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Article

Statistical physical modeling of anomalous diffusion behavior in non-uniform media

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Abstract: The non-uniformity of the medium and the flow field causes the diffusion process to deviate from Fick's law, resulting in anomalous diffusion. Anomalous diffusion is not only an important fundamental research topic in theoretical physics and statistical mechanics, but also a basic physical process of common concern in fields such as environment, hydrology, and engineering, with practical application backgrounds. The study addresses the issue that the classical convection-diffusion model cannot effectively describe the migration laws of gases from the perspective of flow modeling, and establishes a variable-order time fractional convection-diffusion equation model and numerically solves it using the finite difference method. It is used to simulate the migration laws and characteristics of gases, and to compare and analyze the experimental data with the simulation results. The results show that the fractional-order derivative model can well fit the anomalous diffusion phenomenon of the experimental data, and the time order characterizes the non-uniformity of the storage medium structure. The smaller the order, the stronger the non-uniformity. This verifies the accuracy and effectiveness of the model. This study solves the anomalous diffusion phenomenon that cannot be accurately described by traditional integer-order equations, providing a theoretical guidance for predicting the groundwater pollution risk during shale gas extraction under the dual-carbon goals.

Keywords: Variable-order fractional derivative model; Anomalous diffusion; Non-uniform medium; Statistical physics; Numerical simulation

1. Introduction

Heterogeneous media refer to media whose physical properties such as permeability, porosity, and saturation show significant variations in space [1-2]. Unlike homogeneous media, the internal parameter distribution of heterogeneous media has random, anisotropic, or multi-scale characteristics, which determines that the fluid movement laws in the seepage process are much more complex than those in homogeneous media [3-4]. In engineering fields such as oil and gas reservoir development, groundwater pollution prevention and control, and geothermal resource exploitation, reservoir media are almost all heterogeneous - for example, the permeability of different sedimentary microfacies in sandstone reservoirs can differ by 3 to 4 orders of magnitude, and the difference in fracture and matrix permeability of carbonate rock reservoirs can be 4 to 6 orders of magnitude [5-7]. This heterogeneity makes seepage research require a shift from the "averaging" thinking to "refinement" characterization.

The gradient law and exponential function relationship in traditional integer-order derivative models are generally insufficient to accurately describe the mechanical behavior of heterogeneous media [8-9]. For example, in groundwater solute transport, due to the preferential flow paths in fractured porous rock layers, the solute transport speed may be higher than the predicted result of Fick diffusion law, presenting a "fast diffusion" phenomenon; at the same time, the underground aquifer may also exhibit "slow diffusion" due to the quality exchange between low-permeability and high-permeability regions. Abnormal diffusion behavior in heterogeneous media often reflects power-law characteristics, and the fitting formula of the experimental data has the form of a power function [10-11]. For example, the average displacement data of particle diffusion can be fitted by a power function of time, the particle acceleration distribution of turbulence can be characterized by Levy stable distribution, extended Gauss distribution, Tsallis distribution, etc., the relaxation and creep functions of complex viscoelastic materials are more suitable to be fitted by a power function of time, the attenuation coefficient of ultrasonic waves in biological tissues can be accurately fitted by a power function with respect to the frequency of the sound source, and statistical physical modeling can better describe the above power-law characteristics.

This paper introduces the variable time fractional convection-diffusion model into the anomalous diffusion behavior of gas seepage in dual porous media, and uses finite difference method for numerical discretization and iterative solution. The shifted Grunwald formula is used to discretize the variable fractional derivative, and a classical implicit Euler difference scheme is established based on this. The existence and uniqueness of the solution of this scheme are discussed, the compatibility, stability and convergence of the method are analyzed, and the validity of the scheme is proved. An attempt is made to explore the physical meaning of the parameters of the variable fractional derivative model corresponding to practical problems, explore the application and prospects of the variable fractional derivative model in oil and gas resource exploitation, and effectively predict the situation of underground water resource pollution.

2. Anomalous diffusion behavior in heterogeneous media and modeling

2.1. Abnormal Diffusion

Abnormal diffusion is a complex diffusion process that cannot be described by standard statistical physical methods as a non-equilibrium process [12]. The solutions of general linear diffusion equations follow a Gaussian distribution, but the solutions of abnormal diffusion equations do not follow this rule. Therefore, this type of diffusion cannot be simulated using Fick's second law. The fundamental reason is that Fick's law is applicable to diffusion in uniform media or diffusion where the directional displacement is linear with time. However, most porous media generally have fractal structures and anisotropic characteristics. Due to the presence of internal pores that provide channels for gas diffusion, the heterogeneity and fractal structure of the pore channels affect the normal diffusion of gas within the medium. Due to the existence of some blocked pores, diffusion is delayed, resulting in a tailing phenomenon. Alternatively, the presence of large pores connected by different diameter pore channels and preferential paths also accelerates gas diffusion, leading to an early breakthrough phenomenon. Eventually, the diffusion within the medium deviates from a Gaussian distribution. These phenomena can be characterized by abnormal diffusion. Therefore, a fractal-fractal order differential equation is established to describe this abnormal diffusion problem.

