Fourth-order numerical solution of a fractional PDE with the nonlinear source term in the electroanalytical chemistry

M. ABBASZADE AND A. MOHEBBI[1]

Department of Applied Mathematics, Faculty of Mathematical Science, University of Kashan, Kashan, Iran

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ABSTRACT

The aim of this paper is to study the high order difference scheme for the solution of a fractional partial differential equation (PDE) in the electroanalytical chemistry. The space fractional derivative is described in the Riemann-Liouville sense. In the proposed scheme we discretize the space derivative with a fourth-order compact scheme and use the Grunwald-Letnikov discretization of the Riemann-Liouville derivative to obtain a fully discrete implicit scheme and analyze the solvability, stability and convergence of proposed scheme using the Fourier method. The convergence order of method is $O(\tau + h^4)$. Numerical examples demonstrate the theoretical results and high accuracy of proposed scheme.

Keywords: Electroanalytical chemistry, reaction-sub-diffusion, compact finite difference, Fourier analysis, solvability, unconditional stability, convergence.

1. INTRODUCTION

In recent years there has been a growing interest in the field of fractional calculus [6, 16, 22, 26]. Fractional differential equations have attracted increasing attention because they have applications in various fields of science and engineering [4]. Many phenomena in fluid mechanics, viscoelasticity, chemistry, physics, finance and other sciences can be described very successfully by models using mathematical tools from fractional calculus, i.e., the theory of derivatives and integrals of fractional order. Some of the most applications are given in the book of Oldham and Spanier [19] and the papers of Metzler and Klafter [15], Bagley and Trovik [1]. Many considerable works on the theoretical

[1] Corresponding author: Email : a_ mohebbi@kashanu.ac.ir

analysis [5, 25] have been carried on, but analytic solutions of most fractional differential equations cannot be obtained explicitly. So many authors have resorted to numerical solution strategies based on convergence and stability analysis[4, 10, 13, 24]. Liu has carried on so many work on the finite difference method of fractional differential equations [14, 11, 12]. There are several definitions of a fractional derivative of order $\alpha > 0$ [22, 19]. The two most commonly used are the Riemann-Liouville and Caputo. The difference between two definitions is in the order of evaluation [18]. We start with recalling the essentials of the fractional calculus. The fractional calculus is a name for the theory of integrals and derivatives of arbitrary order, which unifies and generalizes the notions of integer-order differentiation and n-fold integration. We give some basic definitions and properties of the fractional calculus theory.

Definition 1. For $\mu \in \Re$ and $x > 0$, a real function $f(x)$, is said to be in the space C_μ if there exists a real number $p > \mu$ such that $f(x) = x^p f_1(x)$, where $f_1(x) \in C(0,\infty)$, and for $m \in \mathrm{N}$ it is said to be in the space C_μ^m if $f^m \in C_\mu$.

Definition 2. The Riemann-Liouville fractional integral operator of order $\alpha > 0$ for a function $f(x) \in C_\mu$, $\mu \geq -1$ is defined as

$$J^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-t)^{\alpha-1} f(t)dt, \qquad \alpha > 0,\ x > 0,\ J^0 f(x) = f(x).$$

Also we have the following properties

$$\bullet J^\alpha J^\beta f(x) = J^{\alpha+\beta} f(x),$$

$$\bullet J^\alpha J^\beta f(x) = J^\beta J^\alpha f(x),$$

$$\bullet J^\alpha x^\gamma = \frac{\Gamma(\gamma+1)}{\Gamma(\alpha+\gamma+1)} x^{\alpha+\gamma}.$$

