Lattice Boltzmann method for fractional advection-diffusion equation

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Abstract

Mass transport such as movement of phosphorus in soils and solutes in rivers is a natural phenomenon and its study plays an important role in science and engineering. It is found that there are numerous practical diffusion phenomena that do not obey the classical advection-diffusion equation (ADE). Such diffusion is called abnormal or super diffusion and is well described using a fractional advection-diffusion equation (FADE). The FADE finds a wide range of applications in various areas with great potential for studying complex mass transport in real hydrological systems. However, solution to the FADE is difficult and the existing numerical methods are complicated and inefficient. In this study, a fresh lattice Boltzmann method is developed for solving the fractional advection-diffusion equation (LabFADE). For the first time the FADE is transformed into an equation similar to an advection-diffusion equation and solved using the lattice Botlzmann method. The LabFADE has all the advantages of the conventional lattice Boltzmann method and avoids a complex solution procedure, unlike other existing numerical methods. The method has been validated through simulations of several benchmark tests: a point source diffusion, a boundary value problem of steady diffusion, and an initial-boundary value problem of unsteady diffusion with the coexistence of source and sink terms. In addition, by including the effects of the skewness β, the fractional order α and the single relaxation time τ, the accuracy and convergence of the method have been assessed. The numerical predictions are compared with the analytical solutions and indicate that the method is 2^{nd} order accurate. The new method will allow the FADE to be more widely applied to complex mass transport problems in science and engineering.

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I. INTRODUCTION

Understanding and studying mass transport play an essential role in science and engineering. For example, the transport and fate of sediments and solutes in flowing waters are critically important for unravelling the impacts of land-based pollutants on downstream water quality and ecological status against a background of future climate and land use change [1]. Such mass transport is often caused by advection arising from flow velocity and diffusion from non-uniform distribution of the mass, or hydrodynamic dispersion from heterogeneous flow characteristics. The phenomenon often becomes complicated under complex flows within an arbitrary geometry in practical applications. Conventionally it is described using a standard advection-diffusion equation (ADE), which is a spatially explicit second-order partial differential equation [2]. The ADE is extensively studied using different solution methods including the lattice Boltzmann method and applied in various areas of science and engineering. Solutions to the ADE can predict the spreading of contaminants in homogeneous porous media [3, 4], drug injection in the treatment of diseases [5], the biochemical reactions during blood coagulation [6], the evolution of a phytoplankton species [7], and solute transport in water flows [8], leading to good understanding and control of the phenomenon.

In recent years it has been observed that many transport phenomena in nature, such as mass transport in groundwater and stream waters do not follow the ADE. This has been confirmed in both field studies and experimental investigations [9–12], and the ADE can produce results with large errors. The main reason is that mass transport seldom occurs uniformly in heterogeneous media, such as soil and sediment, but often exhibits a skewed distribution with a heavy tail in the concentration compared to that produced from the ADE. This phenomenon is recognised as super or abnormal diffusion and investigated using various methods including (a) fractional Brownian motion [13], (b) generalised diffusion equations [14], (c) continuous time random walk models [15], and (d) the aggregated dead zone model [16, 17]. The research shows that one successful general approach is the continuous time random walk (CTRW), which is demonstrated as a very good model for mass transport in real complicated systems [18–21]. In particular, the CTRW model reduces to a fractional advection-dispersion equation (FADE) and becomes a Lèvy motion when the jump length is approximated as a Lèvy flight [9, 22]. The FADE contains the non-local fractional Laplacian operator unlike the local Laplacian in the ADE and is proposed to model non-local diffusion [23]. Although such non-local behaviour may not be suitable for all abnormal diffusion, it has been demonstrated that the FADE is a successful model for many situations of abnormal diffusion in mass transport and its study attracts much interest in various fields of science and engineering. Caffarelli and Silvestre [24] introduce an important dimensional reduction technique for the fractional Laplacian and provide an analytical method for many problems. Saichev and Zaslavsky [25] discuss the fractional operators in theory. Solving the FADE greatly improves predictions of mass transport in real systems [9, 12, 26]. However, for general mass transport there is no direct analytical solution to the FADE like that to the ADE except for a simple case such as a diffusion/dispersion of a one-dimensional (1D) point source. Instead, its solution can only be obtained by using a numerical method. Furthermore, as a fractional order of derivative is involved, there exists a great difficulty to develop a simple and efficient numerical method to solve the FADE. The available solution methods often contain complex procedures and are inefficient in applications to general mass transport problems in practice, e.g., the numerical methods presented by Diethelm et al. [27], the finite-volume method described by Zhang et al. [26], and the characteristic difference method by Shen et al. [28].

On the other hand, the lattice Boltzmann method (LBM) has been shown to be a very successful alternative numerical method in computational fluid dynamics for capturing complex flows, such as those through porous media, which still challenges competing methods [29, 30]. Compared to conventional numerical methods, it involves only simple arithmetic calculations, efficiently handles complicated boundary conditions and is naturally amenable for parallel programming [31], which is crucial for modelling real-time large-scale mass transport under complex flows. Xia et al. recently developed a first LBM based on a multi-speed mode to solve the FADE [32]. However, the method is far more complicated than the standard lattice Boltzmann method, and loses the aforementioned advantages of the LBM over conventional numerical methods such as the finite-difference method.

In this paper, we develop an efficient lattice Boltzmann method to solve the fractional advection-diffusion equation (LabFADE). Firstly we rewrite the FADE in an expression similar to the standard advection-diffusion equation; then we formulate a simple lattice Boltzmann method to solve it; and finally we validate the proposed method through simulations and analyses of several benchmark tests including comparisons with analytical solutions, convergence order and model parameter effect on solutions.

II. FRACTIONAL ADVECTION-DIFFUSION EQUATION

In the present study, we consider the following fractional advection-diffusion equation with a source or sink term [9],

$$\frac{\partial C}{\partial t} + \frac{\partial (uC)}{\partial x} = D\left[\beta \frac{\partial^\alpha C}{\partial_+ x^\alpha} + (1-\beta)\frac{\partial^\alpha C}{\partial_- x^\alpha}\right] + S_c, \tag{1}$$

where C is the concentration and has SI dimension of $[ML^{-3}]$ in base dimensions of length [L], mass [M] and time [T]; t is time [T]; x is the Cartesian coordinate [L]; D is a fractional diffusion coefficient $[L^\alpha/T]$; u is the flow velocity $[LT^{-1}]$; S_c stands for a source or sink term $[ML^{-3}T^{-1}]$; α is a dimensionless constant and represents the order of fractional differentiation; and β is a dimensionless constant and defined as a skewness parameter. α takes a value in a range of $1 < \alpha \leq 2$ as founded in the existing researches [9–12]. β takes a value in a range of $0 \leq \beta \leq 1$; it is found in theory that $\beta > 0.5$ produces a solution that is skewed backward, while $\beta < 0.5$ produces a solution that is skewed forward. Eq. (1) reduces to the classical advection-diffusion equation when $\alpha = 2$ and $\beta = 0.5$.

If the reference dimensional concentration is C_0, time t_0, velocity u_0, and length x_0 together with bars over the original variables for their corresponding non-dimensional ones such as $\bar{C}$, after setting

$$C = C_0\bar{C}, \quad t = t_0\bar{t}, \quad u_j = u_0\bar{u}_j, \quad x = x_0\bar{x}, \quad D = \bar{D}x_0^\alpha/t_0, \tag{2}$$

Eq. (1) can be written in a non-dimensional equation as follows

$$\frac{\partial \bar{C}}{\partial \bar{t}} + \frac{\partial (\bar{u}\bar{C})}{\partial \bar{x}} = \bar{D}\left[\beta \frac{\partial^\alpha \bar{C}}{\partial_+ \bar{x}^\alpha} + (1-\beta)\frac{\partial^\alpha \bar{C}}{\partial_- \bar{x}^\alpha}\right] + \bar{S}_c, \tag{3}$$

on condition that $x_0 = u_0 t_0$. In the above equation, $\bar{S}_c = S_c t_0/C_0$ and the reciprocal of $\bar{D}$ may be defined as the Peclet number for fractional diffusion, i.e.

$$P_{ei} = \frac{1}{\bar{D}} = \frac{u_0 x_0^{\alpha-1}}{D}. \tag{4}$$

If all the overbars are dropped in Eq. (3), it will become identical to Eq. (1). For convenient presentation they are dropped in the rest of the paper.