2.2. Fractional Derivatives

Fractional derivatives are mathematically defined as convolution integrals. They represent the temporal memory of physical processes or the interaction of physical quantities between different spatial points (also known as non-locality) by using power functions as the integration kernel. The traditional integer-order derivative limit definition can be regarded as a simple local memory description. The fractional derivative model characterizes the strength of memory through fractional derivatives [13]. Fractional derivatives have various forms of definitions, and these definitions are essentially consistent in characterizing memory, and the forms can also be mutually transformed. The most frequently used and mathematically rigorous definition for anomalous diffusion modeling is the Riemann-Liouville definition, expressed as follows:

$$\frac{\partial^{\alpha} u(x)}{\partial x^{\alpha}} = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{dx^n} \int_a^x (x-\varepsilon)^{n-1-\alpha} u(\varepsilon) d\varepsilon \qquad (1)$$

$$n-1 \le \alpha < n$$

Here, α represents the order of the fractional derivative, and n is the smallest integer greater than α. If the above definition is transformed into a discrete form, it can lead to the Grünwald-Letnikov definition; if the order of integration and differentiation is reversed, it can result in the Caputo definition; the Riesz definition in the high-dimensional case can also be regarded as an extension of the above definition; the spatial fractional Laplacian operator is essentially the same as the above definition.

2.3. Characterization of anomalous behavior diffusion in non-uniform media

2.3.1. Fractional-order flux form diffusion model

In 1965, Professor Mandelbrot from Yale University in the United States proposed the concept of fractals. He pointed out that there are numerous fractional-dimensional phenomena in nature and in science and technology. The diffusion and transmission process in fractal media is related to the entire time and space, indicating that this phenomenon is non-local. This diffusion movement is called anomalous diffusion. Systems in environments such as turbulence, plasma, growing surfaces, and cells also exhibit characteristics deviating from normal Brownian motion. In these phenomena, the movement of a free particle no longer satisfies Fick's law. The average displacement of the particle over time is proportional to the fractional power of time, and is a nonlinear function of time, that is, for $0 < \alpha < 2$, $\langle (c-\overline{c})^2 \rangle \sim t^{\alpha}$. When $\alpha = 1$, it is normal diffusion; when $0 < \alpha < 1$, it has an abnormal diffusion index, which is an anisotropic diffusion process; when $1 < \alpha < 2$, it is a superdiffusion process. Therefore, the fractional-order diffusion flux was proposed:

$$J = -a(x)\nabla_M^{\gamma} c \tag{2}$$

Instead of the integer-order flux, where $0 \le \gamma \le 1$, substitute it into the mass conservation relation, and then obtain the following fractional-order flux form of the diffusion equation:

$$\frac{\partial c}{\partial t} = \nabla \cdot \left(a(x)\nabla_M^{\gamma} c \right) + f(x) \tag{3}$$

Here, $\nabla_M^{\gamma} c = \int_{\|\theta\|=1} \theta D_{\theta}^{\gamma} c M(\theta) d\theta$ can be understood as the weighted sum of the fractional-order directional derivatives θ generated along various directions by the pollutant concentration $D_{\theta}^{\gamma} c$.

In one-dimensional space, there are only two directions: the positive direction $\theta = 1$ and the negative direction $\theta = -1$. If the measure M is a point mass along each direction, that is, when $\theta = 1$, $M(\theta) = r$; when $\theta = -1$, $M(\theta) = 1 - r$, then the fractional gradient can be simplified as:

$$\nabla_M^{\gamma} c = r D_{\theta=1}^{\gamma} c - (1-r) D_{\theta=-1}^{\gamma} c = {}_0 D_x^{\gamma} c - (1-r)_x D_1^{\gamma} c \tag{4}$$

Let $\gamma = 1 - \beta$, thereby obtaining the fractional-order flux form of the diffusion equation in one-dimensional space of order $2 - \beta$:

$$\frac{\partial c}{\partial t} = D \left\{ {}_0 D_1^{1-\beta} c - (1-r)_x D_1^{1-\beta} c \right\} + f(x) \tag{5}$$

This is the fractional-order Fokker-Planck equation, and the corresponding steady-state equation is:

$$-D \left\{ {}_0 D_1^{1-\beta} c - (1-r)_x D_1^{1-\beta} c \right\} = f(x) \tag{6}$$

It is called the fractional-order flux form of the diffusion equation.

