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FRACTIONAL DIFFUSION MODEL FOR TRANSPORT THROUGH POROUS MEDIA

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ABSTRACT

We model the transport of fluid through porous media in terms of fractional diffusion equation (FDE) for the pressure p(x,t). Potential application could be to shale gas recovery in tight porous media. Specifically, we pose the time FDE in a finite domain of length L,

 $_{0}D_{t}^{\alpha}p = Ap + f(x,t), \quad 0 \le x \le L, \quad t > 0,$ where *A* is a linear differential operator given by

 $A \equiv \frac{\partial}{\partial x} \left(a \frac{\partial}{\partial x} \right)$, where $a = \frac{\kappa}{\mu}$, κ is the permeability

and μ is the viscosity, f(x,t) is a source term. ${}_{0}D_{t}^{\alpha}$ is the time-fractional derivative of order α , $0 < \alpha \le 1$. The initial and boundary conditions are, p(x,0) = g(x), and $p_{x}(0,t) = c$, $p_{x}(L,t) = 0$. The main goal is to study numerically the pressure distribution p(x,t) in one-dimensional porous reservoirs for different α , and for different cases of f(x,t) and g(x).

INTRODUCTION

Fractional calculus methods have the ability to represent non-Gaussian statistical processes which leads to socalled anomalous diffusion regimes in which the mean square displacement $\langle x^2 \rangle$ behaves like $\langle x^2 \rangle \propto t^{\alpha}$, where $\alpha < 1$ (sub-diffusion), $\alpha > 1$ (super-diffusion), and $\alpha = 1$ is the standard (Gaussian) diffusion. Applications of fractional calculus abound in many areas of science, from biological systems [1, 8] to reservoir studies [17].

The transport of fluids through porous media is a complex process which requires a deep understanding of the underlying physics and the geometry of the system [6, 7]. Fluid flow through porous media occurs because

of different physical phenomena, such as diffusion of the particles through the pores, advection of some of the fluid, and perhaps due to some external forces, like gravity. Porous medium with the extremely low permeability and porosity exhibits different flow conditions, such as viscous flow, slip flow and transition flow [21]. We often see a departure from the conventional Darcy's law [9].

Different strategies are applied to understand diffusion in porous media [2, 3]. Among them the most realistic approaches are the use of random walk processes, especially the continuous time random walk (CTRW) approach [14, 15]. In CTRW, the mean squared displacement of the particles is described by the nonlinear power law, that is, $\langle x^2 \rangle \propto t^{\alpha}$, where $0 < \alpha \le 1$. For $\alpha = 1$, we recover the conventional linear relationship which corresponds to the standard diffusion process. The probability density function p(x,t) which describes the location of the particle at the position x at the time t satisfies a time fractional diffusion equation, as explained in [12].

1 Fundamental Ideas of Fractional Calculus

The history of fractional calculus dates back to era of Newton and Leibniz, when the question of non-integer order derivatives was posed [13]. The problem attracted the attention of many researchers and the answer came in the form of general definitions of fractional order derivatives and integrals by many mathematicians, such as, Riemann, Liouville, and Ries. In the recent years, the interest in the subject has risen because of its ability to explain the history dependent processes. The basic definitions of fractional calculus are provided here, for more details the readers are referred to [4, 5, 10, 16].

Riemann-Liouville fractional integral of an absolutely integrable function f(t) is defined by

$$\left({}_{0}I_{t}^{\alpha}f\right)(t)=\frac{1}{\Gamma(\alpha)}\int_{0}^{t}\frac{f(\tau)}{\left(t-\tau\right)^{1-\alpha}}d\tau, \quad t>0, \ \alpha\in R^{+}.$$

For $\alpha = 1$, it reduces to ordinary integral and for $\alpha = 0$, it becomes identity operator.

Riemann-Liouville fractional derivative of an absolutely continuous function f(t) is defined by

$${}_{0}D_{t}^{\alpha}f(t) = \frac{1}{\Gamma(1-\alpha)}\frac{\partial}{\partial t}\int_{0}^{t}\frac{f(\tau)}{(t-\tau)^{\alpha}}d\tau, \quad 0 < \alpha < 1.$$

For $\alpha = 1$, it reduces to ordinary derivative and for $\alpha = 0$, it becomes identity operator.

Caputo fractional derivative of a differentiable function f(t) is defined by

$$\int_{o}^{C} D_{t}^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_{0}^{t} \frac{f'(\tau)}{(t-\tau)^{\alpha}} d\tau, \quad 0 < \alpha < 1.$$

Grunwald-Letnikov fractional derivative of order $0 < \alpha < 1$ of a differentiable function f(t) is defined by

 $\int_{o}^{GL} D_t^{\alpha} f(t) = \lim_{h \to 0} \frac{1}{h^{\alpha}} \sum_{k=0}^{\lfloor t/h \rfloor} \omega_k^{\alpha} f(t-kh), \quad t \ge 0,$ where [t/h] is the integer part of t/h, and $\omega_k^{\alpha} = (-1)^k \begin{pmatrix} \alpha \\ k \end{pmatrix}$ are the generalized binomial

coefficients.

