\int_a^t \frac{f^{(m)}(s)\mathrm{d}s}{(t-s)^{\alpha-m+1}} \tag{4} $$

$$ \frac{\partial^{2\beta_1} u(x)}{\partial |x|^{2\beta_1}} := -\frac{1}{2\cos(\pi\beta_1)}\left[\frac{1}{\Gamma(2-2\beta_1)}\frac{\partial^2}{\partial x^2}\int_0^x \frac{u(s)\mathrm{d}s}{(x-s)^{2\beta_1-1}} + \frac{1}{\Gamma(2-2\beta_1)}\frac{\partial^2}{\partial x^2}\int_x^{l_1} \frac{u(s)\mathrm{d}s}{(s-x)^{2\beta_1-1}}\right] \tag{5} $$

where α, β_1, and β_2 are fractional orders, which are related with the two-scale fractal dimensions of the porous medium [20-22]. This multi-scale AI model can describe the memory effect in time, symmetric diffusion in isotropous nanofiber membranes, while the convection process is considered in a traditional way.

There are numerous analytical methods for solving fractional differential equations, including the homotopy perturbation method [23-26], the variational iteration method [27-29], and the exp-function method [30, 31]. This paper studies eq. (1) by the variational-based numerical method [32].

Numerical simulation

The variational principle is widely studied in engineering [33-38], it is the theoretical bases for both analytical analysis and numerical simulation. This paper gives a variational-based numerical approach to eq. (1), detailed discussion on the numerical algorithm was given in [10, 32]. Time is discretized by L_1 scheme formula and space is discretized by the implicit finite volume method, this discretization method guarantees a fast convergence ratio [32].

Here we consider the case when D_c =1.0, f = 0.0001, and α = 0.1, the numerical results for different values of β, γ are illustrated in fig.1, and the evolution process is given in figs. 2 and 3.

As illustrated in fig. 1, an elevated porosity (decreased values of β and γ) facilitates a more rapid convection diffusion process. This finding aligns with the experimental outcomes documented in [39]. When the porosity is equal to one, β and γ are both equal to zero, indicating that only convection occurs. Conversely, when the porosity is equal to zero, neither convection nor diffusion occurs.

Figure 2 illustrates the evolution of the concentration, demonstrating a discernible acceleration in the rate of change. From t = 0.01 to t = 0.05, the concentration undergoes a change:

$$\frac{\Delta C}{\Delta t}=\frac{5.6425\cdot 10^{-6}-1.7163\cdot 10^{-6}}{0.05-0.01}=9.8155\cdot 10^{-5} \tag{6}$$

While the concentration change from $t = 0.2$ to $t = 20$ is:

$$\frac{\Delta C}{\Delta t}=\frac{8.8987\cdot 10^{-6}-8.3944\cdot 10^{-6}}{20-0.2}=2.8016\cdot 10^{-7} \tag{7}$$

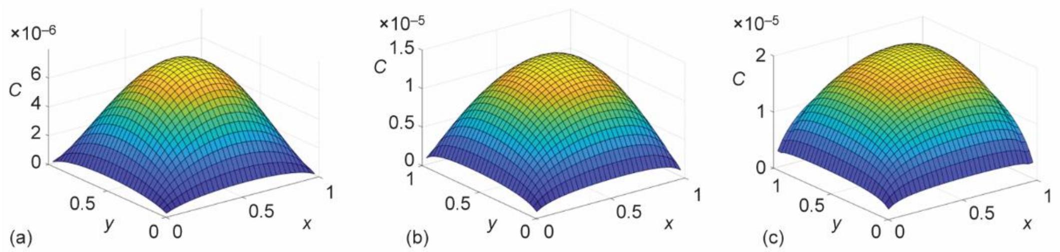

Figure 1. The diffusion process for different *β*, *γ* at *t* = 1.0, *u* = 1.0, and *v* = 1.0; (a) *β* = *γ* = 0.1, (b) *β* = *γ* = 0.5, and (c) *β* = *γ* = 0.99

The rate of change in concentration from $t = 0.01$ to $t = 0.05$ is 350 times faster than that observed for the period from $t = 0.2$ to $t = 20$. The rapid alteration of the concentration is of paramount importance for the optimal design of a nanofiber membrane. Li *et al.* [40] have revealed the fractal nature of the porosity of nanofiber members in the electrospinning process, so that the nanofiber membrane geometry becomes controllable by the bubble electrospinning [41-44]. For different values of α as shown as in fig. 3, a smaller α implies a faster evolution process with low memory effect.