2.3.2. Fractional-order divergence form diffusion model

The mass conservation of fluids in porous media stems from continuum mechanics. The underlying concept is based on the classical definition of divergence in vector fields: when the diameter h of the control volume V approaches zero, the limit of the ratio of the mass within the control volume V enclosed by the closed surface S to the volume V is considered:

$$divJ = \lim_{h \to 0} \frac{1}{V} \int_S J \cdot n dS \tag{7}$$

Here, n represents the unit outward normal vector of the surface S. The basic assumption for the divergence in this definition is that when the diameter of the control volume V approaches zero, this limit exists. This condition is satisfied for homogeneous porous media, but for inhomogeneous anisotropic media, this limit may not necessarily exist. Therefore, it is not appropriate to derive the diffusion equation using integer-order mass conservation laws.

Meerschaert et al. can utilize the generalized continuity equation (fractional-order mass conservation law) generated by the fractional-order divergence:

$$\nabla_M^{\gamma} \cdot J = -\frac{\partial c}{\partial t} + f(x) \tag{8}$$

Instead of the classical continuity equation (the integer-order law of mass conservation). Here, when $0 \le \gamma \le 1$, the fractional-order divergence is defined as:

$$\nabla_M^{\gamma} \cdot J = \int_{\|\theta\|=1} \left(D_{\theta}^{\gamma} J \cdot \theta \right) M(\theta) d\theta \tag{9}$$

In one-dimensional space, the motion of the particle is confined to two directions, $\theta = 1$ or -1. Let $\gamma = 1 - \beta$, the fractional derivative degenerates to:

$$\nabla_M^{\gamma} \cdot J = r_0 D_x^{1-\beta} J - (1-r)_x D_1^{1-\beta} J \tag{10}$$

Specifically, when $\gamma = 1$, $\nabla_M^{\gamma} \cdot J$ is exactly the familiar integer-order divergence $\nabla \cdot J = \frac{\partial J}{\partial x}$, and (9) reduces to the classical first-order mass conservation law.

Thus, in one-dimensional space, by using the integer-order Fick's law and the fractional-order mass conservation law, we obtain the $2-\beta$ order fractional-order divergence form of the spatial fractional diffusion equation:

$$\frac{\partial c}{\partial t} = \left\{ r_0 D_x^{1-\beta} - (1-r)_x D_1^{1-\beta} \right\} (a(x)Dc) + f(x) \tag{11}$$

The corresponding steady-state equation is:

$$-\left\{ r_0 D_x^{1-\beta} - (1-r)_x D_1^{1-\beta} \right\} (a(x)Dc) = f(x) \tag{12}$$

It is called the fractional-order divergence form of the diffusion equation.

The above discussion derived the fractional-order diffusion equation from a macroscopic perspective. Similar to the situation in deriving integer-order diffusion equations, from a microscopic perspective, that is, under the condition that the assumptions of finite average free path and average waiting time are not satisfied, the probability density function (PDF) of the molecular random transport process that follows the independent and identically distributed (IID) rule can be derived to satisfy the fractional-order diffusion equation.

2.3.3. Diffusion Model of Fractional Laplacian Operator

In many engineering and technical applications, fractional-order Laplacian operators are frequently used to describe diffusion processes such as phase field models and inverse scattering problems, for example, the Allen–Cahn equation:

$$\frac{\partial u}{\partial t} + (-\Delta)^s u = f(x,u), x \in R^n \tag{13}$$

$$\left(-\Delta u(x,t)\right)^s = C_s \int_{R^n} \frac{u(x) - u(y)}{|x-y|^{n+2s}} dy, 0 < s < 1 \tag{14}$$

$$u(x,0) = \phi(x), x \in R^n \tag{15}$$

A detailed discussion has been provided on the solvability, regularity and corresponding difference techniques of such fractional diffusion equations defined by fractional-order Laplace operators.

3. Fractional derivative modeling of gas migration in non-uniform media

3.1. Fractional-order derivative model

Regarding the migration characteristics of gas in shale reservoirs (non-uniform media), previous studies have indicated that nonlinear integer derivative models and variable coefficient models can describe abnormal diffusion processes under certain special circumstances. However, they have shortcomings such as numerous physical parameters, unclear physical meanings, and narrow application scope. The fractional derivative equation is a non-local operator expressed in the form of differential-integral, which can better represent the historical memory and global correlation of particle movement. By introducing the time fractional derivative term into the traditional convection-diffusion equation, a time fractional convection-diffusion equation model is established as follows:

$$\frac{\partial^{\alpha} C(x,t)}{\partial t^{\alpha}} = -v\frac{\partial C(x,t)}{\partial x} + D\frac{\partial^{2} C(x,t)}{\partial x^{2}}, 0 < \alpha \leq 1 \tag{16}$$