Definition 3. If m be the smallest integer that exceeds α, the Caputo Riemann-Liouville fractional derivatives operator of order $\alpha > 1$ is defined as, respectively,

$$ {}_0^C D_t^\alpha f(x) = \begin{cases} \dfrac{1}{\Gamma(m-\alpha)} \displaystyle\int_0^x (x-t)^{m-\alpha-1} \left. \frac{d^m f(x)}{dx^m} \right|_{x=t} dt, & m-1 \langle \alpha \langle m,\ m \in \mathrm{N} \\ \dfrac{d^m f(x)}{dx^m}, & m = \alpha, \end{cases} \tag{1.1}$$

$$
{}_0D_t^{\alpha} f(x)=\begin{cases} \dfrac{d^m}{dx^m}\dfrac{1}{\Gamma(m-\alpha)}\int\limits_0^x (x-t)^{m-\alpha-1} f(t)\,dt \;, m-1 \langle \alpha \langle m \;, m\in \mathrm{N} \\ \dfrac{d^m f(x)}{dx^m}, \qquad m=\alpha. \end{cases} \tag{1.2}
$$

Due mainly to the works of Oldham and his co-authors [7, 8, 9, 20, 21], electrochemistry is one of those fields in which fractional-order integrals and derivatives have a strong position and bring practical results. Although the idea of using a half-order fractional integral of current, ${}_0D_t^{-1/2}i(t)$, can be found also in the works of other authors, it was the paper by Oldham [20] which definitely opened a new direction in the methods of electrochemistry called semi-integral electroanalysis. One of the important subjects for study in electrochemistry in the determination of the concentration of analyzed electroactive species near the electrode surface. The method suggested by Oldham and Spanier [21] allows, under certain conditions, replacement of a problem for the diffusion equation by a relationship on the boundary (electrode surface). Based on this idea, Old ham [20] suggested the utilization in experiment the characteristec described by the function

$$
m(t) ={}_0 D_t^{-\frac{1}{2}} i(t)
$$

which is the fractional integral of the current $i(t)$, as the observed function, whose values can be obtained by measurements. Then the subject of main interest, the surface concentration Cs(t) of the electroactive species, can be evaluated as

$$
C_s(t)=C_0-k_0 D_t^{-\frac{1}{2}} i(t), \tag{1.3}
$$

where k is a certain constant described below, and C_0 is the uniform concentration of the electroactive species throughout the electrolytic medium at the initial equilibrium situation characterized by a constant potential, at which no electrochemical reaction of the considered species in possible. The relationship (1.3) was obtained by considering the following problem for a classical diffusion equation [9]

$$
\begin{aligned}
&\frac{\partial C(x,t)}{\partial t}=D_{\bullet}\left[\frac{\partial^2 C(x,t)}{\partial x^2}\right], \quad 0\langle x\langle \infty, \quad t\rangle 0, \\
&C(\infty,0)=C_0\,, \quad C(x,0)=C_0\,, \\
&D_{\bullet}\left[\frac{\partial C(x,t)}{\partial t}\right]_{x=0}=\frac{i(t)}{n\,AF}
\end{aligned} \tag{1.4}
$$

Where $D_{\bullet}$ is diffusion coefficient. A is the electrode area, F is Faraday's constant and n is the number of electrons involved in the reaction, the constant k in (1.3) is expressed as

$$k=\frac{1}{n\,AF\,\sqrt{D_{\bullet}}}.$$

Instead of the classical diffusion equation (1.4), it is possible to consider the fractional order diffusion equation [23]

$$\frac{\partial C(x,t)}{\partial t}={}_0D_t^{1-\gamma}\left[\frac{\partial^2 C(x,t)}{\partial x^2}\right], \tag{1.5}$$

where $0<\gamma<1$. In this paper, we consider the generalized form of the Eq. (1.5) with the nonlinear source term and on a bounded domain with the following form

$$\begin{aligned}&\frac{\partial u(x,t)}{\partial t}={}_0D_t^{1-\gamma}\left[\kappa_1\frac{\partial^2 u(x,t)}{\partial x^2}-\kappa_2 u(x,t)\right]+f(u(x,t),x,t),\\ &0\le x\le L, \qquad\qquad 0\le t\le T,\end{aligned} \tag{1.6}$$