In the present study, we adopt the Riemann-Liouville definition [26, 33] for the left and right fractional derivatives as

$$\frac{\partial^\alpha C}{\partial_+ x^\alpha} = \frac{1}{\Gamma(m-\alpha)}\frac{\partial^m}{\partial x^m}\int_0^x \frac{C(\xi,t)}{(x-\xi)^{(\alpha-m+1)}}d\xi, \tag{5}$$

and

$$\frac{\partial^\alpha C}{\partial_- x^\alpha} = \frac{(-1)^m}{\Gamma(m-\alpha)}\frac{\partial^m}{\partial x^m}\int_x^L \frac{C(\xi,t)}{(\xi-x)^{(\alpha-m+1)}}d\xi, \tag{6}$$

where m is the smallest integer greater than α; Γ is the gamma function; and L is the length of the domain under consideration. In Eq. (3), $1 < \alpha \leq 2$, which gives $m = 2$, and the above definitions become

$$\frac{\partial^\alpha C}{\partial_+ x^\alpha} = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_0^x \frac{C(\xi,t)}{(x-\xi)^{(\alpha-2+1)}}d\xi, \tag{7}$$

and

$$\frac{\partial^\alpha C}{\partial_- x^\alpha} = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_x^L \frac{C(\xi,t)}{(\xi-x)^{(\alpha-2+1)}}d\xi. \tag{8}$$

Let Z^+ and Z^- stand for the integrals in Eqs. (7) and (8), respectively,

$$Z^+ = \int_0^x \frac{C(\xi,t)}{(x-\xi)^{(\alpha-2+1)}}d\xi, \tag{9}$$

and

$$Z^- = \int_x^L \frac{C(\xi,t)}{(\xi-x)^{(\alpha-2+1)}}d\xi. \tag{10}$$

Substitution of Eqs. (7) - (10) into Eq. (3) leads to

$$\frac{\partial C}{\partial t} + \frac{\partial(uC)}{\partial x} = \frac{D}{\Gamma(2-\alpha)}\frac{\partial^2 Z}{\partial x^2} + S_c, \tag{11}$$

in analogy to an ordinary advection-diffusion equation, where

$$Z = \left[\beta Z^+ + (1-\beta)Z^-\right]. \tag{12}$$

III. LATTICE BOLTZMANN METHOD

The fractional advection-diffusion equation (11) is simulated by using the following lattice Boltzmann equation,

$$f_\theta(x + e_\theta \Delta t, t + \Delta t) = f_\theta - \frac{1}{\tau}(f_\theta - f_\theta^{eq}) + \frac{S_c}{b}\Delta t, \tag{13}$$

where f_θ is the particle distribution function; τ is the single relaxation time; Δt is the time step; b is the lattice link number; and e_θ is the particle velocity vector of particle θ and defined as $e_0 = 0$ for $\theta = 0$ or the still particle, $e_\theta = e$ for $\theta = 1$, and $e_\theta = -e$ for $\theta = 2$, which gives $b = 3$, where $e = \Delta x/\Delta t$ and Δx is the lattice size.

We define the following local equilibrium distribution function,

$$f_\theta^{eq} = \begin{cases} C - \lambda Z, & \theta = 0, \\ \frac{1}{2}\lambda Z + \frac{e_\theta u}{2e^2} C, & \theta = 1, \ \& \ 2, \end{cases} \tag{14}$$

where

$$\lambda = \frac{D}{\Delta t(\tau - 1/2)e^2\Gamma(2-\alpha)}, \ \ \alpha = 1, \ \& \ 2. \tag{15}$$

It can be shown that Eq. (14) has the properties,

$$\sum_\theta f_\theta^{eq} = C, \tag{16}$$

$$\sum_\theta e_\theta f_\theta^{eq} = uC, \tag{17}$$

and

$$\sum_\theta e_\theta e_\theta f_\theta^{eq} = \lambda e^2 Z. \tag{18}$$

The concentration C is calculated from

$$C = \sum_\theta f_\theta. \tag{19}$$

Z^+ and Z^- defined in Eqs. (9) and (10) are two definite integrals. In numerical calculations, the former at lattice point x_i is the integration from Point x_1 to x_i and the latter at lattice point x_i is the integration from Point x_i to x_N, where N is the total lattice number covering the domain length L. Consequently, they can be evaluated respectively as

$$\begin{aligned} Z^+ =& \int_0^{x_i} \frac{C(\xi, t)}{(x_i - \xi)^{(\alpha-1)}} d\xi \\ =& \sum_{j=1}^{j=i} C(x_j, t) \frac{(x_i - x_j)^{(2-\alpha)} - (x_i - x_{j+1})^{(2-\alpha)}}{(2-\alpha)}, \end{aligned} \tag{20}$$

and

$$\begin{aligned} Z^- =& \int_{x_i}^{L} \frac{C(\xi, t)}{(\xi - x_i)^{(\alpha-1)}} d\xi \\ =& \sum_{j=i}^{j=N} C(x_j, t) \frac{(x_{j+1} - x_i)^{(2-\alpha)} - (x_j - x_i)^{(2-\alpha)}}{(2-\alpha)}. \end{aligned} \tag{21}$$

Through the Chapman-Enskog Ansatz, it can be shown that the described lattice Boltzmann model can correctly simulate the FADE. The complete recovery of the FADE from the lattice Boltzmann equation (13) is given in the appendix.

IV. SOLUTION PROCEDURE

The solution procedure may be summarised as:

1. Give an initial concentration C,
2. Determine Z^+ and Z^- from Eqs. (20) and (21),
3. Calculate f_θ^{eq} from Eq. (14),
4. Compute f_θ via the lattice Boltzmann equation (13),
5. Update the concentration C according to Eq. (19),
6. Repeat Steps (2) - (5) until a solution is obtained.

The boundary condition for 1D FADE is straightforward. If the concentration is given at an inflow boundary, the only unknown distribution function f_1 is determined using $f_1 = C - f_0 - f_2$; if the concentration gradient is known, the concentration at the inflow boundary can be calculated using an interpolation method and then f_1 is calculated as $f_1 = C - f_0 - f_2$. The outflow boundary condition can be treated similarly.

V. VERIFICATION

In order to verify the new lattice Boltzmann method for the fractional advection-diffusion equation (LabFADE), a number of benchmark tests are simulated and presented. This includes a point source release, steady and unsteady diffusion from a combination of source and sink terms. In addition, the effect of the skewness β, the fractional order α and the single relaxation time τ on solutions as well as convergence order, and accuracy are analysed. All the calculations are carried out on a PC with Intel i5 CPU and 4GB RAM, and take about 8 minutes or less.

A. Point source

Firstly, a 1D point source is considered. A unit point source is released at $x = 500$ cm initially. The FADE is solved with $\alpha = 1.7$ and $\beta = 0.5$, which is the same test problem as