In the equation, $C(x,t)$ represents the gas concentration, v and D are the average velocity and diffusion coefficient in the medium, and α is the time fractional order. When $\alpha = 1$, the equation simplifies to the classical convection-diffusion equation. The geological structure of shale gas reservoirs is complex, and fracturing or natural connected fractures constitute the migration channels for methane gas. The migration process is affected by factors such as the porosity of the gas reservoir, the curvature and roughness of the path, and the physical properties of the fluid, and it changes over time. The constant-order model cannot accurately depict the anomalous gas transport process in strongly heterogeneous shale reservoirs that changes with time. The time fractional-order variable-order convection-diffusion model has been considered suitable for characterizing the groundwater and solute migration process in highly heterogeneous fractures or disordered porous media. The model is as follows:

$$\frac{\partial^{\alpha(t)} C(x,t)}{\partial t^{\alpha(t)}} = -v\frac{\partial C(x,t)}{\partial x} + D\frac{\partial^{2} C(x,t)}{\partial x^{2}}, 0 < \alpha(t) \leq 1 \tag{17}$$

Considering the transformation of the formula for the fractional-order Caputo derivative, Coimbra proposed a formula for the fractional-order differential operator used in physical modeling as follows:

$${}_{0}^{C}D_{t}^{\alpha(t)} f(t) = \frac{1}{\Gamma(1-\alpha(t))}\int_{0}^{t}(t-\tau)^{-\alpha(t)} f'(\tau)d\tau + \frac{\left(f(0^{+}) - f(0^{-})\right)t^{-\alpha(t)}}{\Gamma(1-\alpha(t))} \tag{18}$$

This definition refers to the fact that the memory of the system changes over time and is determined by the current time instant. If $\alpha(t)$ is a constant, it can be simplified to the constant-order Caputo definition. The operator ${}_{0}^{C}D_{t}^{\alpha(t)}$ represents the time-varying fractional derivative operator in the Caputo sense, and can also be defined as follows:

$${}_{0}^{C}D_{t}^{\alpha(t)} C(x,t) = \begin{cases} \dfrac{1}{\Gamma(1-\alpha(t))}\displaystyle\int_{0}^{t}\frac{1}{(t-\xi)^{\alpha(t)}}\frac{\partial C(x,\xi)}{\partial \xi}d\xi, & 0 < \alpha(t) < 1 \\ \dfrac{\partial C(x,t)}{\partial t}, & \alpha(t) = 1 \end{cases} \tag{19}$$

In the formula, $\Gamma(\cdot)$ represents the gamma function.

3.2. Solution of the Diffusion Equation by Finite Difference Method

To establish the difference scheme, the region $[L,R]\times[0,T]$ is divided. The spatial step size is set as $h = \frac{(R-L)}{K}$, and the time step size is Δt. $t_n = n\Delta t\ (n = 0,\cdots,N)$, and $N = \left\lfloor \frac{T}{\Delta t} \right\rfloor$. $x_i = L + ih\ (i = 0,\cdots,K)$, c_i^n represents the difference approximation of $c(x_i,t_n)$ at the point (x_i,t_n), that is, $c_i^n \approx c(x_i,t_n)$.

Let $d_i = d(x_i)$, $v_i = v(x_i)$, $p_i = p(x_i)$, and $f_i^n = f(x_i,t_n)$. Using the shifted Grunwald formula, we define the spatial fractional derivative as:

$$\frac{\partial c^{\alpha}(x_i,t_{n+1})}{\partial x^{\alpha}} = \frac{1}{h^{\alpha}}\sum_{k=0}^{i+1} g_k c(x_{i-k+1},t_{n+1}) + O(h) \tag{20}$$

Here, g_k represents the Grunwald weighting coefficient:

$$g_k = \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)} = (-1)^k\frac{\alpha(\alpha-1)\cdots(\alpha-k+1)}{k!} \tag{21}$$

Define first-order space and time derivatives:

$$\begin{aligned}\frac{\partial c}{\partial t}(x_i,t_{n+1}) &= \frac{c(x_i,t_{n+1})-c(x_i,t_n)}{\Delta t}+O(\tau)\\ \frac{\partial c}{\partial x}(x_i,t_{n+1}) &= \frac{c(x_i,t_{n+1})-c(x_{i-1},t_{n+1})}{h}+O(h)\end{aligned} \tag{22}$$

Among them, $\tau=\Delta t$, thus, we can obtain:

$$\begin{aligned}\frac{c(x_i,t_{n+1})-c(x_i,t_n)}{\Delta t} &= -v_i\frac{c(x_i,t_{n+1})-c(x_{i-1},t_{n+1})}{h}\\ &\quad +\frac{d_i}{h^\alpha}\sum_{k=0}^{i+1}g_k c(x_{i-k+},t_{n+1})-p_i c(x_i,t_{n+1})+f_i^{n+1}+R_{i,n+1}\end{aligned} \tag{23}$$