The boundary and initial conditions are

$$u(0,t)=\varphi_1(t),\quad u(L,t)=\varphi_2(t),\quad 0<t<T, \tag{1.7}$$

$$u(x,0)=\psi(x),\quad 0<x<L. \tag{1.8}$$

where $0<\gamma\le 1$, $\kappa_1>0$, $\kappa_2\ge 0$ and the source term $f(u,x,t)\in C^1[0,L]$. The symbol ${}_0D_t^{1-\gamma}$ is the Riemann-Liouville fractional derivative operator and is defined as

$${}_0D_t^{1-\gamma}u(x,t)=\frac{1}{\Gamma(\gamma)}\frac{\partial}{\partial t}\int_0^t\frac{u(x,\eta)}{(t-\eta)^{1-\gamma}}d\eta,$$

Where $\Gamma(.)$ is the gamma function. Also, let $f(u,x,t)$ satisfies the Lipschitz condition with respect to u:

$$|f(\bar{u},x,t)-f(\tilde{u},x,t)|\le\ell|\bar{u}-\tilde{u}|,\qquad \forall\bar{u},\tilde{u}$$

where ℓ is the Lipschitz constant. The aim of this paper is to propose a numerical scheme of order $O(\tau+h^4)$ for the solution of Eq. (1.6). We apply a fourth order difference scheme for discretizing the spatial derivative and Grunwald-Letnikov discretization for the Riemann-Liouville fractional derivative. We will discuss the stability of proposed method is a by the Fourier method and show that the compact finite difference scheme converges with the spatial accuracy of fourth order using matrix analysis. The outline of this paper is as follows. In Section 2, we introduce the derivation of new method for the solution of Eq. (1.6). This scheme is based on approximating the time derivative of mentioned equation by a scheme of order $O(\tau)$ and spatial derivative with a fourth order compact finite difference scheme. In this section we obtain the matrix form of the proposed method and show the solvability of it. In Section 3 we prove the unconditional stability property of method. In Section 4 we present the convergence of method and show that the convergence order is $O(\tau+h^4)$. In Section 5 we report the numerical experiments of solving Eq. (1.1) with the method developed in this paper for several test problems. Finally concluding remarks are drawn in Section 6.

2. DERIVATION OF METHOD

For positive integer numbers M and N, let $h=L/M$ denotes the step size of spatial variable, x, and $\tau = T/N$ denotes the step size of time variable, t. So we define

$$x_j = jh \qquad , \quad j = 0,1,2,\ldots,M \,,$$

$$t_k = k\tau \qquad , \quad k = 0,1,2,\ldots,N \,.$$

The exact and approximate solutions at the point (x_j, t_k) are denoted by u_j^k and U_j^k respectively. We first state the fourth-order compact scheme of second derivative in the following lemma.

Lemma 1([4]). The fourth-order compact difference operator with maintaining three point stencil to approximate the u_{xx} is

$$\frac{\delta_x^2}{h^2\left(1+\frac{1}{12}\delta_x^2\right)} u_j^k = \left.\frac{\partial^2 u}{\partial x^2}\right|_j^k - \frac{1}{240}\left.\frac{\partial^4 u}{\partial x^4}\right|_j^k h^4 + O(h^6), \tag{2.1}$$

in which $\delta_x^2 u_j = (u_{j-1} - 2u_j + u_{j+1})$.

Now using the relationship between the Grunwald-Letnikov formula and the Riemann-Liouville fractional derivative, we can write

$$ {}_0D_t^{1-\gamma} f(t) = \frac{1}{\tau^{1-\gamma}} \sum_{k=0}^{[t/\tau]} \omega_k^{(1-\gamma)} f(t - k\tau) + \mathrm{O}(\tau^p), \tag{2.2} $$

Where $\omega_k^{(1-\gamma)}$ k are the coefficients of the generating function, that is,

