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Finite difference approximations for fractional advection–dispersion flow equations

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Abstract

Fractional advection–dispersion equations are used in groundwater hydrology to model the transport of passive tracers carried by fluid flow in a porous medium. In this paper we develop practical numerical methods to solve one dimensional fractional advection–dispersion equations with variable coefficients on a finite domain. The practical application of these results is illustrated by modeling a radial flow problem. Use of the fractional derivative allows the model equations to capture the early arrival of tracer observed at a field site.

Keywords: Finite difference approximation; Stability; Backward Euler method; Implicit Euler method; Radial dispersion; Radial advection; Fractional diffusion; Fractional derivative; Fractional advection–dispersion; Numerical fractional ADE

1. Introduction

Fractional derivatives are almost as old as their more familiar integer-order counterparts [23,30]. Fractional derivatives have recently been applied to many problems in physics [3,7,8,10,16,19,20,22, 29,31,36], finance [14,25,28], and hydrology [2,4–6,33,34]. Fractional space derivatives are used to model anomalous diffusion or dispersion, where a particle plume spreads at a rate inconsistent with the classical Brownian motion model. When a fractional derivative replaces the second derivative in a diffusion or dispersion model, it leads to enhanced diffusion (also called superdiffusion). For a one dimensional advection–dispersion model with constant coefficients, analytical solutions are available

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using Fourier transform methods [5,10]. However, many practical problems require a model with variable coefficients [3,11].

In this paper, we develop the basic theory of numerical solution for the space-fractional advection–dispersion equation

$$\frac{\partial c(r,t)}{\partial t} = -v(r)\frac{\partial c(r,t)}{\partial r} + d(r)\frac{\partial^{\alpha} c(r,t)}{\partial r^{\alpha}} + f(r,t), \tag{1}$$

on a finite domain $L < r < R$. Physical considerations restrict $1 < \alpha \leqslant 2$, see [33]. We assume $v(r) \geqslant 0$ and $d(r) \geqslant 0$ so that the flow is from left to right. We also assume an initial condition $c(r, t = 0) = F(r)$ for $L < r < R$ and a natural set of boundary conditions for this problem: $c(r = L, t) = 0$ for all $t \geqslant 0$ and $\partial c(r = R, t)/\partial t = 0$ for all $t \geqslant 0$. Physically, the boundary conditions mean that no tracer leaks past the left boundary, and that the tracer moves freely through the right boundary. With these assumptions, we show that the implicit Euler method is unconditionally stable when a modified form of the Grünwald formula is used to approximate the fractional derivative. Without this modification, the implicit Euler method is unstable and therefore its solution does not converge to the true solution. The explicit Euler method is also unstable when the standard Grünwald formula is used.

Eq. (1) uses a Riemann fractional derivative of order α, defined by

$$\frac{\mathrm{d}^{\alpha} f(r)}{\mathrm{d}r^{\alpha}} = \frac{1}{\Gamma(n-\alpha)}\frac{\mathrm{d}^{n}}{\mathrm{d}r^{n}}\int_{L}^{r}\frac{f(\xi)}{(r-\xi)^{\alpha+1-n}}\,\mathrm{d}\xi, \tag{2}$$

where n is an integer such that $n - 1 < \alpha \leqslant n$. In most of the related literature, the case $L = 0$ is called the Riemann–Liouville form, and the case $L = -\infty$ is the Liouville definition for the fractional derivative. Fractional derivatives are nonlocal operators of convolution type [1,12,21]. The value of the fractional derivative at a point r depends on the function values at all the points to the left of the point of interest. With our boundary conditions, the Riemann and Liouville forms in (1) are equivalent. For more details on fractional derivative concepts and definitions, see [23,24,30].

A different method for solving the fractional partial differential Eq. (1) is pursued in the recent paper of Liu et al. [18]. They transform this partial differential equation into a system of ordinary differential equations (Method of Lines), which is then solved using backward differentiation formulas. In another very recent paper, Fix and Roop [13] develop a finite element method for a two-point boundary value problem. We are unaware of any other published work on numerical solutions of fractional partial differential equations.

2. Numerical methods

In this section we develop the basic theory for numerical solution of the fractional advection–dispersion Eq. (1) on a finite domain $L < r < R$ with the initial condition $c(r, t = 0) = F(r)$ for $L \leqslant r \leqslant R$, and the boundary conditions $c(r = L, t) = 0$ and $\partial c(r = R, t)/\partial t = 0$ for all $t \geqslant 0$. A discrete approximation to the fractional derivative term may be defined from the standard Grünwald formula

$$\frac{\partial^{\alpha} c(r,t)}{\partial r^{\alpha}} = \frac{1}{\Gamma(-\alpha)}\lim_{M\to\infty}\frac{1}{h^{\alpha}}\sum_{k=0}^{M}\frac{\Gamma(k-\alpha)}{\Gamma(k+1)}c(r-kh,t), \tag{3}$$

where M is a positive integer, $h=(r-L)/M$ and $\Gamma(\cdot)$ is the gamma function [23,24,30]. Note that the value of the fractional derivative at a point r depends on the function values at that point and all the points to the left of that point of interest.