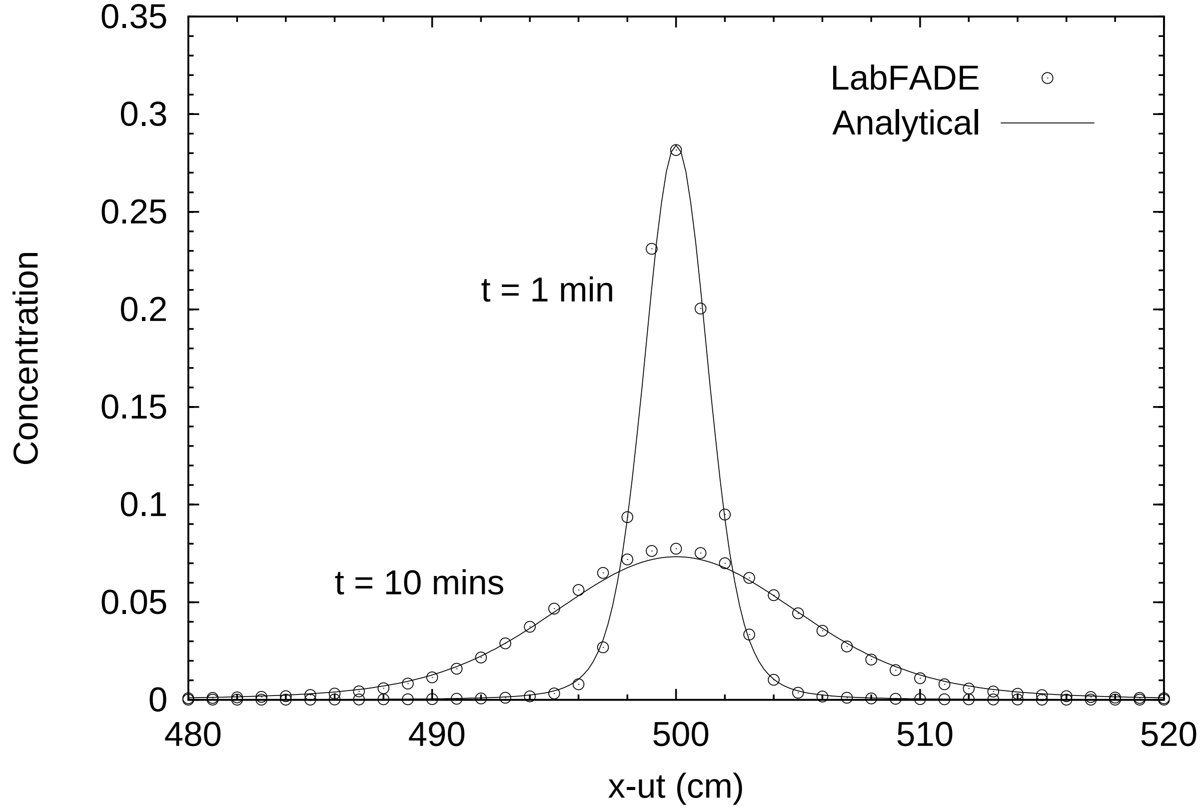

FIG. 1: Comparison of the present numerical results at times $t = 1$ minute and $t = 10$ minutes with the analytical solutions for a unit point source released at $x = 500\ cm$ initially ($\alpha = 1.7$, $\beta = 0.5$, $D = 1\ cm^{1.7}/min$ and $u = 1\ cm/min$).

that used by Zhang et al. using a finite-volume method [26]. In the numerical simulation, $D = 1\ cm^{1.7}/min$ and $u = 1\ cm/min$ together with $\Delta x = 1\ cm$ and $\Delta t = 0.1\ min$. The point source is specified at one lattice point, which is located at $x = 500\ cm$. In theory, the analytical solution to the normal advection-diffusion equation, i.e., $\alpha = 2$ and $\beta = 0.5$, is the Gaussian distribution, and the analytical solution to the fractional advection-diffusion equation (3) is the α-stable distribution [9]. Such an α-stable distribution can be obtained using the numerical procedure and the software described by Nolan [34], which is used to compare with the present numerical solutions in Fig. 1 and shows good agreement. We also simulate this problem using $\beta = 1.0$, which again generates numerical results skewed backward in good agreement with the corresponding analytical solution in Fig. 2.

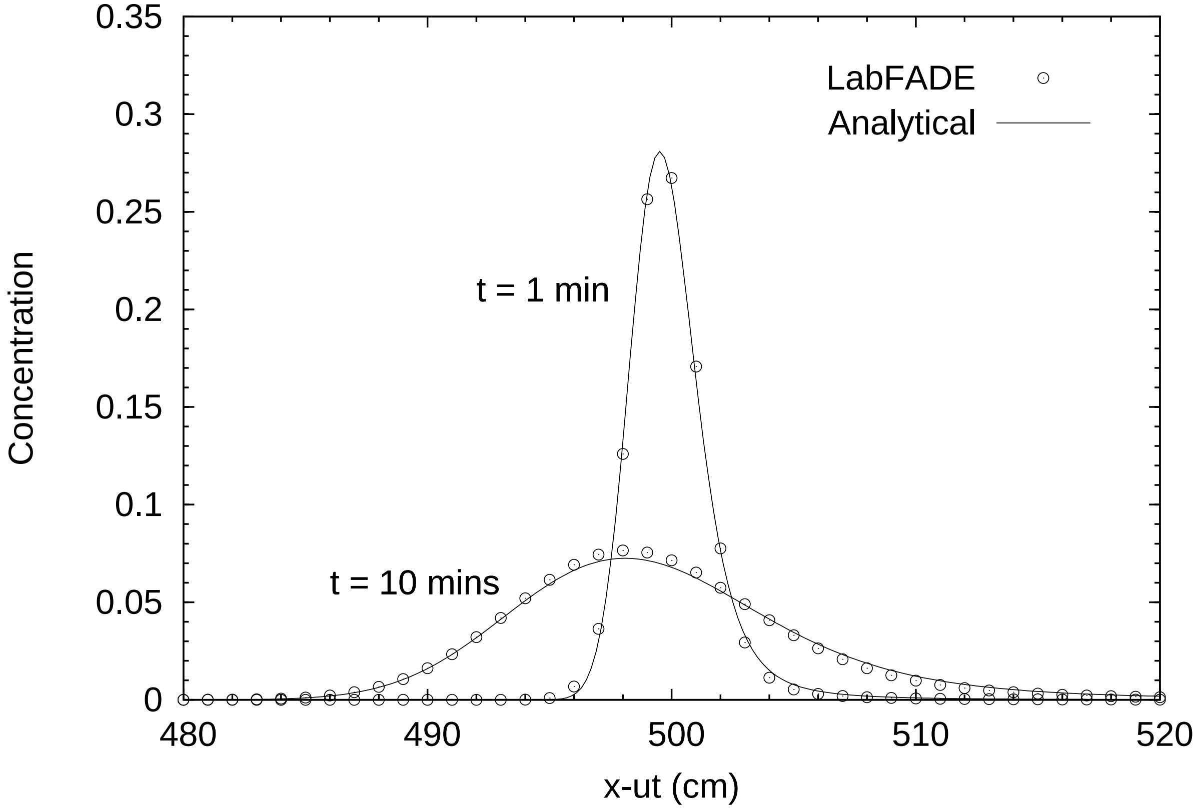

FIG. 2: Comparison of the present skewed numerical results at times $t = 1$ minute and $t = 10$ minutes with the analytical solutions for a unit point source released at $x = 500$ cm initially ($\alpha = 1.7$, $\beta = 1.0$, $D = 1$ $cm^{1.7}/min$ and $u = 1$ cm/min).

B. Effect of skewness parameter β

The second benchmark test is run to show the effect of the skewness parameter β on the solution to the transport of a unit point source. Three values of 0, 0.5 and 1 are used for β with $\alpha = 1.6$. $D = 1$ $cm^{1.6}/min$, and the other parameters remain the same as those used in the first test. The numerical results at time $t = 20$ min are shown in Fig. 3, revealing the clear effect of the skewness factor β on the solutions, i.e., fractional advection-diffusion equation predicts faster spreading of the source or a long tail when $\beta < 0.5$, or slower spreading when $\beta > 0.5$ compared to the result by the classic advection-diffusion equation. This is consistent with the results reported in the literature [26].

