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Numerical solutions of time-space fractional advection–dispersion equations

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Summary

This paper establishes a difference approximation on time-space fractional advection-dispersion equations. Based on the difference approximation an ideal numerical example has been solved, and the result is compared with the one of the rigorous time fractional advection-dispersion equation and the rigorous space fractional advection-dispersion equation respectively. The results show: when time fractional order parameter γ=1 or space fractional order parameter α=2, the numerical calculation result of the time-space fractional advection-dispersion equations is in accordance with that of the rigorous time fractional advection-dispersion equation or the rigorous space fractional advection-dispersion equation. The variation law of the result with parameter is also similar to them, that is when γ is smaller, diffusion is slower; when α is smaller, diffusion is faster. The simulation calculation for a practical example indicates that time-space fractional advection-dispersion equations can simulate the skewness and the tail of anomalous diffusion. This paper provides a efficient tool for the research of fractional advection-dispersion equations.

keywords: fractional advection-dispersion equation; anomalous diffusion; time-space relativity; numerical solution

Introduction

In recent years, the phenomenon of the anomalous diffusion (dispersion) has aroused people's broad attention. It has been studied as complicated dynamical system and has had an extensive application in the fields such as semiconductor, porous media, life science, economy finance [1]. Anomalous diffusion is relative to normal diffusion: In normal diffusion, particle motion is Brownian Motion, the Green Function Solution of whose Cauchy problem is the density function of Gaussian distribution, and mean square displacement is the linear function of moving time, while particle diffusion can be described by traditional second order advection-diffusion (dispersion) equation. Anomalous diffusion is essentially regarded as a kind of non-locality motion of non-markovian, so time-space relativity must be considered. Particle motion is not Brownian motion, and mean square displacement is the non-linear function [2, 3, and 4].

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Research indicates that, in order to describe the anomalous diffusion (dispersion), the control equation must be improved and the physical process of diffusion must be described. So we can start with fractional calculus to get fractional advection-diffusion (dispersion) equation [5]. Many studies have discussed the character of the analytic solution of fractional advection-diffusion equation and can commendably explain the phenomenon of anomalous diffusion. In view of the difficulty of fractional advection-diffusion (dispersion) equation relative to the traditional equation, at present many studies intend to get numerical algorithm by means of considering time fraction and space fraction independently[6,7,8,9]. In this paper, the time and space fraction is considered at the same time in fractional advection-diffusion (dispersion) equation to get a numerical solution.

If considering time-space fraction at the same time, the time-space fractional advection-dispersion equation can be obtained (in order to discuss simply, we take the one-dimension space as the object of study), which is defined as follows:

$$\frac{\partial^\gamma C(x,t)}{\partial t^\gamma} = -v\frac{\partial C}{\partial x} + D\frac{\partial^\alpha}{\partial x^\alpha}C(x,t) \tag{1}$$

Where $0<\gamma\leq 1$, $0<\alpha\leq 2$. This equation includes the traditional advection-dispersion equation (when γ=1, α=2). When α=2, the equation is rigorous time fractional advection-dispersion equation; when γ=1, the equation is rigorous space fractional advection-dispersion equation.

Former research indicates that in the process of advection-dispersion, the change law on time and space of the breakthrough curve is when the value of time fraction order γ is increasingly smaller, time relativity is increasingly stronger, the solute diffuses more slowly, and the breakthrough curve becomes smoother. When the value of space fraction order α is increasingly smaller, space relativity is increasingly stronger, the solute diffuses faster, and the breakthrough curve becomes more abrupt. The γ value and α value respectively describe the time and space non-locality relationship between the concentration flux of solute and the concentration. The time relativity causes the concentration of different time in the same point having effect on the concentration flux of current moment. It has memory effect, namely the process of solute diffusion is slower than regularly. The space relativity causes the concentration of all points at the same time having effect on the concentration flux of current point, namely the process of solute diffusion is quicker than regularly.