Given a numerical approximation scheme, we define $t_n=n\Delta t$ to be the integration time $0 \leqslant t_n \leqslant T$, $\Delta r = h > 0$ is the grid size in space, $K=(R-L)/h$, $r_i = L + \mathrm{i}h$ for $i=0,\ldots,K$ so that $L \leqslant r_i \leqslant R$, and c_i^n is the numerical approximation to $c(r_i,t_n)$. Similarly $d_i = d(r_i)$, $v_i = v(r_i)$, $f_i^n = f(r_i,t_n)$.

In what follows, we will demonstrate some surprising results. In the classical ADE, the implicit Euler method (and also the Crank–Nicholson method) is unconditionally stable, and is therefore preferred to the explicit Euler method. For the fractional ADE with the standard Grünwald estimates, the explicit Euler method, the implicit Euler method, and the Crank–Nicholson method are all unconditionally unstable. A shifted Grünwald formula allows the implicit Euler method (and also the Crank–Nicholson method) to be unconditionally stable.

Proposition 2.1. *The explicit Euler method solution to Eq.* (1), *based on the Grünwald approximation* (3) *to the fractional derivative, is unstable.*

Proof. We have

$$\frac{c_i^{n+1}-c_i^n}{\Delta t} = -v_i\,\frac{c_i^n - c_{i-1}^n}{h} + \frac{d_i}{h^\alpha \Gamma(-\alpha)}\sum_{k=0}^{i}\frac{\Gamma(k-\alpha)}{\Gamma(k+1)}\,c_{i-k}^n + f_i^n \tag{4}$$

for $i=1,2,..K-1$. We define the 'normalized' Grünwald weights by

$$g_k = \frac{\Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)}. \tag{5}$$

Note that these normalized weights only depend on the order α and the index k. (For example, the first four terms of this sequence are given by $g_0=1$, $g_1=-\alpha$, $g_2=\alpha(\alpha-1)/2!$, $g_3=-\alpha(\alpha-1)(\alpha-2)/3!$). The resulting equation can be explicitly solved for c_i^{n+1} to give:

$$c_i^{n+1} = \left(1 - \frac{\Delta t}{h}\,v_i + \frac{\Delta t}{h^\alpha}\,d_i\right)c_i^n + \left(\frac{v_i}{h} - \frac{\alpha}{h^\alpha}\,d_i\right)\Delta t c_{i-1}^n + \frac{d_i \Delta t}{h^\alpha}\sum_{k=2}^{i} g_k c_{i-k}^n + f_i^n \Delta t. \tag{6}$$

Assume that c_i^0 is the only term that has an error, so the perturbed value is $\underline{c}_i^0 = c_i^0 + \varepsilon_i^0$. This perturbation produces a perturbed value for c_i^1 given by $\underline{c}_i^1 = c_i^1 + \varepsilon_i^1$. So (6) yields

$$\underline{c}_i^1 = \mu_i \underline{c}_i^0 + \left(\frac{v_i}{h} - \frac{\alpha}{h^\alpha}\,d_i\right)\Delta t c_{i-1}^n + \frac{d_i \Delta t}{h^\alpha}\sum_{k=2}^{i} g_k c_{i-k}^n + f_i^n \Delta t = \mu_i \varepsilon_i^0 + c_i^1,$$

where the factor

$$\mu_i = 1 - \frac{\Delta t}{h}\,v_i + \frac{\Delta t}{h^\alpha}\,d_i.$$

Therefore we have $\varepsilon_i^1 = \mu_i \varepsilon_i^0$. That is, the error is amplified by the factor μ_i when the finite difference equation is advanced by one timestep. After n timesteps, one may write $\varepsilon_i^n = \mu_i^n \varepsilon_i^0$. We refer to μ as the amplification factor (or magnification factor). In order for the explicit Euler method to be stable, it is necessary that $|\mu_i| \leqslant 1$, for all h sufficiently small. But for $\alpha > 1$, this inequality requires that

$h > (d_i/v_i)^{1/(\alpha-1)}$. Hence, although it is true that the errors may not grow for larger values of h, the method is not stable as h is refined, and therefore the numerical solution does not converge to the exact solution of the differential equation. □

Remark 2.2. The finite difference method defined above has a local truncation error of $O(\Delta t) + O(\Delta r)$, since each finite difference formula is locally first order accurate. Refer to [32] for a proof of first order accuracy of the Grünwald estimate for the fractional term (Also see [24, Section 7.4] for a different proof for polynomial functions).

