Comparative Study of Implicit and Crank-Nicolson Finite Difference Scheme for Fractional Radon Diffusion Equation

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Abstract: In this paper, we develop Implicit and Crank-Nicolson finite difference scheme for time fractional radon diffusion equation. We discuss the stability and convergence of both the scheme. As an application of this scheme, we obtain the numerical solutions of the test problem and represented graphically by mathematical software Mathematica and finally, we compare the rate of convergence of both the scheme.

Index Terms – Fractional calculus, Explicit Finite difference, Caputo formula, Stability, Convergence.

1. INTRODUCTION

The subject of fractional calculus that is, calculus of integrals and derivatives of any arbitrary real or complex order has gained considerable popularity and importance during the past four decades and longer, due mainly to its demonstrated applications in numerous seemingly diverse and widespread fields of science and engineering, bio-science, applied mathematics, finance etc. [1, 2, 6]. In the development of fractional calculus and applications anomalous diffusion equation has received great interest. A physical approach to anomalous diffusion equation containing fractional order derivatives in time or space or time-space. As analytical solution of fractional diffusion equation is very difficult to find thus researchers develop the finite difference schemes to find numerical solution [3, 4, 7, 8, 9, 10, 11]. Radon is naturally occurring radioactive gas which is colorless, odorless and comes from the decay of uranium in rocks, soil and groundwater. Radon is present outdoors and indoors. Due to hazards properties of radon researchers have great interest to study the radon transport through soil, activated charcoal, concrete, etc. [5, 12, 13, 14, 15, 16]. In this paper we study the diffusion of radon in an activated charcoal medium. The diffusion theory came from the famous German physiologist Adolf Fick (1829-1901). He stated that the flux density J is proportional to the gradient of concentration. This gives,

\[ J = -D \frac{\partial c}{\partial x} \]

where J is the radon flux density is diffusion coefficient \( \frac{\partial c}{\partial x} \) is gradient of radon concentration and D is diffusivity coefficient of radon.

Now the change in concentration to change in time and position is stated by the Fick’s second law which is the extension of Fick’s first law, that gives,

\[ \frac{\partial C(x, t)}{\partial t} = \frac{\partial^2 C(x, t)}{\partial x^2} - \lambda c(x, t) \]

where \( \lambda = 2.1 \times 10^{-6} \text{s}^{-1} \) is the decay constant. A theoretical study of radon measurements with activated charcoal was studied by Nikezic and Urosevic [17]. In this study we develop the time fractional Implicit and Crank-Nicolson finite difference method for fractional order radon diffusion equation. We consider the following time fractional radon diffusion equation [TFRDE],

\[ \frac{\partial^\alpha C(x, t)}{\partial t^\alpha} = D \frac{\partial^2 C(x, t)}{\partial x^2} - \lambda C(x, t), \quad 0 < x < L, \quad 0 \leq \alpha \leq 1, \quad t \geq 0 \] (1.1)

initial condition : \( C(x, 0) = 0, \quad 0 < x < L \) (1.2) boundary conditions : \( C(0, t) = c_0 \) and \( \frac{\partial C(x, t)}{\partial x} = 0, \quad t \geq 0 \) (1.3)

Definition 1.1:- The Caputo time-fractional derivative of order \( \alpha \), \( 0 < \alpha \leq 1 \) is defined by,

\[ \frac{\partial^\alpha C(x, t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial C(x, \eta)}{\partial \eta} \frac{d\eta}{(t-\eta)^\alpha}; \quad 0 < \alpha < 1 \]

\[ \frac{\partial^\alpha C(x, t)}{\partial \eta} ; \quad \alpha = 1 \]
2. FINITE DIFFERENCE SCHEME:

2.1 Implicit Finite Difference Scheme for TFRDE:

In this section, we develop the time fractional implicit finite difference method for fractional order radon diffusion equation (1.1)-(1.3).