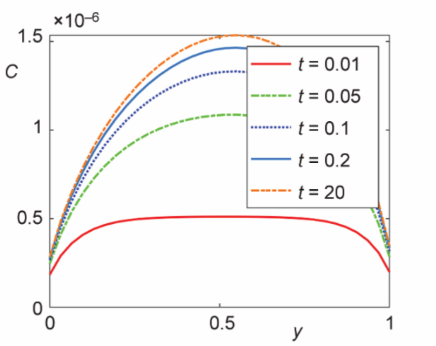

Figure 2. The evolution process with time (α = 0.9, and β = 0.9, γ = 0.9, *u* = 1.0, *v* = 1.0, and D_c = 1.0)

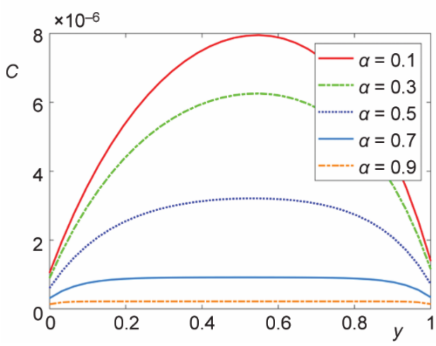

Figure 3. Evolution process with different memory effects (γ = 0.9, β = 0.9, *t* = 0.001, *u* = 1.0, *v* = 1.0, and D_c = 1.0)

Figure 4 illustrates the impact of fluid velocity on the distribution of concentrations. For smaller values of u and v, for example $u = v < 1.0$, the convection process can be considered negligible. Conversely, as the velocity increases, for instance $u = v = 20.0$, the convection and diffusion processes contribute almost equally to the concentration distribution. However, when the velocity reaches a sufficiently high value, for example $u = v = 100.0$, the diffusion process can be disregarded.