Proposition 2.3. *The implicit Euler method solution to Eq.* (1), *based on the Grünwald approximation* (3) *to the fractional derivative, is unstable.*

Proof. In the implicit Euler method, Eq. (1) is discretized so that the right hand side of the equation is evaluated at t_{n+1}. Then we obtain

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} = -v_i \frac{c_i^{n+1} - c_{i-1}^{n+1}}{h} + \frac{d_i}{h^\alpha} \sum_{k=0}^{i} g_k \, c_{i-k}^{n+1} + f_i^{n+1}. \tag{7}$$

Although this is an implicit Euler method, the problem can be solved 'explicitly' by a left-to-right sweep across the r domain, due to the Dirichlet boundary condition at the left boundary. That is, we can compute

$$\left(1 + \frac{v_i \Delta t}{h} - \frac{d_i \Delta t}{h^\alpha}\right) c_i^{n+1} = c_i^n + \left[\frac{v_i c_{i-1}^{n+1}}{h} + \frac{d_i}{h^\alpha} \sum_{k=1}^{i} g_k c_{i-k}^{n+1} + f_i^{n+1}\right] \Delta t. \tag{8}$$

To assess the stability of this implicit Euler method, consider the propagation of an error only in c_i^0 : that is c_i^0 is replaced by $\underline{c}_i^0 = c_i^0 + \varepsilon_i^0$. Then re-write the above equation in the form

$$c_i^{n+1} = \tilde{\mu}_i c_i^n + \tilde{\mu}_i \left[\frac{v_i c_{i-1}^{n+1}}{h} + \frac{d_i}{h^\alpha} \sum_{k=1}^{i} g_k c_{i-k}^{n+1} + f_i^{n+1}\right] \Delta t,$$

where

$$\tilde{\mu}_i = \frac{1}{1 + (v_i \Delta t/h) - (d_i \Delta t/h^\alpha)}. \tag{9}$$

Due to the linearity of this finite difference equation, after some simple manipulations we obtain

$$\underline{c}_i^1 = c_i^1 + \varepsilon_i^1 = \tilde{\mu}_i \underline{c}_i^0 + \cdots = \tilde{\mu}_i (c_i^1 + \varepsilon_i^0) + \cdots = \tilde{\mu}_i c_i^1 + \cdots + \tilde{\mu}_i \varepsilon_i^0 = c_i^1 + \tilde{\mu}_i \varepsilon_i^0.$$

Here $\tilde{\mu}_i$ is the amplification factor (at the grid point r_i). The propagated effect of the error ε_i^0 at time step t_1 is then equal to $\varepsilon_i^1 = \tilde{\mu}_i \varepsilon_i^0$, and at time step t_n this error propagates to become $\varepsilon_i^n = (\tilde{\mu}_i)^n \varepsilon_i^0$. Therefore, in order for the above formulation of the implicit Euler method to be stable, it is necessary that $|\tilde{\mu}_i| \leqslant 1$. However, for any h sufficiently small we will always have $|\tilde{\mu}_i| > 1$, so the implicit Euler method is unstable in this case, and hence its numerical solution does not converge to the exact solution of the differential equation. □

The implicit (Euler) methods are the preferred approach to discretize the classical PDEs due to their unconditional stability (which does not constrain the size of the time step). Unconditional

stability is a hallmark of the implicit Euler method in the classical PDEs. However, the above result shows that stability falls apart in the fractional case when the standard Grünwald formulas are used to approximate the derivatives. A similar conclusion, using similar analysis, is also reached for the Crank–Nicholson discretization of (1) with the form (3) of the Grünwald estimates. To remedy this situation, a variant of the Grünwald formula can be used, in which the function evaluations are shifted to the right. We begin by showing that the shifted Grünwald formula is consistent. We also provide the order of consistency/convergence, since this is important for numerical work.

Theorem 2.4. *Suppose that* $f \in L_1(\mathbb{R})$ *and* $f \in \mathscr{C}^{\alpha+1}(\mathbb{R})$, *and let*

$$A_h f(x) = \frac{1}{\Gamma(-\alpha)} \frac{1}{h^\alpha} \sum_{k=0}^{\infty} \frac{\Gamma(k-\alpha)}{\Gamma(k+1)} f(x-(k-p)h), \tag{10}$$

where p *is a nonnegative integer. Let* $Af(x) = \mathrm{d}^\alpha f(x)/\mathrm{d}x^\alpha$ *be the Liouville fractional derivative as given by* (2) *with* $L = -\infty$. *Then* $A_h f(x) = Af(x) + \mathrm{O}(h)$ *uniformly in* $x \in \mathbb{R}^1$ *as* $h \to 0$.