We define,

\[ t_k = k \tau; \ k = 0,1,2, \ldots, N \text{ and } x_i = i h; \ i = 0,1,2, \ldots, N \]

where

\[ \tau = \frac{T}{N} \text{ and } h = \frac{L}{M} \]

Let \( C(x_i,t_k); i = 0,1,2, \ldots, M \text{ and } k = 0,1,2, \ldots, N \) be the exact solution of time fractional radon diffusion equation (TFRDE) (1.1)-(1.3) at mesh point \( (x_i,t_k) \). Let \( C_i^k \) be the numerical approximation of the point \( C(x_i,t_k) \). The time fractional derivative is approximated by the following scheme,

\[
\frac{\partial^\alpha C(x_i,t_k)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^{k} \frac{C(x_i,t_{j+1}) - C(x_i,t_j)}{\tau} \int_{t_j}^{t_{j+1}} \frac{d\eta}{(t_{k+1} - \eta)^\alpha} + O(\tau)
\]

Now for \( \frac{\partial^2 C}{\partial x^2} \), we adopt a symmetric second order difference quotient in space at time level \( t = t_{k+1} \)

\[
\frac{\partial^2 C}{\partial x^2} = \frac{C(x_{i-1},t_{k+1}) - 2C(x_i,t_{k+1}) + C(x_{i+1},t_{k+1})}{h^2}
\]

Therefore, substituting in equation (1.1), we get

\[
\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left[ C_i^{k+1} - C_i^k \right] + \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=1}^{k} b_j \left[ C_i^{k+j} - C_i^{k-j} \right] = D \frac{C_i^{k+1} - C_i^{k-1}}{h^2} + \lambda C(x_i,t_k)
\]

where \( b_j = (j+1)^{1-\alpha} - j^{1-\alpha}; j = 0,1,2, \ldots, \).

Therefore, the complete fractional approximated initial boundary value problem is,

\[
\begin{align*}
-rc_{i,-1}^k + (1 + 2r)c_i^k - rc_{i+1}^k &= (1 - \mu)c_i^0; & \text{for } k &= 0 \\
-rc_{i-1}^{k+1} + (1 + 2r)c_i^{k+1} - rc_{i+1}^{k+1} &= (1 - \mu - b_1)c_i^k + \sum_{j=1}^{k-1} (b_j - b_{j+1})c_i^{k-j} + b_kc_i^0; & \text{for } k &> 1
\end{align*}
\]

initial condition: \( c_i^0, i = 0,1,2, \ldots, M \)

boundary conditions: \( c_0^k = c_0^0 \text{ and } c_{M+1}^k = c_{M-1}^0; k = 0,1,2, \ldots, N \)

where \( r = \frac{\mu}{h^2} \); \( \mu = \lambda \Gamma(2-\alpha) \tau^\alpha; b_j = (j+1)^{1-\alpha} - j^{1-\alpha}; j = 0,1,2, \ldots, k \); \( \alpha = 0,1,2, \ldots, M \text{ and } k = 0,1,2, \ldots, N \).

The problem (2.1)-(2.4) is a complete discretization of the problem (1.1)-(1.3). Therefore, the fractional approximated initial boundary value problem (2.1)-(2.4) can be written in the following matrix equation form

\[
AC^1 = (1 - \mu)C^0 + E; \text{for } k = 0
\]

\[
AC^{k+1} = (1 - \mu - b_1)C^k + \sum_{j=1}^{k-1} (b_j - b_{j+1})C^{k-j} + b_kC^0 + F; \text{ for } k > 1
\]

where

\[
A = \begin{pmatrix}
1 & 2r & 0 & \cdots & \cdots \\
-2r & 1 & 2r & \cdots & \cdots \\
\vdots & \vdots & \vdots & \ddots & \cdots \\
-2r & -2r & \cdots & 1 & 2r
\end{pmatrix}
\]