Equivalence of Fractional Derivatives: If f(t) is continuous and differentiable and f'(t) is integrable in [0,t], then for every $0 < \alpha < 1$, all fractional derivatives exist and coincide [10, 16].

For numerical approximations, we use Grunwald-Letnikov derivative in the following form [16, 20]:

$${}_{o}^{GL}D_{t}^{\alpha}f(t) = \frac{1}{h^{\alpha}}\sum_{k=0}^{[t/h]}\omega_{k}^{\alpha}f(t-kh) + O(h^{\nu})$$

The binomial coefficients are approximated by the following recursive relation [16, 20],

$$\omega_0^{\alpha} = 1, \quad \omega_k^{\alpha} = \left(1 - \frac{1 + \alpha}{k}\right) \omega_{k-1}^{\alpha}.$$

The generalized binomial coefficients are also generated accurately up to order V by different generating functions. These generating functions are given in [pod]. We use the first order backward difference formula

 $\omega(z,\alpha) = (1-z)^{\alpha}$, as the generating function.

2 Fractional BTCS Method

In this section, we develop a backward in time and centered in space (BTCS) finite difference scheme for the equation

$${}_{0}D_{t}^{\alpha}p = Ap + f(x,t), \quad 0 \le x \le L, \quad t > 0$$
 (1)

The spatial and temporal variables are discretized by placing a uniform grid on the space-time domain, that is, $x_i = j\Delta x$ and $t_m = m\Delta t$. The numerical approximation of the unknown p(x,t) at the point (x_i, t_m) is denoted by P_i^m and it is obtained by $P_i^m \square p_i^m \equiv p(x_i, t_m)$. The time-fractional derivative $_{0}D_{t}^{\alpha}$ is replaced by Grunwald-Letnikov derivative and the space derivative by central difference formula. We obtain the following system of recurrence equations,

$$\frac{1}{\left(\Delta t\right)^{\alpha}} \sum_{k=1}^{m+1} \omega_{k}^{\alpha} p_{j}^{(m+1)-k} + T(x,t)$$

=
$$\frac{a_{j+1}p_{j+1}^{m+1} - (a_{j+1} + a_{j-1})p_{j}^{m+1} + a_{j-1}p_{j-1}^{m+1}}{2\left(\Delta x\right)^{2}} + f_{j}^{m+1}$$

where T(x,t) is the truncation error. After rearranging, we obtain

$$-a_{j-1}S_{\alpha}p_{j-1}^{m+1} + \left[1 + \left(a_{j-1} + a_{j+1}\right)S_{\alpha}\right]p_{j}^{m+1} - a_{j+1}S_{\alpha}p_{j+1}^{m+1} \\ = \left(\Delta t\right)^{\alpha}f_{j}^{m+1} - \sum_{k=2}^{m+1}\omega_{k}^{\alpha}p_{j}^{(m+1)-k}$$
(2)

 $j = 1, 2, \dots, J$; $m = 1, 2, \dots, M$, where and

$$S_{\alpha} = \frac{\left(\Delta t\right)^{\alpha}}{2\left(\Delta x\right)^{2}}.$$

The initial condition, p(x,0) = g(x), is discretized as

$$p_{j}^{1} = g_{j}$$
, for all $j = 1, 2, ..., J$

The Neumann boundary conditions are discretized by the 0th order approximation.

The NBC
$$p_x(0,t) = c$$
 gives $\frac{p_2^m - p_1^{m+1}}{\Delta x} = c$ which
implies $p_1^{m+1} = p_2^m + c\Delta x$, for all $m = 1, 2, \dots, M$,

and the NBC $p_x(L,t) = c$ gives $\frac{p_J^{m+1} - p_{J-1}^m}{\Delta x} = 0$ which implies $p_J^{m+1} = p_{J-1}^m$ for all $m = 1, 2, \dots, M$.