Numerical approximation

The grids which the space step is **h** and the time step is τ is introduced, which is defined as follows:

$$x_j = jh,\ h>0;\ t_n = n\tau,\ \tau>0;\ (j=0,1,2,\cdots;n=0,1,2\cdots) \tag{2}$$

Discretization of the time fractional term

For the left term of the equation(1), the fractional derivative is changed into integral form, which is defined as follows [7,8]:

$$\frac{\partial^\gamma C(x,t)}{\partial t^\gamma}=\begin{cases}\frac{1}{\Gamma(1-\gamma)}\int\limits_0^t (t-\eta)^{-\gamma}\frac{\partial C(x,\eta)}{\partial\eta}d\eta & 0<\gamma<1\\ \frac{\partial C(x,t)}{\partial t} & \gamma=1\end{cases} \tag{3}$$

The integral form can be recast as:

$$\begin{aligned}&\left.\frac{\partial^\gamma C(x,t)}{\partial t^\gamma}\right|_{(x_j,t_n)}=\frac{1}{\Gamma(1-\gamma)}\int\limits_0^t (t-\eta)^{-\gamma}\frac{\partial C(x_j,\eta)}{\partial\eta}d\eta\\ &=\frac{1}{\Gamma(1-\gamma)}\left[\sum_{k=0}^{n-2}\int\limits_{t_k}^{t_{k+1}}(t_n-\eta)^{-\gamma}\frac{\partial C(x_j,\eta)}{\partial\eta}d\eta+\int\limits_{t_{n-1}}^{t_n}(t_n-\eta)^{-\gamma}\frac{\partial C(x_j,\eta)}{\partial\eta}d\eta\right]\end{aligned} \tag{4}$$

The derivative term can be discretized furthermore as follows:

$$\begin{aligned}&\left.\frac{\partial^\gamma C(x,t)}{\partial t^\gamma}\right|_{(x_j,t_n)}\\ &=\frac{1}{\Gamma(1-\gamma)}\left[\sum_{k=0}^{n-2}\frac{C(x_j,t_{k+1})-C(x_j,t_k)}{\tau}\int\limits_{t_k}^{t_{k+1}}(t_n-\eta)^{-\gamma}d\eta+\right.\\ &\left.\frac{C(x_j,t_n)-C(x_j,t_{n-1})}{\tau}\int\limits_{t_{n-1}}^{t_n}(t_n-\eta)^{-\gamma}d\eta\right]\\ &=\frac{\tau^{1-\gamma}}{\Gamma(2-\gamma)}\left[\sum_{k=0}^{n-2}\frac{C(x_j,t_{k+1})-C(x_j,t_k)}{\tau}\left((n-k)^{1-\gamma}-(n-k-1)^{1-\gamma}\right)+\right.\\ &\left.\frac{C(x_j,t_n)-C(x_j,t_{n-1})}{\tau}\right]\end{aligned} \tag{5}$$

At the moment of t_n, $C(x_j,t_k)$ $(k<n)$ is known, so the first term of the equation above is constant which is named A:

$$A=\frac{\tau^{1-\gamma}}{\Gamma(2-\gamma)}\sum_{k=0}^{n-2}\frac{C(x_j,t_{k+1})-C(x_j,t_k)}{\tau}\left((n-k)^{1-\gamma}-(n-k-1)^{1-\gamma}\right) \tag{6}$$

Discretization of the space fractional term

Adopt lemma[10,11]:
if $f(x) \in L_2(R)$ and $f(x) \in C^{\alpha-2}(R)$, $A_h f(x) = Af(x) + O(h)$, where:

$$\begin{aligned} A_h f(x) &= \frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{k=0}^{\infty} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} f(x-(k-1)h) \\ Af(x) &= \frac{\partial^\alpha f(x)}{\partial x^\alpha} \end{aligned} \tag{7}$$

Of the grids having boundary on both sides,

$$\begin{aligned} &\frac{\partial^\alpha f(x)}{\partial x^\alpha}|_{(x_j,t_n)} \\ &= Af(x)|_{(x_j,t_n)} \\ &= A_{h-}(x)|_{(x_j,t_n)} + A_{h+}(x)|_{(x_j,t_n)} \\ &= \frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{k=0}^{j} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} C(x_{j-k+1}, t_{n-1}) + \frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{k=0}^{n-j} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} C(x_{n-k}, t_{n-1}) \end{aligned} \tag{8}$$

The difference approximation of time-space fractional advection-dispersion equation