\[
C^1 = [c_1^1, c_2^1, c_3^1, \ldots, c_M^1]^T; \ C^0 = [c_0^0, c_0^0, c_0^0, \ldots, c_0^0]^T; \ C^k = [c_k^1, c_k^2, c_k^3, \ldots, c_k^M]^T;
\]
\[ E = [r c_0^1, 0, \ldots, \ldots, 0]^T; F = [r c_0^{k+1}, 0, \ldots, \ldots, 0]^T; r = \frac{D\Gamma(2 - \alpha)r^\alpha}{h^2}; \mu = \lambda\Gamma(2 - \alpha)r^\alpha; \\
b_j = (j + 1)^{1 - \alpha} - j^{1 - \alpha}; j = 0, 1, 2, \ldots, k; i = 0, 1, 2, \ldots, M \quad \text{and} \quad k = 0, 1, 2, \ldots, N \]

### 2.1 Crank-Nicolson Finite Difference Scheme for TFRDE:

In this method, we discretize the time fractional derivative by Caputo sense as in previous section and for \(\partial^2x^2\), we adopt the second order central difference scheme in space for each interior grid point \(x_i, 0 \leq i \leq M\). Therefore,

\[
\frac{\partial^2C(x, t_k)}{\partial t^2} = \frac{1}{2}[\delta^2C_i^{k+1} + \delta^2C_i^k] \\
= \frac{1}{2}[c_i^{k+1} - 2c_i^k + c_i^{k-1}] + \frac{\Sigma_{j=1}^{k-1}(b_j - b_{j+1})c_i^j}{h^2}
\]

where \(\delta_{k}\) is the central difference operator.

The fractional approximated initial boundary value problem is

\[-ac_i^0 + (1 + 2\alpha)c_i^1 - ac_i^1 = ac_i^0 + (1 - 2\alpha - \beta)c_i^0 + ac_i^1; \quad \text{for } k = 0, \quad (2.7)\]

For \(k \geq 1\), we have,

\[-ac_i^{k+1} + (1 + 2\alpha)c_i^{k+1} - ac_{i+1}^{k+1} \\
= ac_i^{k+1} + (1 - 2\alpha - \beta - b_1)c_i^k + ac_{i+1}^{k+1} + \Sigma_{j=1}^{k-1}(b_j - b_{j+1})c_i^j + b_kc_i^0 \quad \text{for } k = 1, \ldots, M \quad (2.8)\]

The initial condition, \(c_i^0 = 0, i = 0, 1, 2, \ldots, M\)

The boundary conditions, \(c_0^k = c_0^0 = 0, \quad k = 0, 1, 2, \ldots, M \quad (2.9)\)

where \(\alpha = \frac{D\Gamma(2 - \alpha)r^\alpha}{2h^2}, \quad \beta = \lambda\Gamma(2 - \alpha)r^\alpha \quad (2.10)\)

The fractional approximated initial boundary value problem can be written in the following matrix equation form,

\[ PC^{k+1} = QC^0 + S \quad (2.11) \]

\[ PC^k = Cc^k + \Sigma_{j=1}^{k-1}(b_j - b_{j+1})c^{k-j} + b_kc^0 + S \quad (2.12) \]

Where,

\[ P = \begin{pmatrix} 1 + 2\alpha & -\alpha & \cdots & \cdots \\
-\alpha & 1 + 2\alpha & -\alpha & \cdots \\
\vdots & \vdots & \ddots & \ddots \\
-\alpha & -2\alpha & 1 + 2\alpha & \cdots \end{pmatrix}; \]

\[ Q = \begin{pmatrix} 1 - 2\alpha - \beta & \alpha & \cdots & \cdots \\
\alpha & 1 - 2\alpha - \beta & \alpha & \cdots \\
\vdots & \vdots & \ddots & \ddots \\
\alpha & -2\alpha & 1 - 2\alpha - \beta & \cdots \end{pmatrix}; \]