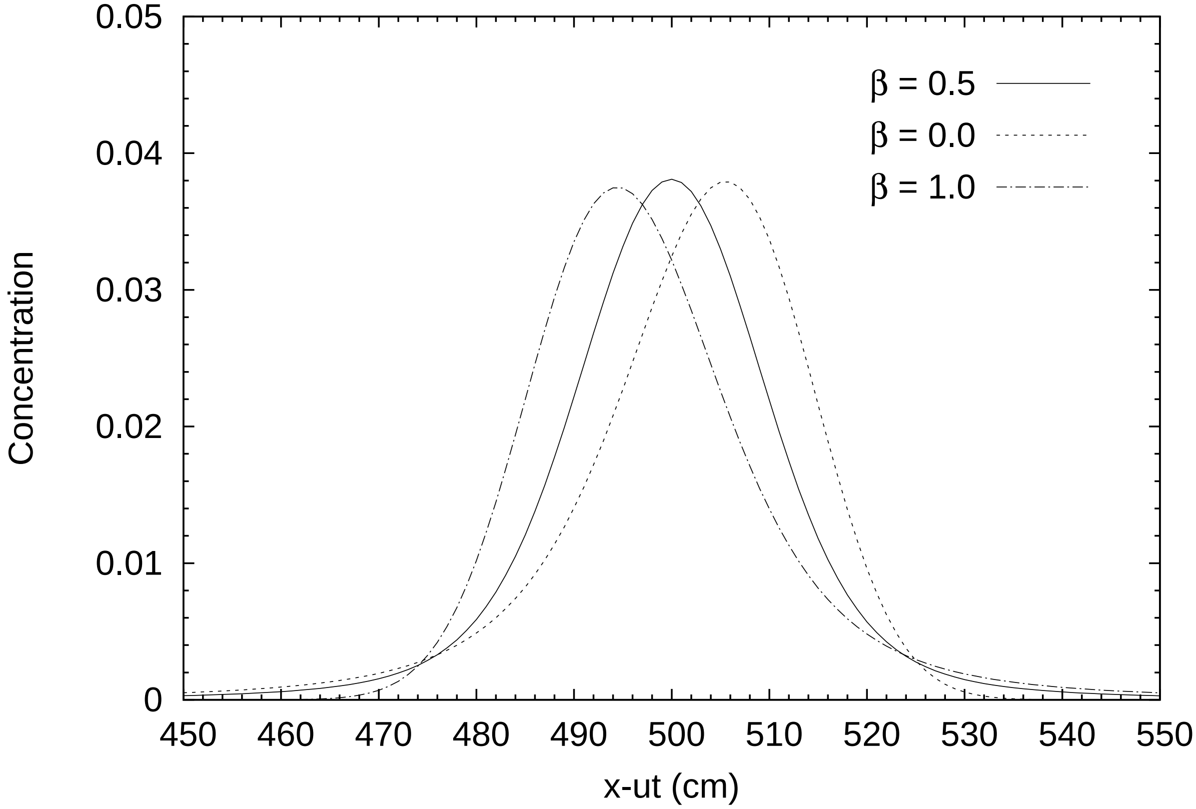

FIG. 3: Effect of skewness parameter β on numerical solutions, showing forward skewness of $\beta = 0$ and backward skewness of $\beta = 1$ as well as the normal case without skewness of $\beta = 0.5$ at time $t = 20$ minutes ($\alpha = 1.6$ and $D = 1\ cm^{1.6}/min$).

C. Effect of fractional order α

In the third benchmark test, the effect of the fractional order α on the solution to a unit point source is carried out. The parameters used in the simulations are $\beta = 0$, $D = 1\ cm^{\alpha}/min$, $\Delta x = 1.0\ cm$, $\Delta t = 1.0\ min$ and $u = 0$, and the domain size is [0, 400 cm]. The simulations are run with three different α values, i.e., $\alpha = 1.4,\ 1.6$, and 1.8. The solutions at time $t = 400\ min$ are shown in Fig. 4, which demonstrates that the smaller the α value, the faster the concentration of the point source diffuses downstream. The figure also includes the result from usual diffusion of $\alpha = 2$, making strong contrast with the fractional diffusion. Figure 5 shows the concentration profiles at different times for $\alpha = 1.4$. All these results are in excellent agreement with those reported by Zhang et. al. [26], suggesting that the proposed method is accurate for the prediction of mass transport described by the FADE.

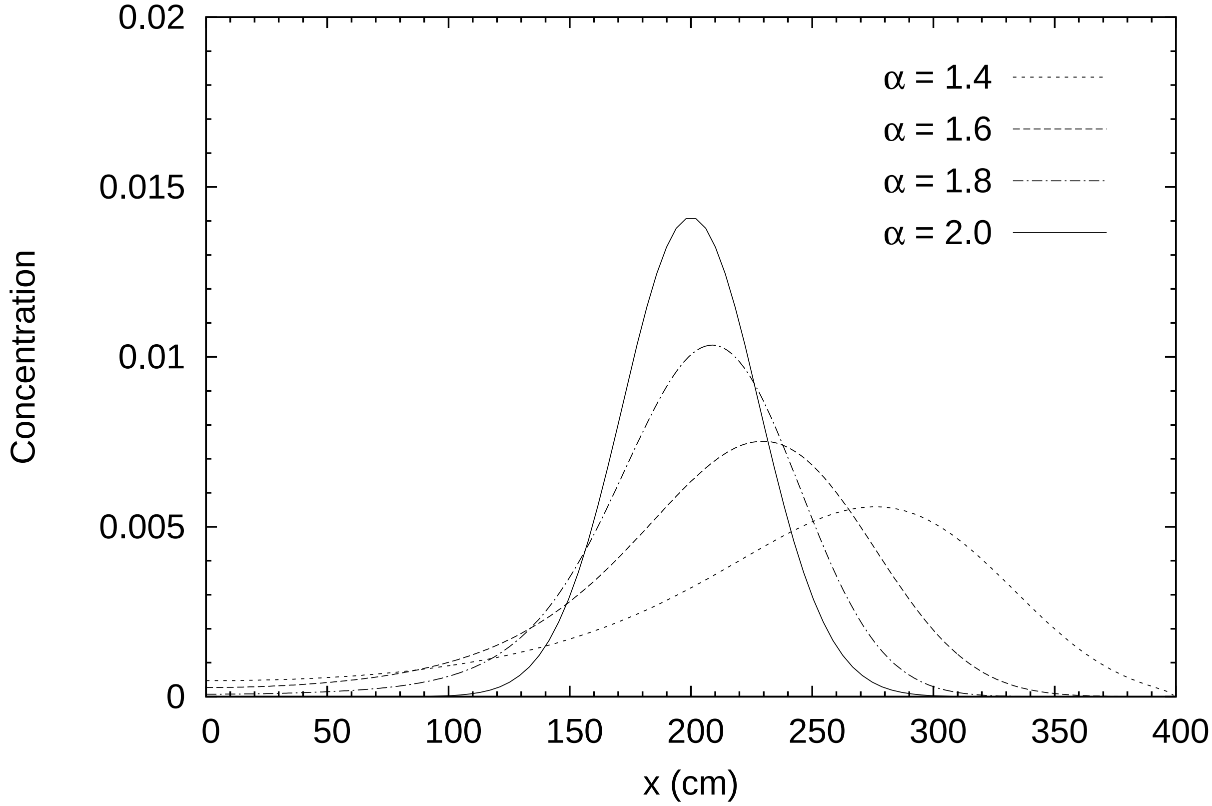

FIG. 4: Effect of the order of fractional differentiation α on the spreading of a point source at time $t = 400$ minutes, indicating faster diffusion downstream for smaller values of α ($\beta = 0$, $D = 1\ cm^{\alpha}/min$, and $u = 0\ cm/min$).