Proof. We adapt the argument that the standard Grünwald formula (3) is $\mathrm{O}(h)$ from Tuan and Gorenflo [32]. Let $\mathscr{F}[f](k) = \hat{f}(k) = \int \mathrm{e}^{\mathrm{i}kx} f(x)\,\mathrm{d}x$ be the Fourier transform of $f(x)$ so that $\mathrm{e}^{\mathrm{i}kh}\hat{f}(k)$ is the Fourier transform of $f(x-h)$. It is well known that

$$(1+z)^\alpha = \sum_{k=0}^{\infty} \binom{\alpha}{k} z^k \tag{11}$$

for any complex $|z| \leqslant 1$ and any $\alpha > 0$, where

$$\binom{\alpha}{k} = \frac{(-1)^k \Gamma(k-\alpha)}{\Gamma(-\alpha)\Gamma(k+1)}.$$

Note that

$$\binom{\alpha}{0} = 1, \binom{\alpha}{1} = \alpha,$$

and

$$\binom{\alpha}{k}(-1)^k = \frac{(-\alpha)(-\alpha+1)\cdots(-\alpha+k-1)}{k!} \quad \text{for all } k \geqslant 2.$$

Take Fourier transforms in (10) and use (11) to see that

$$\begin{aligned}
\mathscr{F}[A_h f](k) &= h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \mathrm{e}^{\mathrm{i}k(m-p)h} \hat{f}(k) \\
&= h^{-\alpha} \mathrm{e}^{-\mathrm{i}khp} (1 - \mathrm{e}^{\mathrm{i}kh})^\alpha \hat{f}(k) \\
&= h^{-\alpha} (-\mathrm{i}kh)^\alpha \left(\frac{1-\mathrm{e}^{\mathrm{i}kh}}{-\mathrm{i}kh} \right)^\alpha \mathrm{e}^{-\mathrm{i}khp} \hat{f}(k) \\
&= (-\mathrm{i}k)^\alpha w(-\mathrm{i}kh) \hat{f}(k),
\end{aligned} \tag{12}$$

where $(iu)^\alpha = \text{sign}(u)|u|^\alpha \exp(i\pi\alpha/2)$ for real u and

$$w(z) = \left(\frac{1-e^{-z}}{z}\right)^\alpha e^{zp} = 1 - \left(p - \frac{\alpha}{2}\right) z + O(|z|^2). \tag{13}$$

Note that $|w(-ix) - 1| \leqslant C|x|$ for all $x \in \mathbb{R}$ for some $C > 0$. Then

$$\begin{aligned}\mathscr{F}[A_h f](k) &= (-ik)^\alpha \hat{f}(k) + (-ik)^\alpha (w(-ikh) - 1)\hat{f}(k) \\ &= \mathscr{F}[Af](k) + \hat{\varphi}(h,k),\end{aligned} \tag{14}$$

where $\hat{\varphi}(h,k) = (-ik)^\alpha (w(-ikh) - 1)\hat{f}(k)$ and

$$\varphi(h,x) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{-ikx} \hat{\varphi}(h,k)\, dk.$$

Since $f \in L_1(\mathbb{R})$ and $f \in \mathscr{C}^{\alpha+1}(\mathbb{R})$ we have

$$I = \int_{-\infty}^{\infty} (1 + |k|)^{\alpha+1} |\hat{f}(k)|\, dk < \infty.$$

Then since

$$|\hat{\varphi}(h,k)| \leqslant |k|^\alpha C|hk|\, |\hat{f}(k)|$$

we also have $|\varphi(h,x)| \leqslant ICh$ for all $x \in \mathbb{R}$. □

Remark 2.5. The universal constant C in the above proof depends on the linear term in the Taylor series (13). Although any shift (even the unshifted form $p = 0$) gives an $O(h)$ consistency, the best performance comes from minimizing $|p - \alpha/2|$. For the fractional advection–dispersion Eq. (1) we have $1 < \alpha \leqslant 2$ so the optimal choice is $p = 1$. If $\alpha = 2$ then this coincides with the centered second difference estimator of the second derivative.