\[ C = \begin{pmatrix} 1 - 2\alpha - \beta & \alpha & \cdots & \cdots \\
\alpha & 1 - 2\alpha - \beta & \alpha & \cdots \\
\vdots & \vdots & \ddots & \ddots \\
\alpha & -2\alpha & 1 - 2\alpha - \beta & \cdots \end{pmatrix}; \]

\[ C^k = [c_1^k, c_2^k, c_3^k, \ldots, \ldots, c_M^k]^T; \]

\[ C^0 = [c_1^0, c_2^0, c_3^0, \ldots, \ldots, c_M^0]^T; \]

\[ S = [rc_0^0, 0, 0, \ldots, \ldots, 0]^T; \]

\[ \alpha = \frac{D\Gamma(2 - \alpha)r^\alpha}{2h^2}; \quad \beta = \lambda\Gamma(2 - \alpha)r^\alpha \]

and \(b_j = (j + 1)^{1 - \alpha} - j^{1 - \alpha}, j = 1, 2, \ldots, k\)

### 3. Stability and Convergence of the Scheme:

#### 3.1 Implicit Finite Difference Scheme for TFRDE:

**Lemma 3.1.1**: [17] If \(\lambda_j(A); j = 1, 2, \ldots, M - 1\) represents eigenvalues of matrix \(A\) then we prove the following results,

1. \(|\lambda_j(A)| \leq 1; j = 1, 2, \ldots, M - 1\)
2. \(|\|A^{-1}\||_2 \leq 1\)

**Theorem (3.1.1)**: The solution of the fractional approximated IBVP \((2.1)-(2.4)\) is unconditionally stable.[17]
Also, the convergence of the approximate finite difference scheme (2.1) - (2.4). Let \( C(x_i, t_k) \) be the exact solution of the TFRDE (1.1)-(1.3) and \( C_i^k \) be the exact solution of the discrete equation (2.1)-(2.4) at the mesh point \((x_i, t_k)\), where \( i = 0, 1, ..., M - 1; k = 1, 2, ..., N\) We define, \( e_i^k = C(x_i, t_k) - C_i^k \), where \( i = 0, 1, ..., M - 1; k = 1, 2, ..., N \) and \( E^k = (e_1^k, e_2^k, ..., e_N^k) \)

Now, we have, \( E^0 = 0, E_0^k = 0 \) and \( E_N^k = 0 \).

From (2.1), we get,

\[
-re_{i-1}^k + (1 + 2r)e_i^k - re_{i+1}^k = (1 - \mu)e_i^0; \text{for } k = 0 \tag{4.1}
\]

From (2.2), we get,

\[
-re_{i-1}^{k+1} + (1 + 2r)e_i^{k+1} - re_{i+1}^{k+1} = (1 - \mu - b_1)e_i^k + \sum_{j=1}^{k-1}(b_j - b_{j+1})e_i^{k-j} + b_ke_i^0; \tag{4.2}
\]

for \( k \geq 1 \)

where \( r = \frac{D(2 - \alpha)\tau^\alpha}{h^2} \); \( \mu = \lambda \Gamma(2 - \alpha)\tau^\alpha; b_j = (j + 1)^{1-\alpha} - j^{1-\alpha}; j = 0, 1, 2, ..., k \); \( i = 0, 1, 2, ..., M \) and \( k = 0, 1, 2, ..., N \).