$\omega(z,\alpha) = \sum_{k=0}^{\infty} \omega_k^{(\alpha)} z^k$ We will discuss the case for $\omega(z,\alpha) = (1-z)^{\alpha}$ and thus p=1. In this case the coefficients are $\omega_0^{(\alpha)} = 1$ *and* $\omega_k^{(\alpha)} = (-1)^k \binom{\alpha}{k} = (-1)^k \frac{\alpha(\alpha-1)\ldots(\alpha-k+1)}{k!}$ for $k \geq 1$ and can be evaluated recursively,

$$ \omega_0^{(\alpha)} = 1, \quad \omega_k^{(\alpha)} = \left(1 - \frac{\alpha+1}{k}\right) \omega_{k-1}^{(\alpha)}, \quad k \geq 1. \tag{2.3} $$

Now, we put

$$ \lambda_l = \omega_l^{(1-\gamma)} = (-1)^l \binom{1-\gamma}{l}, \qquad l = 0,1,\ldots,k. $$

So $\lambda_0 = 1$. If we consider Eq. (1.6)-(1.8) at the point (x_j, t_k), we can write

$$ \frac{\partial u(x_j,t_k)}{\partial t} = ({}_0D_t^{1-\gamma}) \left[\kappa_1 \frac{\partial^2 u(x_j,t_k)}{\partial x^2} - \kappa_2 u(x_j,t_k) \right] + f(u(x_j,t_k), x_j, t_k). \tag{2.4} $$

Since $f(u,x,t)$ has the first order continuous derivative it follows that

$$ f(u(x_j,t_k), x_j, t_k) = f(u(x_j,t_{k-1}), x_j, t_{k-1}) + O(\tau). $$

Also, we can write

$$ \frac{\partial u(x_j,t_k)}{\partial t} = \frac{u(x_j,t_k) - u(x_j,t_{k-1})}{\tau} + O(\tau), $$

$$ \left(1 + \frac{1}{12}\delta_x^2\right) \frac{\partial^2 u(x_j,t_k)}{\partial x^2} = \frac{\delta_x^2 u(x_j,t_k)}{h^2} + O(h^4), $$

$$ {}_0D_t^{1-\gamma} \left(\frac{\partial^2 u(x_j,t_k)}{\partial x^2} \right) = \tau^{\alpha-1} \sum_{l=0}^{k} \lambda_l \frac{\partial^2 u(x_j,t_{k-1})}{\partial x^2} + O(\tau), $$

$$ {}_0D_t^{1-\gamma}u(x_j,t_k)=\tau^{\alpha-1}\sum_{l=0}^{k}\lambda_l u(x_j,t_k)+O(\tau), $$

From Eq. (2.4) and above results, we can obtain

$$ \begin{aligned} \left(1+\frac{1}{12}\delta_x^2\right)u(x_j,t_k)&=\left(1+\frac{1}{12}\delta_x^2\right)u(x_j,t_{k-1})+\mu_1\sum_{l=0}^{k}\lambda_l\delta_x^2u(x_j,t_{k-l})\\ &+\mu_2\sum_{l=0}^{k}\lambda_l\left(1+\frac{1}{12}\delta_x^2\right)u(x_j,t_{k-l})+\tau\left(1+\frac{1}{12}\delta_x^2\right)f_j^{k-1}+R_j^k \end{aligned} \tag{2.5} $$

where, $\mu_1=\kappa_1\dfrac{\tau^\gamma}{h^2}$, $\mu_2=\kappa_2\tau^\gamma$, and

$$ R_j^k=O(\tau^2)\left(1+\frac{1}{12}\delta_x^2\right)+O(h^4)\sum_{l=0}^{k}\left(\kappa_1\tau^\gamma\lambda_l\right). \tag{2.6} $$