Remark 2.6. The Grünwald formula can be viewed as a Riemann sum approximation to the integral definition of the fractional derivative. Under certain conditions (see [24, p. 219]) the fractional derivative (2) may be written in the form

$$\frac{d^\alpha f(r)}{dr^\alpha} = \frac{1}{\Gamma(-\alpha)} \int_L^r f(r-\xi)\xi^{-\alpha-1}\, d\xi. \tag{15}$$

Use Stirling's formula $\Gamma(x+1) \sim \sqrt{2\pi x}\, x^x e^{-x}$ as $x \to \infty$, to see that

$$\begin{aligned}\frac{\Gamma(k-\alpha)}{\Gamma(k+1)} &\sim \frac{\sqrt{2\pi(k-1-\alpha)}(k-1-\alpha)^{(k-1-\alpha)} e^{-(k-1-\alpha)}}{\sqrt{2\pi k} k^k e^{-k}} \\ &= e^{\alpha+1} \sqrt{\frac{k-1-\alpha}{k}}\, \frac{(k-1-\alpha)^{(k-1-\alpha)}}{k^k},\end{aligned}$$

where $\sqrt{(k-1-\alpha)/k} \to 1$ and

$$k^{\alpha+1}\frac{(k-1-\alpha)^{(k-1-\alpha)}}{k^k} = \left(1-\frac{\alpha+1}{k}\right)^k \left(\frac{k}{k-1-\alpha}\right)^{\alpha+1} \to \mathrm{e}^{-\alpha-1}$$

as $k \to \infty$, and therefore

$$\frac{\Gamma(k-\alpha)}{\Gamma(k+1)} \sim k^{-\alpha-1} \tag{16}$$

as $k \to \infty$. Then

$$\frac{1}{\Gamma(-\alpha)}\frac{1}{h^\alpha}\sum_{k=0}^{M}\frac{\Gamma(k-\alpha)}{\Gamma(k+1)}f(r-kh) \approx \frac{1}{\Gamma(-\alpha)}\sum_{k=0}^{M} f(r-kh)(kh)^{-\alpha-1}h$$

which is a Riemann sum approximation to (15). Then the shift in (10) corresponds to replacing $f(r-kh)$ by $f(r-(k-p)h)$ which does not affect the limit as $h \to 0$.

Boundary conditions are usually not treated in the stability analysis of the finite difference scheme, since it is the behavior in the interior region that is of most interest. Below we prove the numerical stability for Eq. (1) with Dirichlet boundary conditions on the right boundary, that is $c(r{=}R,t){=}b_R(t)$. In the fractional advection–dispersion Eq. (1) the order of the fractional derivative is $1 < \alpha \leqslant 2$, so the optimal Grünwald formula is shifted by one grid point to the right. It turns out that this modification also makes the implicit Euler method consistent and unconditionally stable. Then the Lax equivalence theorem in [27, p. 45] implies that the finite difference solution converges to the true solution as $\Delta t \to 0$ and $h = \Delta r \to 0$.

Theorem 2.7. *The implicit Euler method solution to Eq.* (1) *with* $1 < \alpha \leqslant 2$ *on the finite domain* $L \leqslant r \leqslant R$, *with boundary conditions* $c(r=L,t)=0$ *and* $c(r=R,t)=b_R(t)$ *for all* $t \geqslant 0$, *based on the shifted Grünwald approximation*

$$\frac{\partial^\alpha c(r,t)}{\partial r^\alpha} = \frac{1}{\Gamma(-\alpha)}\lim_{M\to\infty}\frac{1}{h^\alpha}\sum_{k=0}^{M}\frac{\Gamma(k-\alpha)}{\Gamma(k+1)}c(r-(k-1)h,t), \tag{17}$$

where $h=(r-L)/M$, *is consistent and unconditionally stable.*

Proof. The left boundary condition $c(L,t)=0$ implies that we can extend the function $c(r,t)=0$ for all $r \leqslant L$ and $t \geqslant 0$. Then the fractional derivative (2) coincides with the Liouville form, the finite sum approximation (17) equals the infinite sum approximation in (10), and Theorem 2.4 implies that the truncation error in the shifted Grünwald approximation (17) is $\mathrm{O}(h)$. It follows easily that the method is consistent. Now the approximating formula for the fractional term in (1) is

$$\frac{\partial^\alpha c(r_i,t_n)}{\partial r^\alpha} \approx \frac{1}{h^\alpha}\sum_{k=0}^{i+1} g_k c_{i-k+1}^n. \tag{18}$$

When this shifted Grünwald estimate (18) is substituted in the implicit Euler method, the resulting difference equations are

$$\frac{c_i^{n+1}-c_i^n}{\Delta t} = -v_i\frac{c_i^{n+1}-c_{i-1}^{n+1}}{h} + \frac{d_i}{h^\alpha}\sum_{k=0}^{i+1} g_k c_{i-k+1}^{n+1} + f_i^{n+1}. \tag{19}$$