There exists a positive constant M such that:

$$\left|R_{i,n+1}\right|\le M\left(\tau+h\right) \tag{24}$$

From this equation, the implicit Euler scheme can be established as follows:

$$\frac{c_i^{n+1}-c_i^n}{\Delta t}=-v_i\frac{c_i^{n+1}-c_{i-1}^{n+1}}{h}+\frac{d_i}{h^\alpha}\sum_{k=0}^{i+1}g_k c_{i-k+1}^{n+1}-p_i c_i^{n+1}+f_i^{n+1} \tag{25}$$

$$c_i^0=s(x_i),0\le i\le K-1 \tag{26}$$

$$c_L^n=0,\ c_K^j=b(t_j),0\le t_j\le N \tag{27}$$

From the above, it can be seen that Equations (25) to (27) are consistent with the equation with initial and boundary value conditions.

Equation (25) can be rewritten in the following form:

$$\begin{aligned}&-g_0B_ic_{i+1}^{n+1}+\left(1+E_i-g_1B_i+\Delta tp_i\right)c_i^{n+1}-\left(E_i+g_2B_i\right)\cdot c_{i-1}^{n+1}\\ &-B_i\sum_{k=3}^{i+1}g_k c_{i-k+1}^{n+1}=c_i^n+\Delta tf_i^{n+1}\left(E_i=v_i\Delta t/h,B_i=d_i\Delta t/h^\alpha\right)\end{aligned} \tag{28}$$

The fractional-order equation can be further rewritten in matrix form:

$$AC^{n+1}=C^n+\Delta tF^{n+1} \tag{29}$$

Here: $C^n=(c_1^n,c_2^n,\cdots,c_{K-1}^n)^T$, $C^n+\Delta tF^{n+1}=\left(c_1^n+\Delta tf_1^{n+1},c_2^n+\Delta tf_2^{n+1},\cdots,c_{K-1}^n+\Delta tf_{K-1}^{n+1}+g_0B_{K-1}b_K(t_{n+1})\right)^T$.

$A=[A_{i,j}]$ is a $(K-1)\times(K-1)$ coefficient matrix. When $i=1,\cdots,K-1$ and $j=1,\cdots,K-1$:

$$A_{i,j}=\begin{cases}0, & j\ge i+2\\ -g_0B_i, & j=i+1\\ 1+E_i-g_1B_i+\Delta tp_i, & j=i\\ -E_i-g_2B_i, & j=i-1\\ -g_{i-j+1}B_i, & j\le i-2\end{cases} \tag{30}$$

3.3. Stability and Convergence of the Difference Scheme

Suppose $V_i^j\left(i=0,1,2,\cdots,m;j=0,1,2,\cdots,n\right)$ are the approximations of the difference scheme, and the error $\varepsilon_i^j=V_i^j-u_i^j\left(i=0,1,2,\cdots,m;j=0,1,2,\cdots,n\right)$ satisfies:

$$\left(\frac{\nu hr}{2}-\omega r\right)\varepsilon_{i+1}^1+(1+2r\omega)\varepsilon_i^1-\left(\frac{\nu hr}{2}+\omega r\right)\varepsilon_{i-1}^1=\varepsilon_i^0 \tag{31}$$

$$\left(\frac{\nu hr}{2}-\omega r\right)\varepsilon_{i+1}^{k+1}+(1+2r\omega)\varepsilon_i^{k+1}-\left(\frac{\nu hr}{2}+\omega r\right)\varepsilon_{i-1}^{k+1}$$
$$=c_1\varepsilon_i^k+\sum_{j=1}^{k-1}c_{j+1}\varepsilon_i^{k-j}+b_k\varepsilon_i^0, k>0\left(i=1,2,\cdots,m-1\right) \tag{32}$$

Equations (31) - (32) can be expressed as:

$$\begin{cases} AE^{k+1}=c_1E^k+c_2E^{k-1}+\cdots+c_kE^1+b_kE^0 \\ E^0 \end{cases} \tag{33}$$

Here, $E^k=\left(\varepsilon_1^k,\varepsilon_2^k,\cdots,\varepsilon_{m-1}^k\right)^T$. Through mathematical induction, the following result can be proved:

Let $u\left(x_i,t_k\right)$, $\left(i=1,2,\cdots,m-1;k=1,2,\cdots,n\right)$ be the exact solution of the equation at the grid points (x_i,t_k). Define $e_i^k=u(x_i,t_k)-u_i^k$, $i=1,2,\cdots,m-1$; $k=1,2,\cdots,n$ and $e^k=\left(e_1^k,e_2^k,\cdots,e_{m-1}^k\right)^T$. Substituting $e^0=0$ gives:

$$\left(\frac{\nu hr}{2}-\omega r\right)e_{i+1}^1+\left(1+2r\omega\right)e_i^1-\left(\frac{\nu hr}{2}+\omega r\right)e_{i-1}^1=R_i^1 \tag{34}$$

$$\left(\frac{\nu hr}{2}-\omega r\right)e_{i+1}^{k+1}+\left(1+2r\omega\right)e_i^{k+1}-\left(\frac{\nu hr}{2}+\omega r\right)e_{i-1}^{k+1}$$
$$=c_1e_i^k+\sum_{j=1}^{k-1}c_{j+1}e_i^{k-j}+R_i^{k+1}, k>0\left(i=1,2,\cdots,m-1\right) \tag{35}$$

Here, R_i^{k+1} represents the truncation error, and $\left|R_i^{k+1}\right|\le C\left(\tau^{1+\alpha}+\tau^{\alpha}h^2\right)$, for $i=1,2,\cdots,m-1$; $k=0,1,2,\cdots,n$, where C is a constant.

Lemma 1: $\left\|e^k\right\|_\infty\le Cb_{k-1}^{-1}\left(\tau^{1+\alpha}+\tau^{\alpha}h^2\right)$, for $k=1,2,\cdots,n$, where $\left\|e^k\right\|_\infty=\max_{1\le i\le m-1}\left|e_i^k\right|$, and C is a constant.

And:

$$\lim_{k\to\infty}\frac{b_k^{-1}}{k^{\alpha}}=\lim_{k\to\infty}\frac{k^{-\alpha}}{\left(k+1\right)^{1-\alpha}-k^{1-\alpha}}=\frac{1}{1-\alpha} \tag{36}$$

Therefore, there exists a constant $\tilde{C}$ such that:

$$\left\|e^k\right\|_\infty\le\tilde{C}k^{\alpha}\left(\tau^{1+\alpha}+\tau^{\alpha}h^2\right) \tag{37}$$

Also, since $k\tau\le T$, we have:

$$\left\|e^k\right\|_\infty\le\tilde{C}T^{\alpha}\left(\tau+h^2\right) \tag{38}$$

Therefore, the following theorem is obtained:

Lemma 2 Let u_i^k be the approximate value of $u(x_i,t_k)$ calculated by the difference scheme. Then there exists a positive constant C such that:

$$\left|u_i^k-u(x_i,t_k)\right|\le C\left(\tau+h^2\right), i=1,2,\cdots,m-1;k=1,2,\cdots,n \tag{39}$$

3.4. Verification of Convergence for Difference Schemes

Among them:

$$\alpha=\frac{1}{2},\omega=1,\nu=\frac{1}{4},L=\frac{8\sqrt{7}\pi}{21},T=4,f(x)=\sin\left(\frac{3\sqrt{7}}{8}x\right)e^{\frac{x}{8}} \tag{40}$$

The exact solution of the equation in series form is:

$$u(x,t)=E_{\frac{1}{2}}\left(-t^{\frac{1}{2}}\right)\sin\left(\frac{3\sqrt{7}}{8}x\right)e^{\frac{1}{8}x}=\sum_{n=0}^{\infty}\frac{(-\sqrt{t})^{n}}{\Gamma\left(\frac{n}{2}+1\right)}\sin\left(\frac{3\sqrt{7}}{8}x\right)e^{\frac{1}{8}x} \tag{41}$$

Figure 1 and Figure 2 show the comparison between the numerical solutions and the exact solutions at $t=1$ with $\tau=0.15$, $h=0.2$, and $\tau=0.035$, $h=0.075$. We observe that as the grid refinement becomes finer, the numerical solutions get closer to the exact solutions. Table 1 verifies the convergence of the difference scheme in this paper, demonstrating the effectiveness of the difference scheme.