D. Steady diffusion with a source/sink term

The fourth problem is described by the following steady fractional diffusion equation,

$$\begin{cases} D(x)\frac{\partial^{\alpha} C}{\partial_{+} x^{\alpha}} + D(x)\frac{\partial^{\alpha} C}{\partial_{-} x^{\alpha}} + S_c(x) = 0, \quad 0 < x < 2, \\ C(0) = 0, \quad C(2) = 0, \end{cases} \tag{22}$$

where $\alpha = 1.8$, $D(x) = \Gamma(1.2)$, and S_c is the source and sink term given by

$$S_c(x) = -8\left[(x^{0.2} + (2-x)^{0.2}) - \frac{5}{2}(x^{1.2} + (2-x)^{1.2}) + \frac{25}{22}(x^{2.2} + (2-x)^{2.2})\right]. \tag{23}$$

This is a boundary value problem of a steady-state fractional diffusion and is used by Wang and Nu for verification of a fractional finite-difference method [35]. It has an analytical solution of

$$C(x) = x^2(2-x)^2. \tag{24}$$

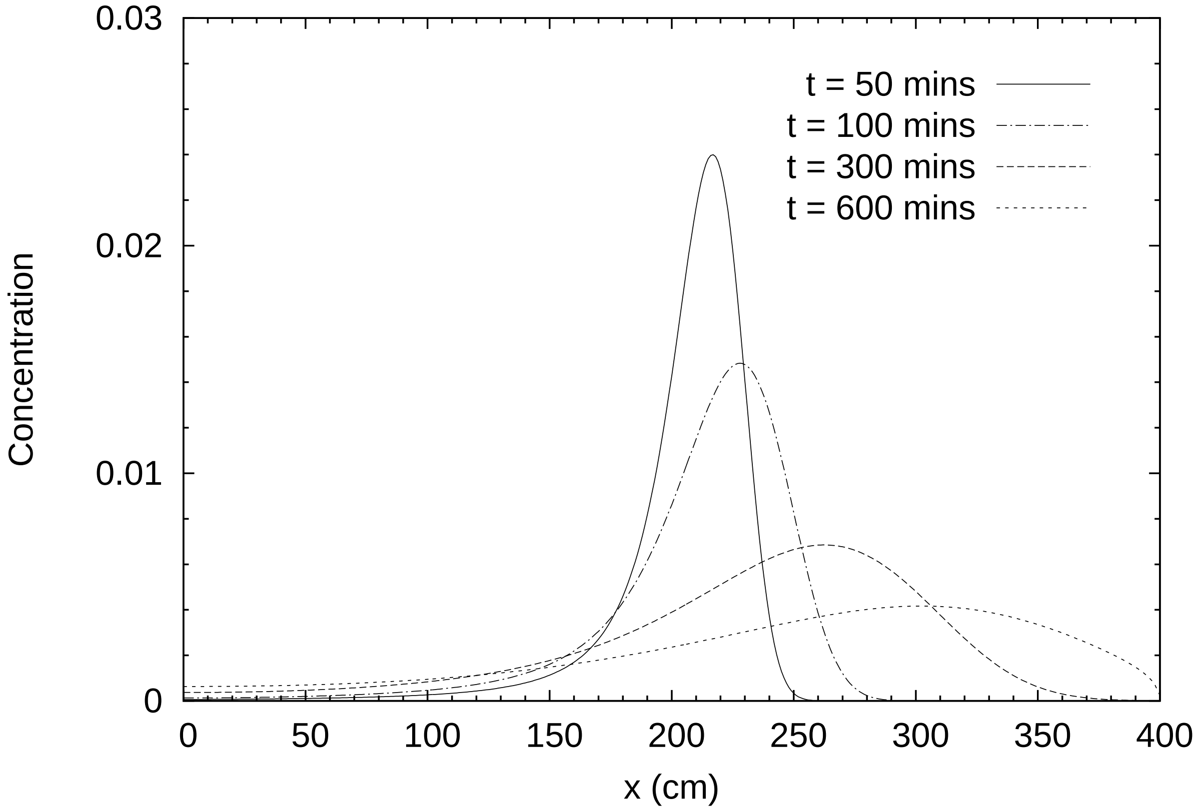

FIG. 5: Spreading of a point source with time depicted with results at times $t = 50$, 100, 300 and 600 minutes for $\alpha = 1.4$, $\beta = 0$, $D = 1\ cm^{1.4}/min$, and $u = 0\ cm/min$.

In the simulation, 200 lattices were used with $\Delta x = 0.01$, $\Delta t = 6.67 \times 10^{-5}$, $\beta = 0.5$ and $D = 2D(x)$. After the 30000^{th} iterations, the steady solution is obtained and the results are compared with the analytical solution in Fig. 6, showing good agreement.

E. Accuracy and convergence

In order to assess the accuracy and convergence of the presented scheme, the boundary value problem described in Section V D has been investigated using 25, 50, 100 and 200 lattices. The relative error is defined as

$$E_r = \frac{1}{N}\sqrt{\sum \left(\frac{C_n - C_a}{C_a}\right)^2}, \tag{25}$$

where C_n and C_a stand for the numerical result and the analytical solution, respectively, and N is the total number of the lattice points. The errors E_r for the results using the various

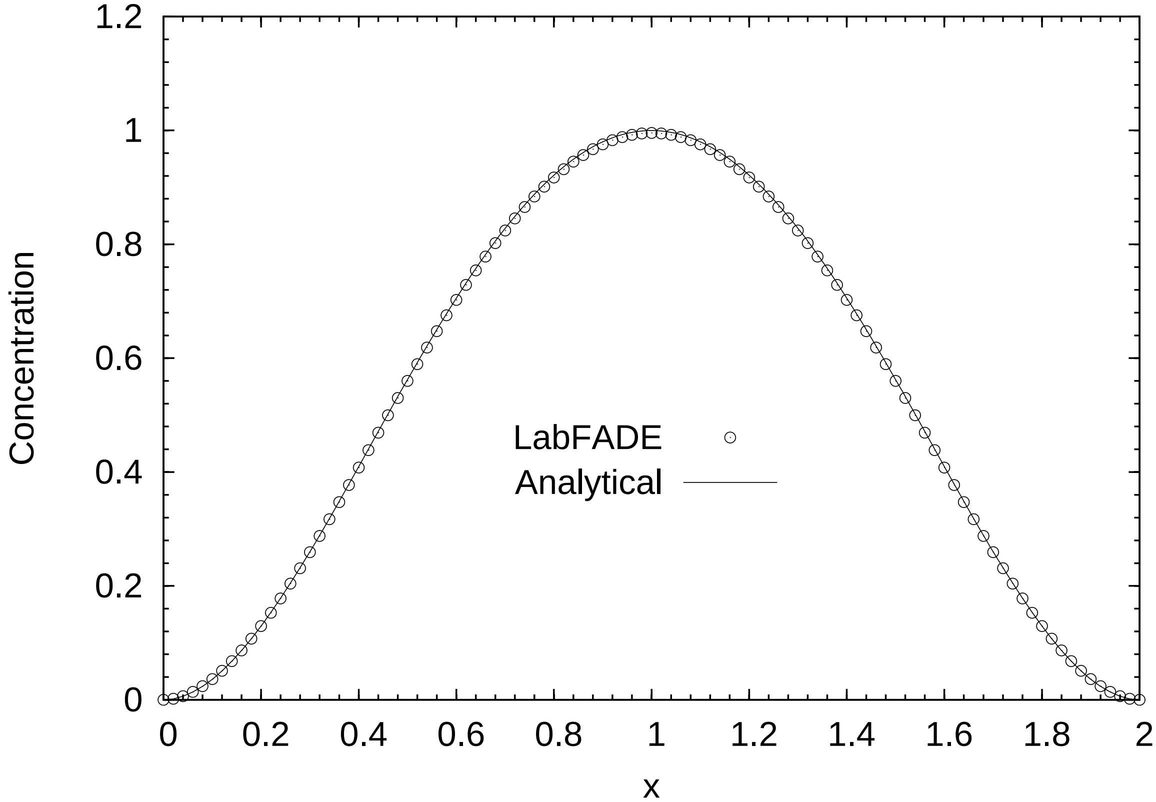

FIG. 6: Comparison of numerical solution with the analytical solution for the steady diffusion with the source term $S_c \neq 0$ and $\alpha = 1.8$, $\beta = 0.5$, $D = 2\Gamma(1.2)$, and $u = 0$.

lattices are listed in Table I and also plotted against the relative lattice size or Knudsen number $k_n = \Delta x/L$ ($L = 2$) in Fig. 7, showing that the proposed model has good accuracy; as seen from the figure, a trendline is best fitted through the points, suggesting that the model is second-order accurate consistent with lattice Boltzmann dynamics although the power of the trendline is 1.86 and slightly smaller than 2 due to the effect of using the first-order accurate boundary conditions.

TABLE I: Relative errors for various lattice sizes and numbers.