**Theorem 3.1.2** [17] The fractional order implicit finite difference scheme (2.1)-(2.4) for TFRDE (1.1)-(1.3) is convergent and the solution \( C_i^k \) of the discrete scheme (2.1)-(2.4) and the solution \( C(x_i, t_k) \) of the equation (1.1)-(1.3) satisfy,

\[
||C(x_i, t_k) - C_i^k|| \leq k||E||_{\infty} + O(\tau^{1-\alpha}, h^2); i = 0, 1, 2, ..., M - 1; k = 0, 1, ..., N
\]

**3.2 Crank-Nicolson Finite Difference Scheme for TFRDE:**

**Lemma 3.2.1:** [18] If \( \lambda_i(P); j = 1, 2, ..., M - 1 \) represents eigenvalues of matrix \( P \) then we prove the following results,

1) \( |\lambda_j(P)| \geq 1; j = 1, 2, ..., M - 1 \)
2) \( \|P^{-1}\| \leq 1 \)
3) \( \|\Delta\| \leq 1 \)
4) \( \|C\| \leq 1 \)

**Theorem 3.2.1:** [18] The solution of the finite difference scheme (2.7)-(2.10) for TFRDE (1.1)-(1.3) is unconditionally stable.

**Theorem 3.2.2:** [18] The finite difference scheme (2.7)-(2.10) for TFRDE (1.1)-(1.3) is unconditionally convergent, that is to prove

\[
||E^k||_2 \leq ||E^0||_2 , \text{as } (h, \tau) \to (0, 0)
\]

**4. COMPARATIVE STUDY OF NUMERICAL SOLUTION OF BOTH THE SCHEME:**

In this section, we obtain the approximated solution of TFRDE of both the Implicit and C-N finite difference schemes with initial and boundary conditions and compare their solutions. To obtain the numerical solution, it is important to use some analytical model. Thus, we present an example to demonstrate that TFRDE can be applied to simulate behavior of a fractional diffusion equation with the following parameters by using Mathematica Software. We consider the following, dimensionless time fractional radon diffusion equation with suitable initial and boundary conditions,

\[
\frac{\partial^\alpha C(x, t)}{\partial t^\alpha} = D \frac{\partial^2 C(x, t)}{\partial x^2} - \lambda C(x, t), 0 < x < L; 0 < \alpha < 1; t > 0
\]

initial condition: \( C(0, t) = 0, 0 < x < L \)

boundary conditions: \( C(L, t) = 0 \) and \( \frac{\partial C(x)}{\partial x} = 0, t \geq 0 \)

with the radon diffusion coefficient \( D = 1.43 \times 10^{-6} Bq/m^3 \). The numerical solutions obtained at \( t = 0.05 \) by considering the parameters \( L = 1.7278 cm \),

\[
\lambda = 2.1 \times 10^{-6} s^{-1}, \tau = 0.05, k = 4 m^2/kg, \rho = 0.5 g/cm^3, C_0 = 200 Bq/m^3,
\]

\[
C(0, t) = 40 \times 10^3, \alpha = 0.9.
\]

The comparison of solutions of RDE of Implicit and Crank Nicolson finite difference scheme respectively for \( \alpha = 0.9 \) is shown in table and graphically as in figure.
Figure. The comparative approximate solution of radon diffusion equation for $\alpha = 0.9$

<table>
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<tr>
<th>Length</th>
<th>Implicit TFRDE</th>
<th>C-N TFRDE</th>
<th>Difference</th>
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<td>0.0000</td>
<td>0.0000</td>
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<td>$2.62202 \times 10^{-6}$</td>
</tr>
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<tr>
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Table. Comparison of solutions of RDE of Implicit and Crank Nicolson finite difference scheme respectively for $\alpha = 0.9$

5. CONCLUSION

We discuss the fractional order Implicit and Crank-Nicolson finite difference scheme for TFRDE and also, the stability and convergence of the scheme. As an application of this method we obtain the numerical solution of text problem and its solution is simulated graphically by mathematical software Mathematica. Also we observe that, the Implicit and Crank Nicolson finite difference scheme for Radon diffusion equation work equally. The difference between the solutions is not significantly differing, but Radon diffusion is very hazardous for human life. Therefore, the small change in solution is also important. The Crank-Nicolson finite difference scheme is more accurate and reliable than the implicit finite difference scheme because it has a higher order accuracy.
6. REFERENCES