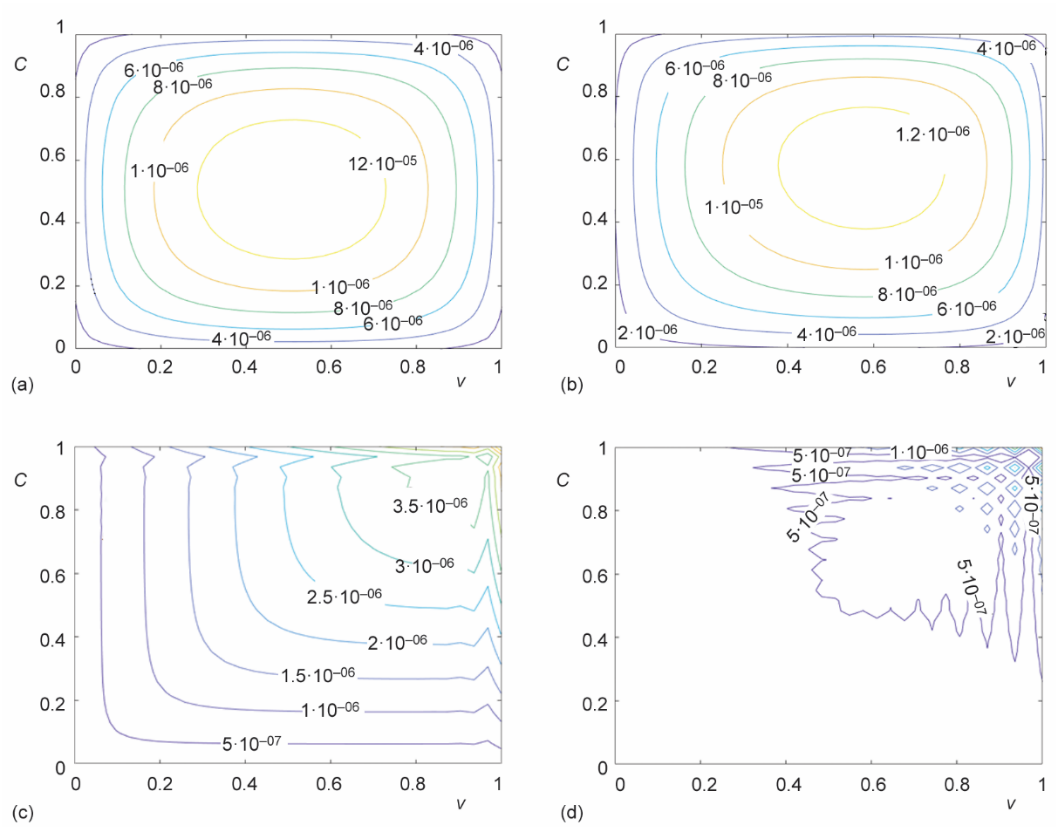

Figure 4. The effect of convection on the fractal diffusion process (α = 0.8, γ = 0.6, β = 0.6, t = 1.0, D_c = 1.0); (a) u = 0.1, v = 0.1, (b) u = 1.0, v = 1.0, (c) u = 20.0, v = 20.0, and (d) u = 100.0, v = 100.0

A comparison of fig. 5 with fig. 4 reveals a similar trend for convection and diffusion processes, with the exception of the concentration at the center, which undergoes a change. The isotropic porous medium exhibits a faster evolution than that observed for the anisotropic ones. Figure 6 provides a clear illustration of the aforementioned differences. The direction of the fluid velocity exerts an influence on the distribution of the concentration, as illustrated in fig. 7. When $u > v$, the diffusant will undergo a more rapid convection process in the x-direction than in the y-direction.

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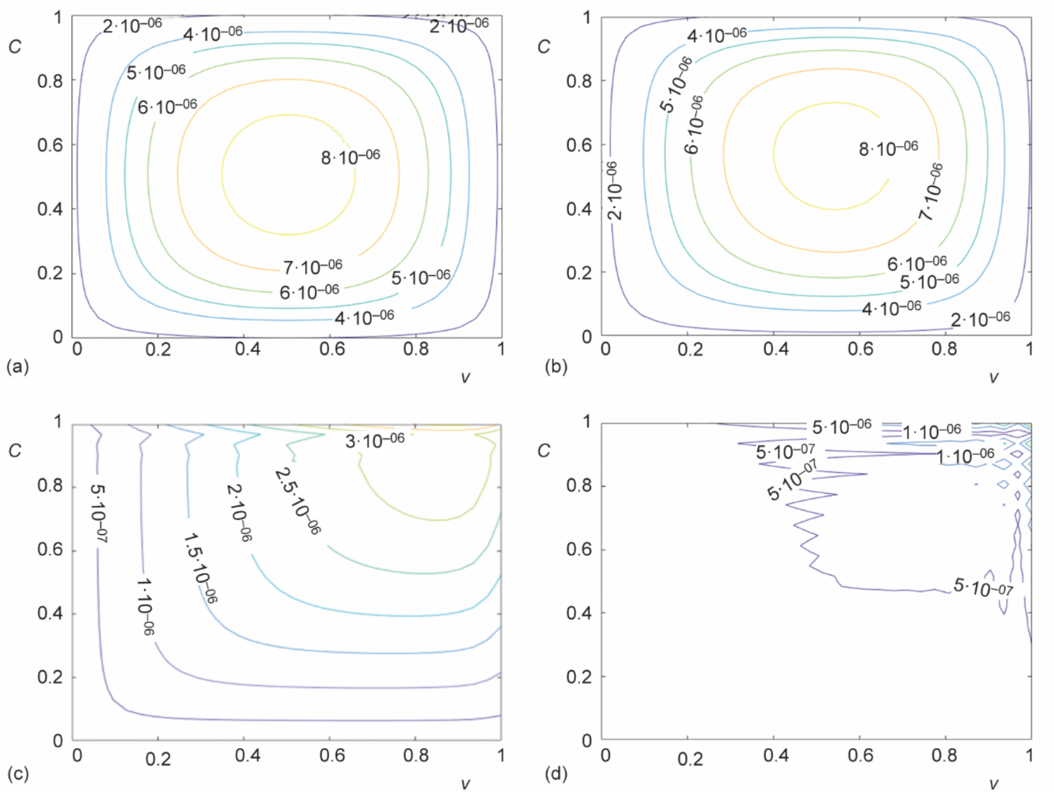