These equations, together with the Dirichlet boundary conditions, result in a linear system of equations whose coefficient matrix is the sum of a lower triangular and a super-diagonal matrices. Defining $E_i = v_i \Delta t/h$, and $B_i = d_i \Delta t/h^\alpha$, then the system defined by (19) can be re-written as

$$c_i^{n+1} - c_i^n = -E_i(c_i^{n+1} - c_{i-1}^{n+1}) + B_i \sum_{k=0}^{i+1} g_k c_{i-k+1}^{n+1} + \Delta t f_i^{n+1}.$$

The above equation can be re-arranged for the like terms to yield

$$-g_0 B_i c_{i+1}^{n+1} + (1 + E_i - g_1 B_i) c_i^{n+1} - (E_i + g_2 B_i) c_{i-1}^{n+1} - B_i \sum_{k=3}^{i+1} g_k c_{i-k+1}^{n+1} = c_i^n + \Delta t f_i^{n+1}.$$

This difference equation defines a linear system of equations $\underline{A}\,\underline{C}^{n+1} = \underline{C}^n + \Delta t \underline{F}^{n+1}$, where

$$\underline{C}^{n+1} = [c_0^{n+1}, c_1^{n+1}, c_2^{n+1}, \ldots, c_K^{n+1}]^{\mathrm{T}}$$

$$\underline{C}^n + \Delta t \underline{F}^n = [0, c_1^n + \Delta t f_1^n, c_2^n + \Delta t f_2^n, \ldots, c_{K-1}^n + \Delta t f_{K-1}^n, b_R(t_{n+1})]^{\mathrm{T}}$$

and $\underline{A} = [A_{i,j}]$ is the matrix of coefficients. These coefficients, for $i = 1, \ldots, K-1$ and $j = 1, \ldots, K-1$ are defined as follows (note that $g_0 = 1,\ g_1 = -\alpha$):

$$A_{i,j} = \begin{cases} 0 & \text{when } j \geqslant i+2, \\ -g_0 B_i & \text{when } j = i+1, \\ 1 + E_i - g_1 B_i & \text{when } j = i, \\ -E_i - g_2 B_i & \text{when } j = i-1, \\ -g_{i-j+1} B_i & \text{when } j \leqslant i-1. \end{cases}$$

while $A_{0,0} = 1,\ A_{0,j} = 0$ for $j = 1, \ldots, K,\ A_{K,K} = 1$, and $A_{K,j} = 0$ for $j = 0, \ldots, K-1$.

Let λ be an eigenvalue of the matrix A, so that $\underline{A}X = \lambda X$ for some nonzero vector X. Choose i so that $|x_i| = \max\{|x_j| : j = 0, \ldots, K\}$. Then $\sum_{j=0}^{K} A_{i,j} x_j = \lambda x_i$, and therefore

$$\lambda = A_{i,i} + \sum_{j=0, j\neq i}^{K} A_{i,j} \frac{x_j}{x_i}. \tag{20}$$

If $i = 0$ or $i = K$, then we get $\lambda = 1$. Otherwise, substituting the values of $A_{i,j}$ into (20) we get

$$\lambda = 1 + E_i - g_1 B_i - g_0 B_i \frac{x_{i+1}}{x_i} - (E_i + g_2 B_i) \frac{x_{i-1}}{x_i} - B_i \sum_{j=0}^{i-2} g_{i-j+1} \frac{x_j}{x_i}$$

$$= 1 + E_i(1 - x_{i-1}/x_i) - B_i \left[g_1 + \sum_{j=0, j\neq i}^{i+1} g_{i-j+1} \frac{x_j}{x_i} \right].$$

Substitute $z = -1$ into (11) to see that $\sum_{k=0}^{\infty} g_k = 0$. Since $1 < \alpha \leqslant 2$, the only negative term in the sequence of Grünwald weights is $g_1 = -\alpha$. Therefore, $-g_1 \geqslant \sum_{k=0, k\neq 1}^{j} g_k$ for any $j = 0, 1, 2, \ldots$.

Since $|x_j/x_i| \leqslant 1$ and $g_j \geqslant 0$ for $j = 0, 2, 3, 4, \ldots$, we get

$$\sum_{j=0, j\neq i}^{i+1} g_{i-j+1}|x_j/x_i| \leqslant \sum_{j=0, j\neq i}^{i+1} g_{i-j+1} \leqslant -g_1.$$

Therefore, we have

$$g_1 + \sum_{j=0, j\neq i}^{i+1} g_{i-j+1} \left|\frac{x_j}{x_i}\right| \leqslant 0.$$