By omitting the small term R_j^k, the implicit compact difference scheme for (1.6)-(1.8) is given as follows:

$$ \begin{cases} \left(1+\mu_2+\left(\dfrac{1}{12}-\mu_1+\dfrac{\mu_2}{12}\right)\delta_x^2\right)U_j^k=\left(1-\lambda_1\mu_2+\left(\dfrac{1}{12}+\lambda_1\mu_1-\dfrac{\lambda_1\mu_2}{12}\right)\delta_x^2\right)U_j^{k-1}\\ \qquad +\mu_1\displaystyle\sum_{l=2}^{k}\lambda_l\delta_x^2U_j^{k-l}-\mu_2\sum_{l=2}^{k}\lambda_l\left(1+\frac{1}{12}\delta_x^2\right)U_j^{k-l}+\tau\left(1+\frac{1}{12}\delta_x^2\right)f_j^{k-1},\\ U_j^0=\psi(x_j),\qquad j=1,2,\ldots,M-1,\\ U_0^k=\varphi_1(t_k),\quad U_M^k=\varphi_2(t_k),\ \ k=1,2,\ldots,N. \end{cases} \tag{2.7} $$

Now we denote the solution vector of order $M-1$ at $t=t_k$ by $\mathbf{U}^k=\mathbf{U}(t_k)=(U_1^k,\ldots,U_{M-1}^k)^T$. We can give the matrix-vector form of (2.7) by

$$A\mathbf{U}^k = \sum_{l=0}^{k-1} B_l \mathbf{U}^l + \mathbf{F}^k, k = 1, 2, 3, \ldots, N, \tag{2.8}$$

in which

$$\mathbf{A} = tri\left[\frac{1}{12}(1+\mu_2) - \mu_1, \frac{5}{6}(1+\mu_2) + 2\mu_1, \frac{1}{12}(1+\mu_2) - \mu_1\right],$$

$$\mathbf{B}_l = \lambda_l tri\left[\mu_1 - \frac{\mu_2}{12}, -2\mu_1 - \frac{5}{6}\mu_2, \mu_1 - \frac{\mu_2}{12}\right],$$

$$\mathbf{B}_{k-1} = tri\left[\frac{1}{12}(1-\lambda_1\mu_2), \frac{5}{6}(1-\lambda_1\mu_2), \frac{1}{12}(1-\lambda_1\mu_2)\right],$$

$$\mathbf{F}^k = \begin{bmatrix} -\left(\frac{1}{12}(1+\mu_2) - \mu_1\right)U_0^k + \tau\left(1 + \frac{1}{12}\delta_x^2\right)f_1^{k-1} + \left(\frac{1}{12}(1+\lambda_1\mu_2) - \mu_1\right)U_0^k \\ \tau\left(1 + \frac{1}{12}\delta_x^2\right)f_2^{k-1} \\ \vdots \\ \tau\left(1 + \frac{1}{12}\delta_x^2\right)f_{M-2}^{k-1} \\ -\left(\frac{1}{12}(1+\mu_2) - \mu_1\right)U_M^k + \tau\left(1 + \frac{1}{12}\delta_x^2\right)f_{M-1}^{k-1} + \left(\frac{1}{12}(1+\lambda_1\mu_2) - \mu_1\right)U_M^k \end{bmatrix},$$

where $tri\,[a_1 a_2 a_3]_{(M-1)\times(M-1)}$ denotes a $(M-1)\times(M-1)$ tri-diagonal matrix. Each row of this matrix contains the values a_1, a_2 and a_3 on its sub-diagonal, diagonal and super diagonal, respectively. We can state the solvability of proposed scheme in the following theorem.

Theorem 1. The compact difference scheme (2.7) has a unique solution.

Proof. For any possible values of μ_1, μ_2 and h the coefficient matrix A is strictly diagonal dominant so it is nonsingular. Consequently the difference scheme (2.7) has a unique solution.