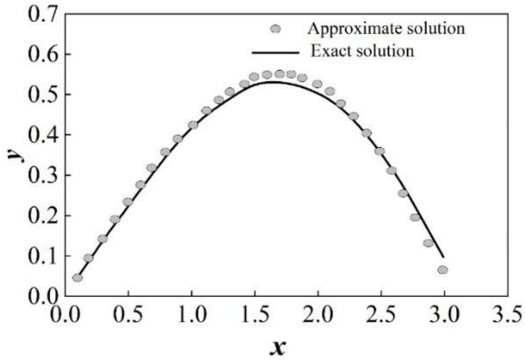


Figure 1. $\tau=0.15, h=0.2$

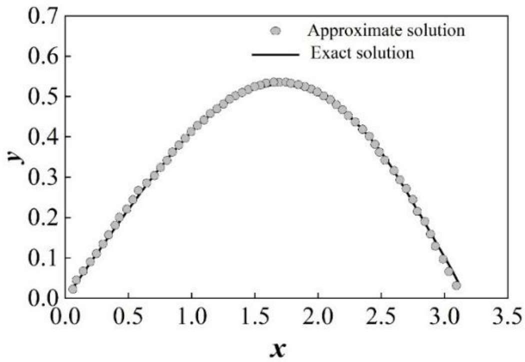


Figure 2. $\tau=0.035, h=0.075$

Table 1. The $\|\bullet\|_\infty$ errors of numerical solution

T	$\tau=0.2, h=0.2$	$\tau=0.1, h=0.1$	$\tau=0.025, h=0.05$	$\tau=0.00625, h=0.0125$
$t=1$	8.0472×10^{-2}	3.6925×10^{-2}	9.7711×10^{-3}	2.4409×10^{-3}
$t=2$	6.7077×10^{-2}	2.9859×10^{-2}	7.7777×10^{-3}	1.9251×10^{-3}
$t=3$	5.8733×10^{-2}	2.5783×10^{-2}	6.6822×10^{-3}	1.6503×10^{-3}
$t=4$	5.2759×10^{-2}	2.3062×10^{-2}	5.9569×10^{-3}	1.4655×10^{-3}

4. Analysis of Numerical Simulation Results

4.1. Example 1

Assuming there is a continuous point source C_{in} at the inlet boundary and gas is continuously introduced into the simulated sample inlet end, and a convective boundary condition is defined at the outlet boundary. The gas concentration curve shows a continuously rising trend until it gradually reaches stability. The initial concentration value is set to 0, and the outlet boundary condition is set to a free boundary condition. Through numerical simulation methods, the transport process of gas particles within a certain medium region is numerically simulated. Several dimensionless concentration penetration curves of gas particles are shown in Figure 3.

In non-uniform medium structures, the fractional derivative model is an effective tool for simulating anomalous particle diffusion. Figure 3 shows that the smaller the fractional order α in the time fractional convection-diffusion model simulation results, the slower the particle transport process and the longer the time required for the concentration to reach its maximum value. By combining the simulation results, it can be inferred that the medium structure is the dominant factor affecting the change of the concentration penetration curve. The order in the fractional model effectively reflects the effect of the medium structure on the particle transport. Due to the strong heterogeneity structure of the oil and gas reservoir matrix, there are dead pores in the dual medium structure, or some transport channels are blocked or filled, which all hinder the gas particle transport process. From Figure 3, it can be seen that as the time order α in the fractional model decreases, the gas transport process becomes slower. When $\alpha = 1$, the classical convection-diffusion model changes in the fastest growth trend before reaching the maximum concentration, until the concentration reaches its peak.

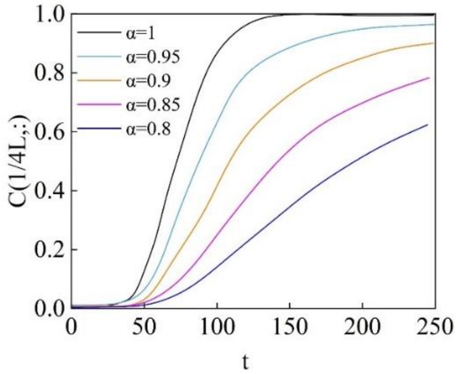
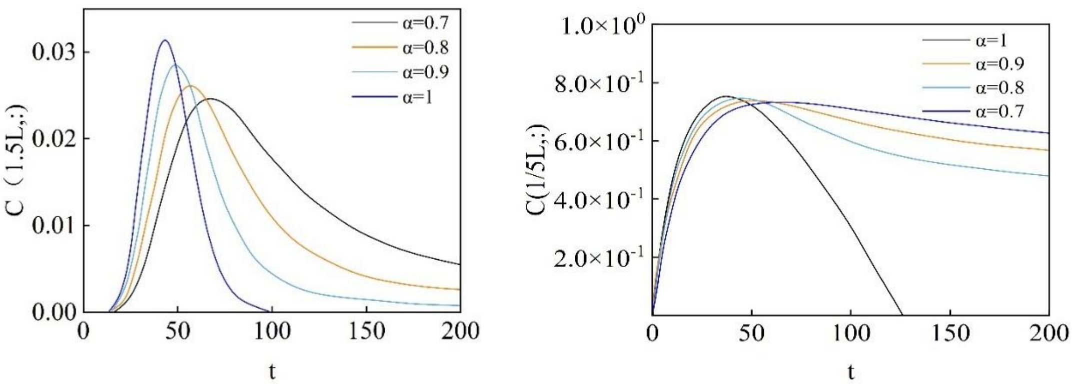


Figure 3. The concentration of the gas particles in the gas particles is through

4.2. Example 2

Assume that an initial value of C_0 is given at the entrance boundary, and the entrance boundary condition is set to 0, while the exit boundary is set as a free boundary condition.