Since, E_1, B_i are both non-negative reals, we conclude that every eigenvalue of $\underline{A}$ satisfies $|\lambda| \geqslant 1$. Then $\underline{A}$ is invertible, and every η eigenvalue of $\underline{A}^{-1}$ satisfies $|\eta| \leqslant 1$. Therefore the spectral radius of the inverse matrix $\rho(\underline{A}^{-1}) \leqslant 1$, and an error $\underline{\varepsilon}^0$ in $\underline{C}^0$ will result in an error in $\underline{C}^1$ given by $\underline{\varepsilon}^1 = \underline{A}^{-1}\underline{\varepsilon}^0$. Thus the error is bounded $\|\underline{\varepsilon}^1\| \leqslant \|\underline{\varepsilon}^0\|$ and therefore the method is unconditionally stable. □

Remark 2.8. The result of Theorem 2.7 also applies to the fractional advection-diffusion Eq. (1) with more general space and time dependent advection and dispersion coefficients, that is, $v = v(r, t) \geqslant 0$, and $d = d(r, t) \geqslant 0$. The proof is essentially unmodified in this case.

Remark 2.9. Note that for $\alpha = 2$, which corresponds to the classical second derivative case, the shifted Grüwald estimate (18) is just the standard centered difference formula for approximating the second derivative ($g_0 = 1, g_1 = -2, g_2 = 1, g_3 = g_4 = \cdots = 0$),

$$\frac{\partial^2 c(r_i, t_n)}{\partial r^2} \approx \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{h^2}. \tag{21}$$

Remark 2.10. The system of equations $\underline{A}\,\underline{C}^{n+1} = \underline{C}^n + \Delta t \underline{F}^{n+1}$ is solved at time t_n to advance the solution to time t_{n+1}. Note that if the timestep Δt is kept constant, since the matrix coefficients are independent of time t (this assumes that $v = v(r)$ and $d = d(r)$), the linear system needs to be solved only once, and the matrix multipliers saved to efficiently solve the resulting system of equations as the solution is marched forward in time.

Remark 2.11. The same approach as in Theorem 2.7 can also be applied with a more general boundary condition of the third kind of the form $c(R, t) + \beta \partial c(R, t)/\partial r = s(t)$ with $\beta \geqslant 0$, as this boundary condition preserves the diagonal dominance of the resulting coefficient matrix.

Remark 2.12. The Crank–Nicholson discretization, using the shifted Grünwald estimates for the fractional derivative, can also be shown to be unconditionally stable. The proof is exactly as in the above case, the only change will be that for the coefficient matrix, E_i, B_i will be replaced by $E_i/2, B_i/2$ respectively. However, the Crank–Nicholson method with the standard Grünwald formula (i.e., with no shift) will be unconditionally unstable. The general preference for the Crank–Nicholson for the classical PDE's is that it provides a stable finite difference method that is second order accurate $O((\Delta t)^2) + O(h^2)$. However the Grünwald estimates are only $O(h)$ accurate, and therefore in the

fractional advection–dispersion differential equations the second order accuracy is not achieved by the use of the corresponding Grünwald finite differences.

3. Radial flow application

A tracer solute is introduced into an aquifer at an injection well, and then pumped out at a second extraction well. We adopt a radial coordinate system centered at the extraction well, and assume that the medium is radially homogeneous. Tracer concentration $c(r,t)$ in the aquifer is related to tracer flux $q(r,t)$ and injection rate $f(r,t)$ according to the conservation equation

$$\frac{\partial c(r,t)}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(rq(r,t)) + f(r,t) \tag{22}$$

where the flux is described by

$$q(r,t) = \frac{v_0}{r}c(r,t) - \frac{d_0}{r}\frac{\partial c(r,t)}{\partial r}. \tag{23}$$

The first term is the advective flux, inversely proportional to r because of the radial geometry. The second term is the dispersive flux, and this empirical formula derives from the fact that dispersion is the effect of differential advection in a porous media, so that advection and dispersion coefficients are roughly proportional.

In a recent field study [9,26,35] at a Nevada test aquifer, 20.81 kg of bromide used as a tracer solute, at an average concentration of 3600 mg/l, was introduced at the injection well for a period of 85 h at the rate of 67.8 l/h. The distance from injection well to the extraction well was 30 m, and the radius of extraction well was 0.127 m. The velocity coefficient and the dispersion constant were estimated to be of the same order of magnitude. Measured concentrations over time at the extraction well show early breakthrough that cannot be explained by the classical radial flow model.