Lattice Size, Δx	0.08	0.04	0.02	0.01
Lattice number, N	25	50	100	200
Relative Error, E_r	1.35×10^{-2}	9.37×10^{-3}	9.60×10^{-4}	3.95×10^{-4}

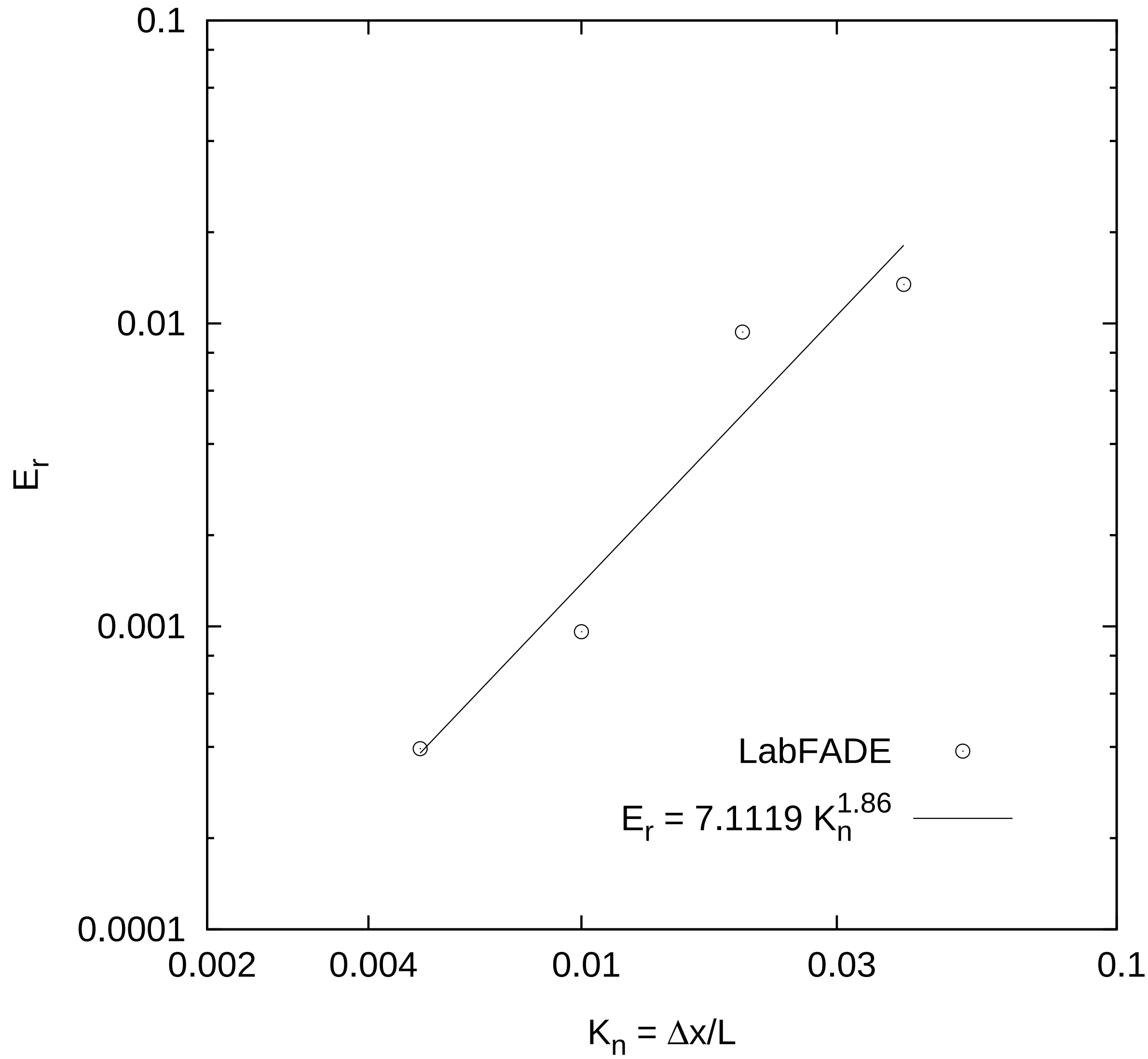

FIG. 7: Relative errors against lattice sizes for steady fractional diffusion phenomenon with the source term $S_c \neq 0$ and $\alpha = 1.8$, $\beta = 0.5$, $D = 2\Gamma(1.2)$, and $u = 0$.

F. Effect of single relaxation time τ

In order to study the effect of the single relaxation time τ on the method, the above steady fractional diffusion problem is simulated using values of 0.92, 0.95, 1.0, 1.3, 1.5 and 2.0 for the single relaxation τ. It is found that the model is stable with the use of these values but becomes unstable for a value less than 0.92. The stable numerical results are plotted in Fig 8, which shows that use of $0.92 \leq \tau \leq 1.5$ can provide accurate solutions to this test.

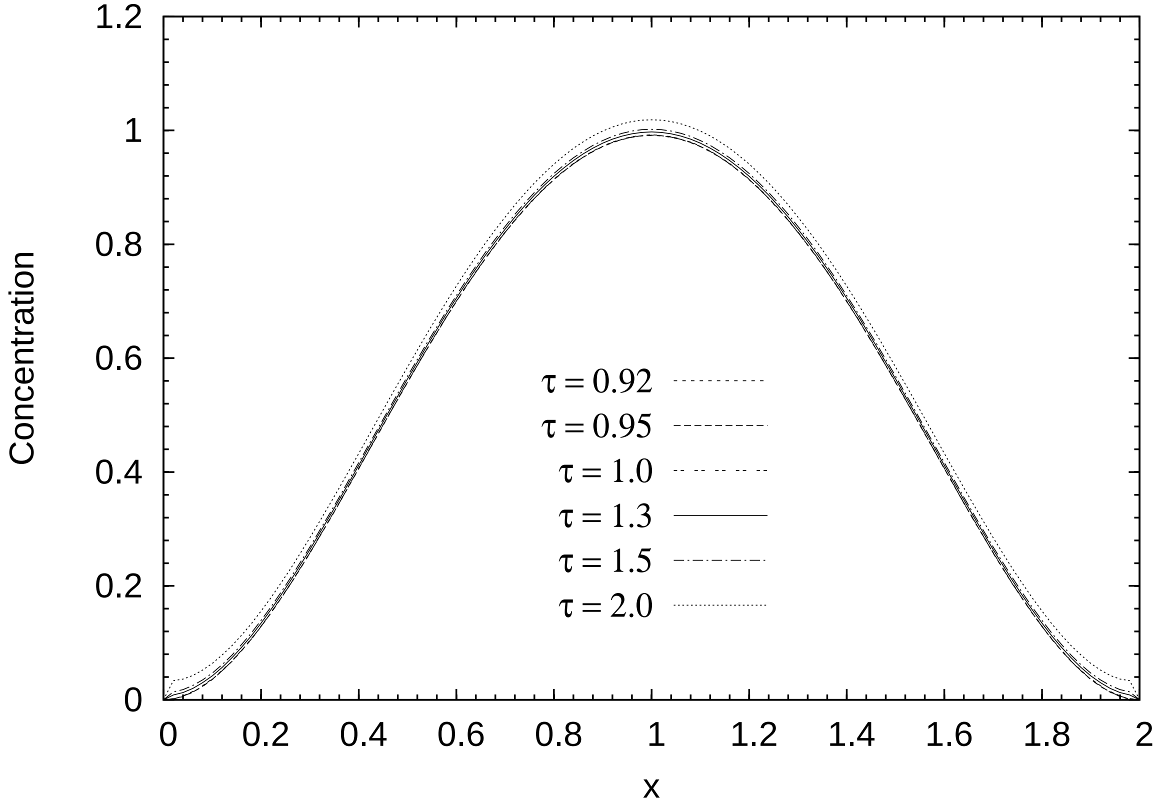

FIG. 8: Effect of the single relaxation time τ on solutions for steady fractional diffusion phenomenon with the source term $S_c \neq 0$ and $\alpha = 1.8$, $\beta = 0.5$, $D = 2\Gamma(1.2)$, and $u = 0$.