Figure 5. The effect of convection on the fractal diffusion process (α = 0.8, β = 0.6, γ = 0.9 t = 1.0, and D_c = 1.0); (a) u = 0.1, v = 0.1, (b) u = 1.0, v = 1.0, (c) u = 20.0, v = 20.0, and (d) u = 100.0, v = 100.0

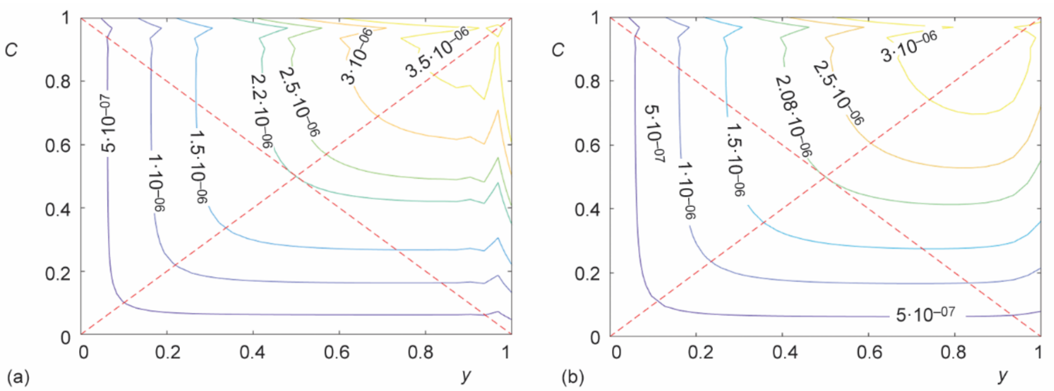

Figure 6. Comparison of the evolution process between the isotropic and anisotropic porous media; (a) α = 0.8, γ = 0.6, β = 0.6, t = 1.0, D_c = 1.0 and (b) α = 0.8, γ = 0.9, β = 0.6, t = 1.0, D_c = 1.0

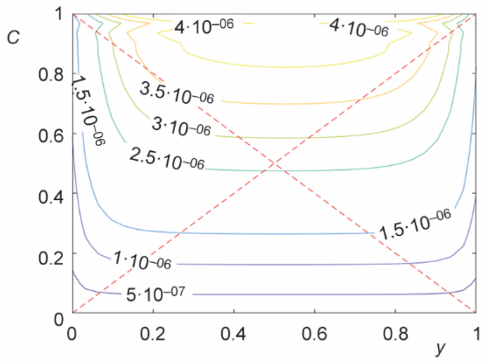

Figure 7. Effect of convection direction on the distribution of the concentration (u = 20, v = 1, t = 1.0, α = 0.8, and $\beta = \gamma$ = 0.6)

Discussion and conclusions

This paper presents a numerical study of the fascinating phenomenon of fractal convection-diffusion within porous media. In the context of the convection-diffusion problem, the temporal Caputo fractional derivative is employed to illustrate the evolution of the concentration of the diffusant, while the spatial Riesz fractional derivative is utilized to represent the diffusion process. The traditional derivative is applied to the convection process. The convection-diffusion process exerts a profound impact on the permeability of the nanofiber membrane. This paper examines the impact of the convection-diffusion process on the concentration of diffusants. The numerical results demonstrate that the evolution process is significantly influenced by the porosity of the porous media. In the case of relatively low fluid velocity, the diffusion process assumes a dominant role. Nevertheless, at a specific threshold, the convection process becomes the dominant phenomenon. The direction of fractal convection-diffusion of the nanofiber membrane's permeability is predominantly influenced by the direction of the fluid-fow.

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