3. STABILITY OF PROPOSED METHOD

In the section we will analyze the stability of the finite difference scheme (2.7) by using the Fourier analysis. For x = (x_1, x_2, …, $x_{M-1})^T \in \Re^{M-1}$, we define a discrete l^2-norm by $\left\|x^k\right\|_{\ell^2} = (h\sum_{j=1}^{M-1} x_j^2)^{1/2}$. Let $\widetilde{U}_j^k$ be the approximate solution of (2.7) and define

$$\rho_j^k = U_j^k - \widetilde{U}_j^k, \quad k = 0,1,\ldots,N, \quad j = 0,1,\ldots,M,$$

with corresponding vector

$$\rho^k = \left(\rho_1^k, \rho_2^k, \ldots, \rho_{M-1}^k\right)^T.$$

We obtain the following round off error equation

$$\begin{aligned}&\left(1+\mu_2+(\frac{1}{12}-\mu_1+\frac{\mu_2}{12})\delta_x^2\right)\rho_j^k = \left(1-\lambda_1\mu_2 + \left(\frac{1}{12}+\lambda_1\mu_1-\frac{\lambda_1\mu_2}{12}\right)\delta_x^2\right)\rho_j^{k-1}\\&+\mu_1\sum_{l=2}^{k}\lambda_l\,\delta_x^2\,\rho_j^{k-l} - \mu_2\sum_{l=2}^{k}\lambda_l\left(1+\frac{1}{12}\delta_x^2\right)\rho_j^{k-l} + \tau\left(1+\frac{1}{12}\delta_x^2\right)\left(f_j^{k-1} - \widetilde{f}_j^{k-1}\right), \qquad (3.1)\\&1 \le j \le M-1, \qquad 1 \le k \le N,\end{aligned}$$

with

$$\rho_0^k = \rho_M^k = 0.$$

in which $\widetilde{f}_j^{k-1} = f(\widetilde{U}_j^{k-1}, x_j, t_{k-1})$ We define the grid function

$$\rho^k(x) = \begin{cases}\rho_j^k & x_j - \frac{h}{2} < x \le x_j + \frac{h}{2},\\ 0 & 0 \le x \le \frac{h}{2} \quad or \quad L - \frac{h}{2} < x \le L.\end{cases}$$

We can expand the $\rho^k(x)$ in a Fourier series [5]

$$\rho^k(x) = \sum_{l=-\infty}^{\infty} d_k(l) e^{i\,2\pi l x/L}, k = 1, 2, \ldots, N,$$

where

$$d_k(l) = \frac{1}{L}\int_0^L \rho^k(x) e^{i\,2\pi l x/L} dx.$$

Also we introduce the following norm

$$\left\|\rho^k\right\|_2 = \left(\sum_{j=1}^{M-1} h\left|\rho_j^k\right|^2\right)^{\frac{1}{2}} = \left[\int_0^L \left|\rho^k(x)\right|^2 dx\right]^{\frac{1}{2}}.$$

By applying the Parseval equality

$$\int_0^L \left|\rho^k(x)\right|^2 dx = \sum_{l=-\infty}^{\infty} \left|d_k(l)\right|^2,$$

we obtain

$$\left\|\rho^k\right\|_2^2 = \sum_{l=-\infty}^{\infty} \left| d_k(l)\right|^2. \tag{3.2}$$

Now we can suppose that the solution of equation (3.1) has the following form

$$\rho_j^k = d_k e^{i\sigma jh},$$

where $\sigma = \frac{2\pi l}{L}$. Substituting the above expression into (3.1) and putting $\theta = \sigma h$, we obtain

$$d_k = \frac{1}{\mu}\left[\hat{\mu} + \varpi \sum_{l=2}^{k} \lambda_l\, d_{k-1} + \tau\left(1 + \frac{1}{12}\delta_x^2\right)\left(f_j^k - \tilde{f}_j^k\right)\right] \tag{3.3}$$

where

$$\mu = \frac{1}{3}\cos^2\frac{\theta}{2} + 4\mu_1 \sin^2\frac{\theta}{2} + \frac{\mu_2}{3}\cos^2\frac{\theta}{2} + \frac{2}{3}\mu_2 + \frac{2}{3},$$

$$\hat{\mu} = \frac{1}{3}\cos^2\frac{\theta}{2} - 4\lambda_1\mu_1 \sin^2\frac{\theta}{2} - \frac{\lambda_1\mu_2}{3}\cos^2\frac{\theta}{2} - \frac{2}{3}\lambda_1\mu_2 + \frac{2}{3}, \tag{3.4}$$

$$\varpi = -4\mu_1 \sin^2\frac{\theta}{2} - \frac{\mu_2}{3}\cos^2\frac{\theta}{2} - \frac{2}{3}\mu_2.$$