To address this situation, we employ a model with a fractional dispersive flux:

$$q(r,t) = \frac{v_0}{r}c(r,t) - \frac{d_0}{r}\frac{\partial^\beta c(r,t)}{\partial r^\beta} \tag{24}$$

for some $0 < \beta \leqslant 1$. The fractional term models anomalous dispersion due to velocity contrasts resulting from the interaction with a porous medium. Note that v_0 and d_0 in Eq. (24) are not the same as in the classical flux Eq. (23) and the d_0's do not even have the same dimensions. The v_0 and d_0 are fitted parameters. We have emphasized the numerical approximation method here. See [35] for the details of the tested aquifer and associated parameters. Also, see [33] for a physical derivation of the fractional flux based on statistical mechanics. The classical model corresponds to a value of $\beta = 1$. Values of $\beta < 1$ lead to superdispersion, in which solute spreads faster than the classical model predicts. See [6,15] for some practical methods of estimating the order β of the fractional derivative from data. In the limiting case of $\beta = 0$, the dispersion process is replaced by an advection process in the differential equation. Substituting (24) with $\alpha = \beta + 1$ into the radial conservation law (22) we get

$$\frac{\partial c(r,t)}{\partial t} = -\frac{v_0}{r}\frac{\partial c(r,t)}{\partial r} + \frac{d_0}{r}\frac{\partial^\alpha c(r,t)}{\partial r^\alpha} + f(r,t). \tag{25}$$

Note that Eq. (25) is the same as Eq. (1) with $v(r) = v_0/r$ and $d(r) = d_0/r$. We consider this equation and its numerical solution in the case $1 \leqslant \alpha \leqslant 2$, for $L < r < R$, and $0 < t \leqslant T$. We take

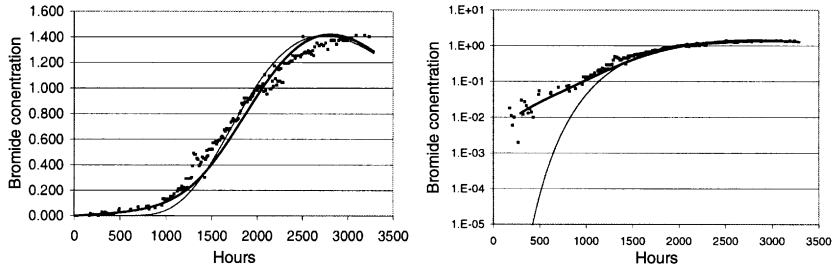

Fig. 1. Concentration of bromide tracer (gm/m^3) at extraction well. Fractional radial flow model (25) with $v_0=4.0$, $d_0=2.4$ and $\alpha=1.6$ (thick line) captures early breakthrough better than classical radial flow model with $v_0=3.5$, $d_0=5.0$ and $\alpha=2$ (thin line).

$L=-60.127$ and $R=-0.127$. The injection well is at $r=-30.127$ meters, the extraction well is centered at $r=0$, with its wall at $r=R=-0.127$ meters. The left boundary is set to be upstream and sufficiently far from the injection well so that no measurable bromide concentration reaches the left boundary during the time of interest. In doing so, we keep the numerical solution mass preserving. So, we may assume $c(r=L,t)=0$, and $\partial c(r=R,t)/\partial r=0$. The injection of bromide is modeled by a forcing function $f(r=-30.127,\ t)=5.93\ g/m^3/day$ for $0\leqslant t\leqslant 3.54$ days, based on some additional assumptions about aquifer thickness and porosity, and the volume over which the initial injection spreads. A graph of bromide concentration at the extraction well as a function of time, along with the results of numerical estimates using the shifted implicit Euler method are shown in Fig. 1. In the numerical simulation, the r-interval $[-60.127,\ -0.127]$ was divided into $K=60$ subintervals, so that $h=\Delta r=1.00$ meter, and a value of $\Delta t=1.00$ day was used. The shifted Grünwald estimate (18) at each gridpoint r_i uses the terms at $r_{i+1},r_i,r_{i-1},\ldots,r_0$ with the associated Grünwald weights $g_0,g_1,g_2,\ldots,g_{i+1}$ to set up the coefficient matrix $\underline{A}$. The parameters $v_0=4.0$, $d_0=2.4$ and $\alpha=1.6$ were fit empirically. The fractional radial flow model captures the early breakthrough of tracer at the extraction well. As shown, the best-fitting curve from the classical radial flow model greatly under-estimated early arrival. We also remark that this solute flow model and its numerical solution match the test data closely only up to the peak. Additional (mobile/immobile) solute flow modeling to address the late time arrival of the solute has been recently carried out. For details, see [35].

4. Conclusions

Fractional derivatives in space can be used to model anomalous dispersion/diffusion, where particles spread faster than the classical models predict. Fractional advection–dispersion equations with variable coefficients allows velocity to vary over the domain, which is important in applications. An implicit Euler method, based on a modified Grünwald approximation to the fractional derivative, is consistent and unconditionally stable. If the usual Grünwald approximation is used, the implicit Euler method is always unstable. This simple numerical method is useful for solving the fractional radial flow equation, where the fluid velocity increases as flow converges on an extraction well. The fractional derivative allows the model to more accurately describe early arrival, which is important in modeling groundwater contamination.

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