For j = 2, we have,

$$\begin{bmatrix} 1 + (a_1 + a_3) S_{\alpha} \end{bmatrix} p_2^{m+1} - a_3 S_{\alpha} p_3^{m+1}$$
$$= (\Delta t)^{\alpha} f_2 + a_1 S_{\alpha} p_1^{m+1} - \sum_{k=2}^{m+1} \omega_k^{\alpha} p_2^{(m+1)-k}$$

But with $p_1^{m+1} = p_2^m + c\Delta x$, this becomes $\left[1 + (a_1 + a_3)S_{\alpha}\right]p_2^{m+1} - a_3S_{\alpha}p_3^{m+1}$ $= (\Delta t)^{\alpha} f_2 + a_1S_{\alpha}(p_2^m + c\Delta x) - \sum_{k=1}^{m+1} \omega_k^{\alpha} p_2^{(m+1)-k}$

For
$$j = J - 1$$
, we get,
 $-a_{J-2}S_{\alpha}p_{J-2}^{m+1} + \left[1 + (a_{J-2} + a_J)S_{\alpha}\right]p_{J-1}^{m+1}$

$$= (\Delta t)^{\alpha} f_{J-1} + a_J S_{\alpha} p_J^{m+1} - \sum_{k=2}^{m+1} \omega_k^{\alpha} p_{J-1}^{(m+1)-k}$$

and with
$$p_J^{m+1} = p_{J-1}^m$$
, this becomes
 $-a_{J-2}S_{\alpha}p_{J-2}^{m+1} + \left[1 + (a_{J-2} + a_J)S_{\alpha}\right]p_{J-1}^{m+1}$
 $= (\Delta t)^{\alpha} f_{J-1} + a_JS_{\alpha}p_{J-1}^m - \sum_{k=2}^{m+1}\omega_k^{\alpha}p_{J-1}^{(m+1)-k}$

For $j = 3, 4, \dots, J - 2$, it is same as above

In matrix form it can be written as $Qp^{m+1} = b$, Where Q is $(J-2) \times (J-2)$ matrix whose main diagonal entries are $q_{jj} = 1 + (a_j + a_{j+2})S_{\alpha}$, where j = 1, 2, ..., J - 2. The entries of the sup-diagonal are $q_{j,j+1} = -a_{j+2}S_{\alpha}$ with j = 1, 2, ..., J - 3, and the entries of the sub-diagonal are given as $q_{j,j-1} = -a_jS_{\alpha}$ where j = 2, 3, ..., J - 2. The vector p^{m+1} represents $p^{m+1} = [p_2^{m+1}, ..., p_{J-1}^{m+1}]^T$ and b is a column vector of length J-2, whose entries are

$$b_{1} = (\Delta t)^{\alpha} f_{2} + a_{1}S_{\alpha} (p_{2}^{m} + c\Delta x) - \sum_{k=2}^{m+1} \omega_{k}^{\alpha} p_{2}^{(m+1)-k}$$

$$b_{J-2} = (\Delta t)^{\alpha} f_{J-1} + a_{J}S_{\alpha} p_{J-1}^{m} - \sum_{k=2}^{m+1} \omega_{k}^{\alpha} p_{J-1}^{(m+1)-k} ,$$

and for
$$j = 2, 3, ..., J - 3$$
,
 $b_j = (\Delta t)^{\alpha} f_j - \sum_{k=2}^{m+1} \omega_k^{\alpha} p_j^{(m+1)-k}$.

3 Stability of the Fractional BTCS Method

We use the discrete von Neumann stability criterion to derive the stability condition for the implicit finite difference scheme (1). The von Neumann stability method is discussed in [19]. Yuste and Acedo [20] applied the method to find the stability condition for the explicit finite difference scheme of time fractional diffusion equation, Sweilam [18] derived the stability condition for the explicit finite difference echeme of time fractional wave equation by using von Neumann stability criterion.

First, we assume a solution (a sub-diffusive mode or eigenfunction) with the form $p_j^m = \zeta_m e^{iqj\Delta x}$, equation (2) gives

$$\left[1+4S_{\alpha}\sin^{2}\left(\frac{q\Delta x}{2}\right)\right]\zeta_{m+1}=-\sum_{k=2}^{m+1}\omega_{k}^{\alpha}\zeta_{(m+1)-(k-1)}.$$

The stability of the solution is determined by the behavior of ζ_m , which is a function of *t*., and assuming that $\zeta_{m+1}(t) = \xi \zeta_m(t)$, where ξ is independent of *t*. We obtain

$$\left[1+4S_{\alpha}\sin^{2}\left(\frac{q\Delta x}{2}\right)\right]\xi = -\sum_{k=2}^{m+1}\omega_{k}^{\alpha}\xi^{-k+2}$$

If $|\xi| > 1$, the temporal factor goes to infinity and the mode is unstable. Considering the extreme value $\xi = -1$, we obtain the following bound on S_{α} :

$$4S_{\alpha}\sin^{2}\left(\frac{q\Delta x}{2}\right) \leq \sum_{k=1}^{m+1} (-1)^{k} \omega_{k}^{\alpha} .$$

As $m \to \infty$, we obtain $S_{\alpha} \leq \frac{1}{2^{2-\alpha}}$.