Lemma 2([14]). The coefficients λ_l satisfy

$$(1)\ \lambda_0 = 1,\ \lambda_1 = \gamma - 1,\ \lambda_l < 0,\ \ l = 1, 2, \ldots,$$

$$(2)\ \sum_{l=0}^{\infty} \lambda_l = 0,\ -\sum_{l=1}^{n} \lambda_l < 1,\ \forall n \in N.$$

Lemma 3. The coefficient μ in (3.4) satisfies in $0 \le \frac{1}{\mu} \le 3$.

Proof. Since μ_1 and μ_2 are positive so from (3.4) we can write

$$1 \le 3\mu = \cos^2\frac{\theta}{2} + 12\mu_1 \sin^2\frac{\theta}{2} + \mu_2 \cos^2\frac{\theta}{2} + 2\mu_2 + 2,$$

which gives $0 \le \frac{1}{\mu} \le 3.$

Proposition 1. Suppose that $d_k\ (1 \le k \le N)$ are defined by (3.3), then we have

$$|d_k| \le (1 + 3L\tau)^k\, |d_0|, \qquad k = 1, 2, \ldots, N.$$

Proof. We will use mathematical induction to complete the proof. For $k = 1$, from (3.3) and using Lemma 3 we can write

$$\begin{aligned}
|d_1| &\le \frac{1}{\mu}\left(\hat{\mu}|d_0| + \tau\left(1 + \frac{1}{12}\delta_x^2\right)e^{-ij\theta}\left|f_j^0 - \tilde{f}_j^0\right|\right) \\
&\le \frac{1}{\mu}\left(\hat{\mu}|d_0| + \tau\left(1 + \frac{1}{12}\delta_x^2\right)e^{-ij\theta}\, L\left|U_j^0 - \tilde{U}_j^0\right|\right) \\
&\le \frac{1}{\mu}\left(\hat{\mu}|d_0| + \tau\left(1 + \frac{1}{12}\delta_x^2\right)e^{-ij\theta}\, L|d_0|e^{ij\theta}\right) \\
&= \left(\frac{\hat{\mu} + L\tau}{\mu}\right)|d_0| \le (1 + 3L\tau)|d_0|.
\end{aligned}$$

Now suppose

$$|d_n| \le (1 + 3L\tau)^n\, |d_0|, \qquad n = 1, 2, \ldots, k-1.$$

From (3.3) and induction hypothesis, we can write

$$|d_k| \le \frac{|d_0|}{\mu}(1+3L\tau)^{k-1}\left\{\hat{\mu}+|\varpi|\sum_{l=0}^{k-2}|\lambda_{k-l}|\right\}+\frac{1}{\mu}\left(\tau\left(1+\frac{1}{12}\delta_x^2\right)e^{-ij\theta}\left|f_j^{k-1}-\tilde{f}_j^{k-1}\right|\right)$$

$$\le \frac{|d_0|}{\mu}(1+3L\tau)^{k-1}\left\{\hat{\mu}+|\varpi|\sum_{l=0}^{k-1}(|\lambda_{k-l}|-|\lambda_1|)\right\}+\frac{1}{\mu}\left(\tau\left(1+\frac{1}{12}\delta_x^2\right)e^{-ij\theta}L\left|U_j^k-\tilde{U}_j^k\right|\right)$$

$$\le \frac{|d_0|}{\mu}(1+3L\tau)^{k-1}\left\{\hat{\mu}+|\varpi|\sum_{l=1}^{k}(-\lambda_l-|\lambda_1|)\right\}+\frac{1}{\mu}\left(\tau\left(1+\frac{1}{12}\delta_x^2\right)e^{-ij\theta}L|d_{k-1}|e^{ij\theta}\right)$$

$$\le \frac{|d_0|}{\mu}(1+3L\tau)^{k-1}\{\hat{\mu}+|\varpi|(1-(1-\gamma))+L\tau\}$$

$$=(1+3L\tau)^k\,|d_0|,$$

which completes the proof.