The numerical simulation results of the fractional derivative model are shown in Figure 4. The figure shows that in the time fractional derivative model, the concentration penetration curves under several different time orders α are obtained through numerical methods. In the fractional convection-diffusion model, when $0 < \alpha < 1$, the fractional order α has a strong influence on the gas migration process. At the fixed control position 1/5L, as the order α decreases, the concentration peak becomes smaller, and abnormal diffusion shows a slow decay. As can be seen from Figure 4, the tail slope of the concentration penetration curve changes with the order α, and the smaller the order, the more severe the power-law tailing phenomenon, and the longer the tail. This is because the particle migration channel is blocked and the gas movement is hindered. Figure 4 (b) is a semi-logarithmic coordinate graph, and it can be observed that the tail slope of the concentration penetration curve under different time orders α is different, indicating that the time order α is the main parameter affecting the tailing phenomenon.



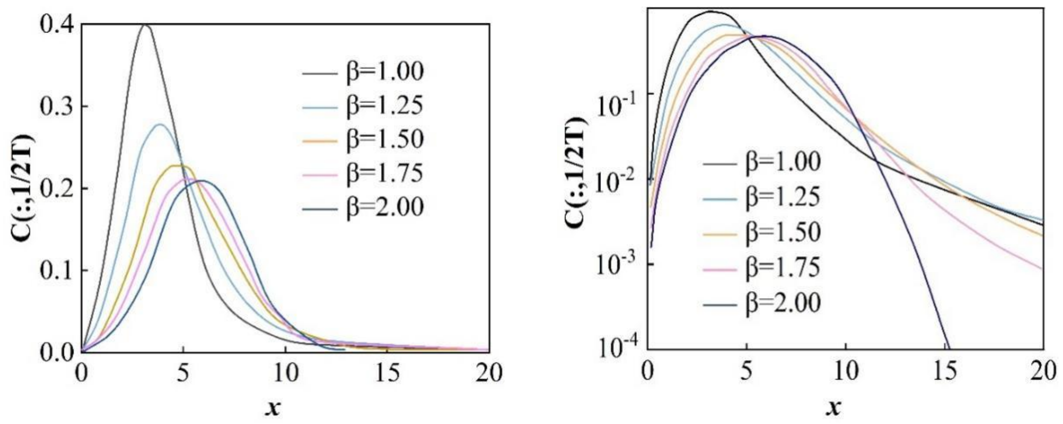
(a) Concentration penetration curve (b) Semilogarithmic coordinate

Figure 4. Numerical simulation of fractional derivative model

4.3. Example 3

A point source at a specific instant is set at the boundary, and the particle transport law is simulated using the spatio-temporal fractional convection-diffusion model. The initial value is C_0, the inlet boundary value is 0, and the right boundary condition is a free boundary. The numerical simulation results are shown in Figure 5.

From Figure 5, it can be concluded that the spatial fractional convection-diffusion model can well simulate the early arrival phenomenon of particles. As the spatial order decreases, the early arrival phenomenon becomes more obvious. Based on the analysis of the actual situation, if particles move in a dual porous medium, there are large-scale fracture channels in the medium, which promote the acceleration of particle movement, thus resulting in an early super-diffusion phenomenon. The gas transport process in the dual porous medium is closely related to the pore structure and spatial distribution. In summary, the fractional derivative model is an effective tool for describing the gas transport process with memory effects.



(a) α=2 Semilogarithmic graph (b) α=1 Semilogarithmic graph

Figure 5. The numerical results of the diffusion model simulation

5. Conclusion

Although the research on anomalous diffusion has a long history, it was initially concentrated in the field of statistical physics. Since the 1980s, theoretical research on fractional derivative diffusion equation models has gradually begun. In the past decade, fractional diffusion models have gradually become a research hotspot in multiple fields of environmental fluid mechanics. From the perspective of flow modeling, the classical convection-diffusion model cannot effectively describe the migration laws of gases. Considering the characteristics of heterogeneous media, a variable-time fractional derivative model that can accurately describe the migration process with historical dependence has been established, and numerical simulation has been carried out using the finite difference method. From the numerical simulation results, the fractional derivative model can accurately depict the anomalous diffusion phenomenon of particles. By changing the time or spatial order in the fractional derivative model, different degrees of sub-diffusion or super-diffusion phenomena can be reflected.

At present, the fractional derivative modeling and application of anomalous diffusion mainly focus on mechanism research and experimental data analysis. The application scope and depth in engineering need to be expanded. In particular, the combination of fractional diffusion models with hydrological processes such as surface runoff and subsurface flow exchange to solve environmental fluid mechanics problems will be an important research direction in this field. At the same time, the actual movement process of solutes or particles often involves multi-field coupling problems. The analysis of a single physical process cannot effectively solve practical engineering problems. Therefore, the theoretical analysis and application of fractional anomalous diffusion models under multi-physical field coupling conditions are important research topics.

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