Based on discrete difference of the time and space fractional term in the sections above, the difference approximation can be obtained as follows:
implicit difference schemes:

$$\begin{aligned} &\frac{\tau^{1-\gamma}}{\Gamma(2-\gamma)} \frac{C(x_j,t_n) - C(x_j,t_{n-1})}{\tau} + A = -v \frac{C(x_{j+1},t_n) - C(x_j,t_n)}{h} + \\ &D\left[\frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{k=0}^{j} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} C(x_{j-k+1}, t_{n-1}) + \frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{k=0}^{n-j} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} C(x_{n-k}, t_{n-1})\right] \end{aligned} \tag{9}$$

explicit difference schemes:

$$\begin{aligned} &\frac{\tau^{1-\gamma}}{\Gamma(2-\gamma)} \frac{C(x_j,t_{n+1}) - C(x_j,t_n)}{\tau} + A = -v \frac{C(x_{j+1},t_n) - C(x_j,t_n)}{h} + \\ &D\left[\frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{k=0}^{j} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} C(x_{j-k+1}, t_{n-1}) + \frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{k=0}^{n-j} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} C(x_{n-k}, t_{n-1})\right] \end{aligned} \tag{10}$$

Numerical calculation example and discussion

This paper adopts an ideal test case done by Xia Yuan and Wu Jichun [6]. The case is calculated by different numerical calculation algorithms each with different parameters. Then the results are compared with each other. In one dimension space (0,100), an instantaneous point source of solute is set in x=50. The concentration of solute put in is 100 units, and in other points initial concentration are all 0. Time step length is 0.1. Focusing on dispersion, let advection term coefficient v=0, diffusion term coefficient D=0.8, in order to observe the phenomenon of anomalous diffusion better.

Comparison with traditional advection-dispersion equation

In the space-time correlative fractional advection-dispersion equation, we take γ=1, α=2. Then at x=45, get the comparison of numerical solutions with the ones of traditional advection – dispersion, which is showed in figure 1.

When γ=1, α=2, the numerical solutions of time-space correlative fractional advection -dispersion equation and traditional advection-dispersion equation are in complete agreement.

Comparison with rigorous time fractional advection-dispersion equation

For α=2, γ=0.6, 0.8, we first get the numerical solutions of time-space fractional advection-dispersion equation using the same ideal example. Then compare the numerical solutions with the numerical results of rigorous time fractional equation (fig. 2). For saving the amount of calculation, only the first 3000 time steps are adopted.

Figure. 2 displays the results for α=2, as it can be seen that the variation law of anomalous diffusion caused by changing γ are the same, while the corresponding numerical solutions are in full accordance, of either time-space fractional advection-dispersion equation or rigorous time fractional advection-dispersion equation.

Comparison with rigorous space fractional advection-dispersion equation

With γ=1, α=1.2, 1.6, get the numerical solutions of time-space correlative fractional advection-dispersion equation respectively. Then compare it with the results of rigorous space fractional advection-dispersion equation for α=1.2, 1.6, as shown in figure. 3.

As shown in Figure. 3, the variation law of anomalous diffusion caused by changing α are also the same, while the corresponding numerical solutions are in full accordance, of either time-space fractional advection-dispersion equation or rigorous space fractional advection-dispersion equation.

Computation example

Data sources used for computation came from references [12]. In this labora-

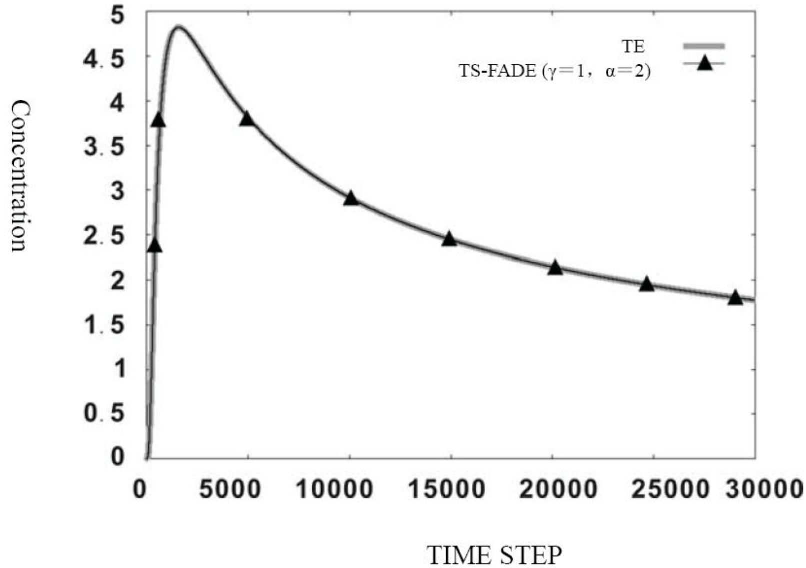

Figure 1: The comparison of breakthrough curve of time-space fractional advection-dispersion (TS-FADE) equation with the one of traditional equation (TE) at x=45, when γ=1, α=2.