G. Unsteady diffusion with a source term

The final problem is described by the following unsteady fractional diffusion equation,

$$\begin{cases} \frac{\partial C}{\partial t} = D(x,t)\frac{\partial^\alpha C}{\partial_+ x^\alpha} + D(x,t)\frac{\partial^\alpha C}{\partial_- x^\alpha} + S_c(x), \quad 0 < x < 2, \; 0 < t \leq 1 \\ C(0,t) = 0, \quad C(2,t) = 0, \quad 0 \leq t \leq 1 \\ C(x,0) = x^2(2-x)^2, \quad a \leq x \leq 2, \end{cases} \tag{26}$$

where $\alpha = 1.8$, $D(x) = \Gamma(1.2)t$, and S_c is the source term given by

$$S_c(x) = -e^{-t}x^2(2-x)^2 - 8te^{-t}\left[(x^{0.2} + (2-x)^{0.2}) - \frac{5}{2}(x^{1.2} + (2-x)^{1.2}) + \frac{25}{22}(x^{2.2} + (2-x)^{2.2})\right]. \tag{27}$$

This is an initial-boundary value problem of an unsteady-state fractional diffusion and is used by Wang and Nu for verification of a fractional finite-difference method [35]. It also has an analytical solution of

$$C(x) = e^{-t}x^2(2-x)^2. \tag{28}$$

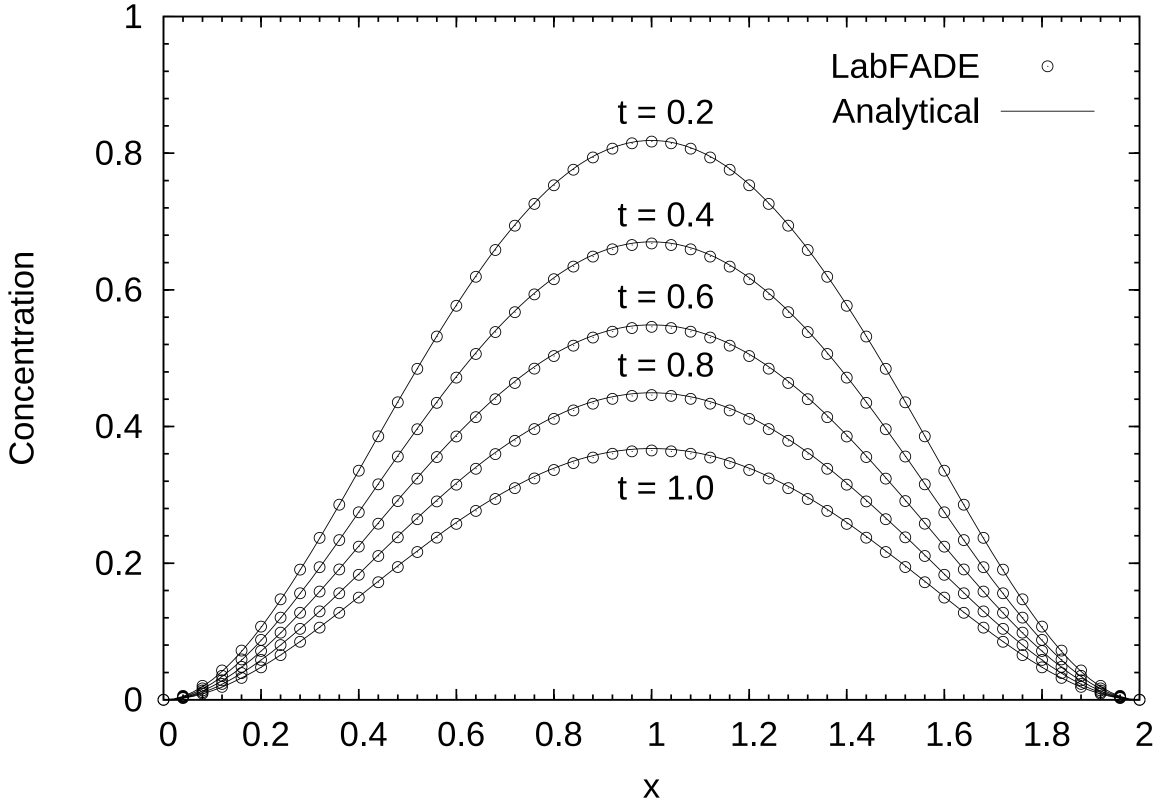

FIG. 9: Comparisons of numerical results with the analytical solutions for unsteady fractional diffusion phenomenon with the source term S_c and $\alpha = 1.8$, $\beta = 0.5$, $D = 2t\Gamma(1.2)$, and $u = 0$.

In the simulation, 100 lattices were used with $\Delta x = 0.02$, $\Delta t = 2 \times 10^{-4}$, $\beta = 0.5$ and $D = 2D(x)$. The numerical results at different times $t = 0.2,\ 0.4,\ 0.6,\ 0.8$, and 1.0 are shown in Fig. 9, and are further compared with the corresponding analytical solutions, demonstrating excellent agreements. This again confirms that the described scheme is able to produce accurate solutions to unsteady fractional diffusion phenomena with a complicated source or sink term.

VI. CONCLUSIONS

An efficient lattice Boltzmann method is proposed to solve the fractional advection-diffusion equation for prediction of complicated mass transport in practical hydrological systems (LabFADE). Use of a relaxation time in the range of $0.92 \leq \tau < 1.5$ can produce accurate solutions. The results have shown that the method is second-order accurate at similar accuracy to other more complicated numerical methods for solving the FADE. It retains the simplicity and advantages of the standard lattice Boltzmann method that has been developed for computational fluid dynamics. This enables the new method to be suitable for application of the FADE to a wide range of investigations into complex large-scale mass transport in hydrological sciences and environmental engineering.

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Appendix A: Recovery of the FADE

To prove that the concentration C calculated from Eq. (19) satisfies the fractional advection-diffusion equation (11), we apply the Chapman-Enskog analysis to the lattice Boltzmann equation (13). Assuming that Δt is small and

$$\Delta t = \varepsilon, \tag{A1}$$

substitution of Eq. (A1) into Eq. (13) yields

$$f_\theta(x + e_\theta \varepsilon, t + \varepsilon) - f_\theta(x, t) = -\frac{1}{\tau}(f_\theta - f_\theta^{eq}) + \frac{S_c}{b}\varepsilon. \tag{A2}$$

Taking a Taylor expansion to the left hand side of the above equation in time and space at a point (x, t) leads to

$$\varepsilon \left(\frac{\partial}{\partial t} + e_\theta \frac{\partial}{\partial x} \right) f_\theta \; + \; \frac{1}{2}\varepsilon^2 \left(\frac{\partial}{\partial t} + e_\theta \frac{\partial}{\partial x} \right)^2 f_\theta + \mathcal{O}(\varepsilon^3) = \frac{S_c}{b}\varepsilon - \frac{1}{\tau}(f_\theta - f_\theta^{eq}). \tag{A3}$$

Using the Chapman-Enskog Ansatz, f_θ can be expressed as,

$$f_\theta = f_\theta^{(0)} + \varepsilon f_\theta^{(1)} + \varepsilon^2 f_\theta^{(2)} + \mathcal{O}(\varepsilon^3). \tag{A4}$$

The centred scheme [36] is used for term S_c,

$$S_c = S_c \left(x + \frac{1}{2} e_\theta \varepsilon, t + \frac{1}{2}\varepsilon \right), \tag{A5}$$

which can also be written, via a Taylor expansion, as

$$S_c\left(x + \frac{1}{2}e_\theta\varepsilon, t+\frac{1}{2}\varepsilon\right) = S_c(x,t) + \frac{1}{2}\varepsilon\left(\frac{\partial}{\partial t}+e_\theta\frac{\partial}{\partial x}\right)S_c(x,t)+\mathcal{O}(\varepsilon^2). \tag{A6}$$

After inserting Eqs. (A4) and (A6) into Eq. (A3), the equation to order ε^0 is

$$f_\theta^{(0)} = f_\theta^{eq}, \tag{A7}$$

to order ε

$$\left(\frac{\partial}{\partial t}+e_\theta\frac{\partial}{\partial x}\right)f_\theta^{(0)} = \frac{S_c}{b}-\frac{f_\theta^{(1)}}{\tau}, \tag{A8}$$

and to order ε^2

$$\left(\frac{\partial}{\partial t}+e_\theta\frac{\partial}{\partial x}\right)f_\theta^{(1)} + \frac{1}{2}\left(\frac{\partial}{\partial t}+e_\theta\frac{\partial}{\partial x}\right)^2 f_\theta^{(0)} = \frac{1}{2}\left(\frac{\partial}{\partial t}+e_\theta\frac{\partial}{\partial x}\right)\frac{S_c}{b}-\frac{f_\theta^{(2)}}{\tau}. \tag{A9}$$