5 Truncating Error of the Fractional BTCS Method

The truncating error T(x,t) of the fractional BTCS difference scheme is obtained from equation (2) as follows:

$$T(x,t) = \frac{1}{\left(\Delta t\right)^{\alpha}} \sum_{k=1}^{m+1} \omega_k^{\alpha} p_j^{(m+1)-(k-1)}$$
$$-\frac{a_{j+1}p_{j+1}^{m+1} - (a_{j+1} + a_{j-1})p_j^{m+1} + a_{j-1}p_{j-1}^{m+1}}{2\left(\Delta x\right)^2} + f_j$$

As we have

$$p_{xx} = \frac{p_{j-1}^{m+1} - 2p_j^{m+1} + p_{j+1}^{m+1}}{\left(\Delta x\right)^2} + O\left(\Delta x^2\right),$$

and

$${}_{0}D_{t}^{\alpha}p(x,t) = \frac{1}{\left(\Delta t\right)^{\alpha}}\sum_{k=1}^{m+1}\omega_{k}^{\alpha}p_{j}^{(m+1)-(k-1)} + O\left(\Delta t^{\nu}\right).$$

Thus, we have

 $T(x,t) = O(\Delta t^{\nu}) + O(\Delta x^{2}),$

where ν is the accuracy of the temporal order, which depends on the choice of the generating function that was used to approximate the values of general binomial

coefficients ω_k^{α} . Since we have used the first order

generating function, therefore $\nu = 1$, and hence the truncation error is of the following order,

$$T(x,t) = O(\Delta t) + O(\Delta x^2)$$

Note that $T(x,t) \to 0$ as $\Delta t, \Delta x \to 0$. It is possible to obtain higher order accurate in time formulas by using the higher order generating functions for the binomial coefficients ω_k^{α} , but then the stability bound on S_{α} becomes smaller [20].

6 Numerical Solutions

We test the reliability of the numerical scheme by presenting the numerical solutions of test examples.



Figure 1. Numerical solutions of example 1.

Example 1

Consider the following fractional diffusion equation

$$\frac{\partial^{\alpha} p}{\partial t^{\alpha}} = \frac{\partial^2 p}{\partial x^2}, \qquad 0 < x < 1, \quad 0 < t < 1.$$

The initial condition is p(x,0) = x(1-x), and the boundary conditions are p(0,t) = p(1,t) = 1. We obtain the following numerical solutions by using the numerical scheme given above.



Figure 2. Numerical solutions of example 2.

Example 2

Consider the following fractional diffusion equation

$$\frac{\partial^{\alpha} p}{\partial t^{\alpha}} = \frac{\partial^2 p}{\partial x^2}, \qquad 0 < x < 1, \quad 0 < t < 1.$$

The initial condition is $p(x,0) = \sin(\pi x)$, and the boundary conditions are p(0,t) = p(1,t) = 1. We obtain the following numerical solutions by using the numerical scheme given above.

Example 3

Consider the following fractional diffusion equation

$$\frac{\partial^{\alpha} p}{\partial t^{\alpha}} = \frac{\partial^2 p}{\partial x^2}, \qquad -\infty < x < \infty, \quad 0 < t < 10.$$

The initial condition is $p(x,0) = \delta(x)$, and the boundary conditions are $p(x,t) \rightarrow 0$ as $|x| \rightarrow \infty$. We obtain the following numerical solutions by using the numerical scheme given above.



Figure 3. Numerical solutions of example 3.

Example 4

Consider the following fractional diffusion equation

$$\frac{\partial^{\alpha} p}{\partial t^{\alpha}} = \frac{\partial^{2} p}{\partial x^{2}} + \frac{2x(1-x)t^{2-\alpha}}{\Gamma(3-\alpha)} + 2(t^{2}+1)$$
$$0 < x < 1, \quad 0 < t < 1.$$

The initial condition is p(x,0) = x(1-x), and the boundary conditions are p(0,t) = p(1,t) = 1. We obtain the numerical solutions by using the numerical scheme given above. Numerical solution is plotted together with the exact solution $p(x,t) = x(1-x)(t^2+1)$.



Figure 4: Numerical solutions of example 4.

7 Conclusions

Fractional differential equations are used to describe complex system, such as, anomalous diffusion in porous media. In this study, we consider time-fractional diffusion equation with the source term to describe transport through porous media such as hydrocarbon reservoirs and aquafers. We have developed an implicit finite difference scheme based on the Grunwald-Letnikov derivative for finding the numerical solutions of the fractional diffusion equation. We employ uniform mesh on the space-time domain. The stability of numerical scheme is established by using von-Neumann stability criterion. The stability condition is obtained and which is numerically tested by three examples. The truncation error is found which shows that the above numerical scheme is first order accurate in time and second order accurate in space. Although the higher order accuracy in time can be obtained but that narrows the stability bound.

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