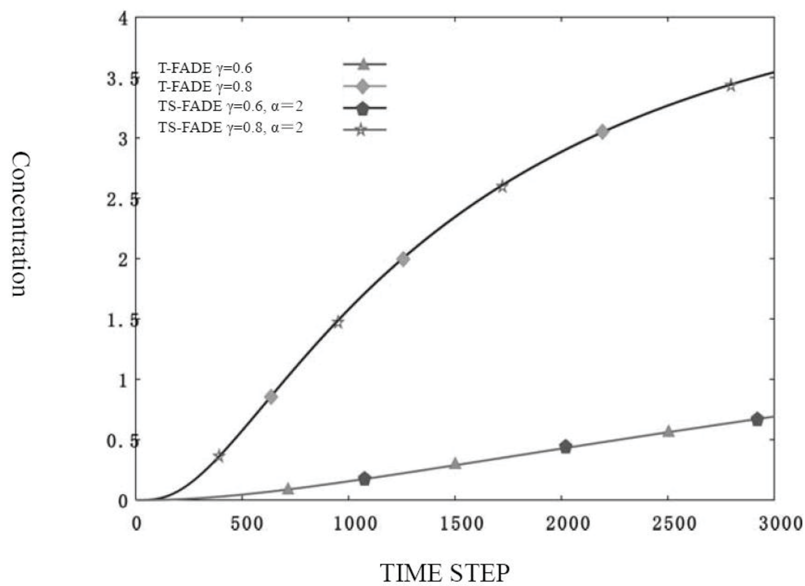

Figure 2: Comparison of numerical solutions of time-space fractional advection-dispersion equation (TS-FADE) at different values of γ with rigorous time advection-dispersion fractional equation (T-FADE), when α=2.

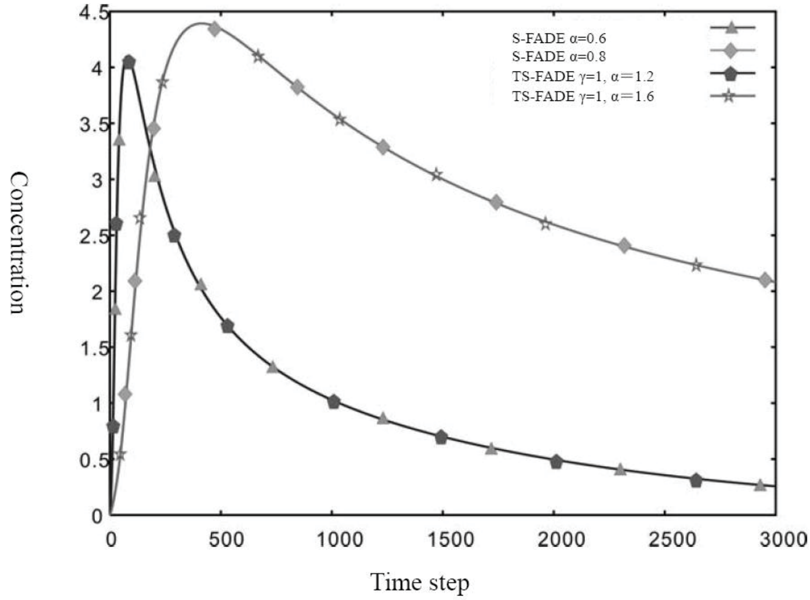

Figure 3: Comparison of numerical solutions of time-space fractional advection-space equation with different α with rigorous space fractional advection-space equation (S-FADE), when γ=1.