Substitution of Eq. (A8) into the above equation gives

$$\left(1-\frac{1}{2\tau}\right)\left(\frac{\partial}{\partial t}+e_\theta\frac{\partial}{\partial x}\right)f_\theta^{(1)} = -\frac{1}{\tau}f_\theta^{(2)}. \tag{A10}$$

Combining Eq. (A8) with ε times Eq. (A10), we obtain

$$\left(\frac{\partial}{\partial t}+e_\theta\frac{\partial}{\partial x}\right)f_\theta^{(0)} + \varepsilon\left(1-\frac{1}{2\tau}\right)\left(\frac{\partial}{\partial t}+e_\theta\frac{\partial}{\partial x}\right)f_\theta^{(1)} = \frac{S_c}{b}-\frac{1}{\tau}(f_\theta^{(1)}+\varepsilon f_\theta^{(2)}). \tag{A11}$$

Now, summing Eq. (A11) over θ provides

$$\frac{\partial}{\partial t}\sum_\theta f_\theta^{(0)} + \frac{\partial}{\partial x}\sum_\theta e_\theta f_\theta^{(0)} + \varepsilon\left(1-\frac{1}{2\tau}\right)\frac{\partial}{\partial x}\sum_\theta e_\theta f_\theta^{(1)} = S_c. \tag{A12}$$

Putting Eq. (A8) into the above equation results in

$$\frac{\partial}{\partial t}\sum_\theta f_\theta^{(0)} + \frac{\partial}{\partial x}\sum_\theta e_\theta f_\theta^{(0)} = \varepsilon\left(\tau-\frac{1}{2}\right)\frac{\partial}{\partial x}\sum_\theta e_\theta e_\theta\frac{\partial f_\theta^{(0)}}{\partial x} + S_c+\varepsilon\left(\tau-\frac{1}{2}\right)\frac{\partial}{\partial x}\frac{\partial}{\partial t}\sum_\theta e_\theta f_\theta^{(0)}. \tag{A13}$$

It can be shown that the last term on the right side of the above equation is much smaller than the first term. If we assume that the characteristic velocity is U_c, length L_c, time t_c, and concentration C_c, the term $(\partial/\partial t \sum_\theta e_\theta f_\theta^{(0)})$ is of order $U_c C_c/t_c$ and the term $(\partial/\partial x \sum_\theta e_\theta e_\theta f_\theta^{(0)})$ is of order $e^2 C_c/L_c$. Thus the ratio of the former to the latter terms has the order of

$$\mathcal{O}\left(\frac{\partial/\partial t \sum_\theta e_\theta f_\theta^{(0)}}{\partial/\partial x \sum_\theta e_\theta e_\theta f_\theta^{(0)}}\right) = \mathcal{O}\left(\frac{U_c C_c/t_c}{e^2 C_c/L_c}\right) = \mathcal{O}\left(\frac{U_c}{e}\right)^2 = \mathcal{O}(M^2), \tag{A14}$$

in which C_s is the sound speed with the same order as e and $M = U_c/C_s$ is the Mach number. It follows that the last term in Eq. (A13) is much smaller compared to the first term and can be neglected if $M << 1$, which is consistent with the lattice Boltzmann dynamics; hence Eq. (A13) becomes

$$\frac{\partial}{\partial t}\sum_\theta f_\theta^{(0)} + \frac{\partial}{\partial x}\sum_\theta e_\theta f_\theta^{(0)} = \varepsilon\left(\tau - \frac{1}{2}\right)\frac{\partial^2}{\partial x^2}\sum_\theta e_\theta e_\theta f_\theta^{(0)} + S_c. \tag{A15}$$

Referring to Eq. (A7), after the terms are evaluated using Eq. (14), the above equation becomes the exact fractional advection-diffusion equation (11).

Appendix B: Pseudocode for the LabFADE

The Pseudocode consists of main programme and one module. The former is used to run the simulation after defining the problem, providing computation parameters and initialising variables and the latter is the core algorithm for implementation of the LabFADE. Only the main programme is required to change for modelling different mass transport. Without loss of generality, the complete set-up main programme for Example D - Steady diffusion with a source/sink term is presented below, which can be changed to reproduce other examples in this paper.

```
program main
------------
```

```
This main code is the complete set-up for Example D
       &   - Steady diffusion with a source/sink term.

call module fracdiff

Notations

a - Lattice link direction
C - Concentration
Dfx - dispersion coefficient
dt - Time step
dx - Lattice size
Lx - Total lattice number
u - Velocity
x - Index
alpha - Fractional differentiation order
Beta -  Skewness parameter
& - Continuation

Basic set up and problem is defined

alpha = 1.8
Beta  = 0.5
Lx = 201
dx = 0.001
dt = 0.000067
Dfx = 1.8363   [= 2*gamma(1.2)]

Define single relaxation time tau = 1.0

Assign particle velocity e(0) = 0, e(1) = e and e(2) = -e
              (e = dx/dt)
```

```
Initialise variables velocity & concentration
u = 0
C = 0

Determine the source/sink term
Sc = - 8*( x**0.2+(2-x)**0.2 - 5/2*(x**1.2+(2-x)**1.2) +
     & 25/22*(x**2.2+(2-x**2.2) )

Calculate local equilibrium distribution function
      using the initial variables feq
call compute_feq

Set f = feq

open a file to save the result

Start the loop for time marching

call collide_stream

Inflow boundary condition f_1 = C-f_0-f_2
outflow boundary condition f_2 = C-f_0-f_1

call solution

update the local equilibrium distribution function feq
call compute_feq

End the loop when a solution is obtained

Output result to the file
```

```
end program main
```

```
module fracdiff
---------------

function collide_stream

Implement lattice Boltzmann equation Eq. (13)

for x = 1: Lx

xp = x+1
xn = x-1

ftemp(0,x) = f(0,x) - (f(0,x)-feq(0,x))/tau + dt/5*Sc(x)
if (xp <= Lx) ftemp(1,xp) = f(1,x) - (f(1,x)-feq(1,x))/tau + dt/5*Sc(x)
if (xe >= 1) ftemp(2,xn) = f(2,x) - (f(2,x)-feq(2,x))/tau + dt/5*Sc(x)

end

end function collide_stream

function solution

Set the global f

f = ftemp
```

```
Calculate the concentration

for x = 1: Lx

Cen(x) = 0.0
for a = 0: 2
Cen(x) = Cen(x) + f(a,x)
end
end

end function solution


function compute_feq

For the local equilibrium distribution function

for x = 1: Lx

Qxp(x) = 0.   [See Eq. (20)]

for xt = 1: x-1

Qxp(x) = Qxp(x) + Cen(xt+1,y)*( (real(x-xt)*dx)**(2-alpha)
       & - (real(x-xt-1)*dx)**(2-alpha) ) /(2-alpha)

end
end

Qxm(Lx) = 0.  [See Eq. (21)]
```

```
for x = 1: Lx-1

Qxm(x) = 0.

for xt = x: Lx-1

Qxm(x) = Qxm(x) + Cen(xt,y)*( (real(xt+1-x)*dx)**(2-alpha)
       & - (real(xt-x)*dx)**(2-alpha) ) /(2-alpha)

end
end

Determine feq     [See Eq. (14)]

for a = 1: 2

feq(a,x) = Dfx/(Gamma2ma*2*dt*(tau-0.5)*e*e)*( Beta*Qxp(x)
         & + (1-Beta*Qxm(x) )
         & + Cen(x)/(2*e*e)* e(a)*u(x)
end

feq(0,x) = Cen(x) - Dfx/(Gamma2ma*dt*(tau-0.5)*e*e)*( Beta*Qxp(x)
         & + (1-Beta)*Qxm(x) )

end function compute_feq

end module fracdiff
```


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