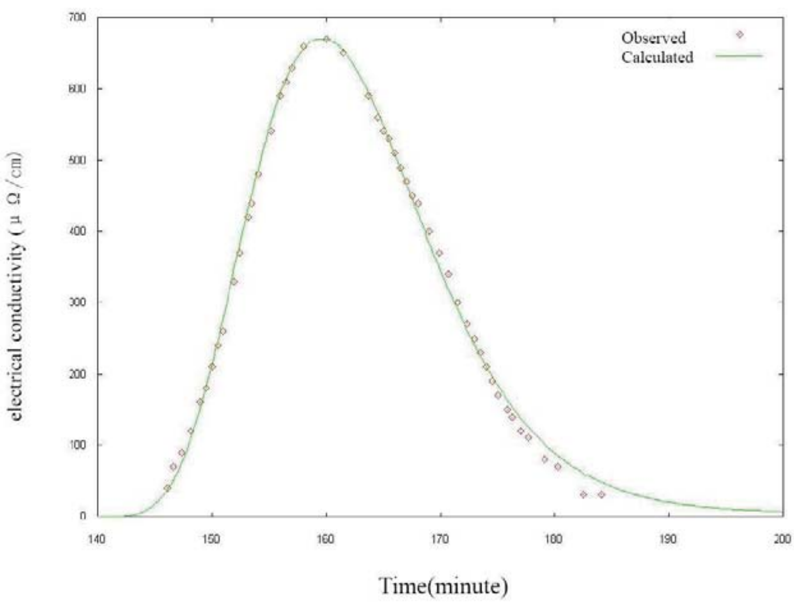

Figure 4: Measured data changed with time and the fitting curve.

tory dispersion experiment, a tracer (NaCl) was first put instantaneously, then the change of electrical conductivity of an observation point was measured, which was 80cm away from the injecting well. The concentration was approximately proportional to the conductivity, and could be directly obtained via multiplying the corresponding electrical conductivity by a coefficient. Using our method, the fitting results were: α=1.76, γ=0.993, D=0.033, v=0.48. The fitting results show in figure. 4.

As it is seen from figure. 4, there are two differences between the fractional stable distribution and the Gaussian distribution. The first difference lies in the body part, of which the measured points' distribution is asymmetric, so it has positive skewness. However, as a normal distribution, the Gaussian distribution is symmetrical. The Gaussian distribution includes two parameters, of which μ used to denote the center point or the location of mean value, while the variance describes discrete degree around the mean value. This is to say, lacking parameters used to describe skewness, the Gaussian distribution cannot be applied to skewed distribution, while the fractional stable distribution has four parameters, among which α could describe the deviation from normality.

The second difference is that tailing phenomenon was observed at the tail of the decline curve. Because of little measured data at the tail from references, the phenomenon in figure 4 was not obvious. However, references [12] to the tailing phenomenon, point out that the Gaussian distribution cannot explain this phenomenon. But the fractional stable distribution has this characteristic, and satisfies the phenomenon well.

Conclusion

1. By comparing the results of different numerical algorithms on the ideal test case, it can be proven that the numerical solution algorithm of time-space fractional advection-dispersion equations put forward in this paper is compatible with rigorous time fractional advection-dispersion equations and rigorous space fractional advection-dispersion equations. That is when γ=1 or α=2, the numerical calculation result of the time-space fractional advection-dispersion equations is absolutely in accordance with that of the rigorous time fractional advection-dispersion equation or the rigorous space fractional advection-dispersion equation.
2. By numerical calculation of time-space fractional advection-dispersion equations with different parameters, it can be shown that when the value of time fraction order γ is increasingly smaller, time relativity is increasingly stronger, the solute diffuses more slowly, and the breakthrough curve becomes smoother; when the value of space fraction order α is increasingly smaller, space relativity is increasingly stronger, the solute diffuses faster, and the breakthrough

curve becomes more abrupt. The variation law of the calculation result with parameters is also similar to that of the rigorous time fractional advection-dispersion equation or the rigorous space fractional advection-dispersion equation, and the result is also in accordance with the analytic solution.

3. By the numerical calculation simulation of practical testing results, the time-space fractional advection-dispersion equation can simulate the skewness and the tail of the breakthrough curve, which is not available with traditional advection-dispersion equations. This means time-space fractional advection-dispersion equation is in accordance with the law of anomalous diffusion. It can be used as a control equation of solute transport simulation, and reflect solute transport phenomenon more accurately.

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