Theorem 2. The compact difference scheme (2.7) is unconditionally stable for any $0<\gamma<1$.

Proof. Applying Proposition 1 and Parseval's equality, we obtain

$$\left\|U^k-\tilde{U}^k\right\|_{l^2}^2=\left\|\rho^k\right\|_{l^2}^2=\sum_{j=1}^{M-1}h\left|\rho_j^k\right|^2=h\sum_{j=1}^{M-1}\left|d_k\,e^{i\sigma jh}\right|^2=h\sum_{j=1}^{M-1}|d_k|^2$$

$$\le h\sum_{j=1}^{M-1}(1+3L\tau)^k|d_0|^2\le h\,e^{3Lk\tau}\sum_{j=1}^{M-1}\left|d_0\,e^{i\sigma jh}\right|^2\le e^{3LT}\left\|\rho^0\right\|_{l^2}^2=e^{3LT}\left\|U^0-\tilde{U}^0\right\|_{l^2}^2,$$

which means that the scheme (2.7) is unconditionally stable.

4. CONVERGENCE OF PROPOSED METHOD

In this section we prove that difference scheme (2.5) converges with the spatial accuracy of fourth order. We need some lemmas and theorems that will be expressed.

Lemma 4([2]). Regarding to the definitions of λ_l, we have

$$\tau^{\gamma-1}\sum_{l=0}^{k}\lambda_l=\frac{1}{\Gamma(\gamma)}+\mathrm{O}(\tau).$$

On the basis (2.6) and Lemma 4, we have

$$R_j^k=\mathrm{O}(\tau^2)\left(1+\frac{1}{12}\delta_x^2\right)+\mathrm{O}(h^4)\sum_{l=0}^{k}\left(\kappa_1\tau^{\gamma}\lambda_l\right)$$

$$=\mathrm{O}(\tau^2)+\tau\mathrm{O}(h^4)\kappa_1\tau^{\gamma-1}\sum_{l=0}^{k}\lambda_l \tag{4.1}$$

$$=\mathrm{O}(\tau^2)+\tau\mathrm{O}(h^4)\kappa_1\left(\frac{1}{\Gamma(\gamma)}+\mathrm{O}(\tau)\right)=\mathrm{O}(\tau^2+\tau h^4),$$

so from (4.1), we can obtain

$$R_j^k=O(\tau^2+\tau h^4),$$

$$k=1,2,\ldots,N,\quad j=1,2,\ldots,M,$$

therefore, there is a positive constant C_1, such that [3]

$$\left|R_j^k\right|\le C_1(\tau^2+\tau h^4). \tag{4.2}$$

Similar to the stability analysis in Section 3, we define the grid functions [3]

$$e^k(x)=\begin{cases} e_j^k \quad \text{when} \quad x_j-\dfrac{h}{2}<x\le x_j+\dfrac{h}{2},\ \ j=1,2,\ldots,M-1,\\ \\ 0 \quad \text{when} \quad 0\le x\le \dfrac{h}{2}\ or\ L-\dfrac{h}{2}<x\le L,\end{cases}$$

and

$$R^k(x)=\begin{cases} R_j^k & \text{when} \quad x_j-\frac{h}{2}<x\le x_j+\frac{h}{2}, \quad j=1,2,\ldots,M-1, \\ 0 & \text{when} \quad 0\le x\le\frac{h}{2} \ or \ L-\frac{h}{2}<x\le L, \end{cases}$$

Thus $e^k(x)$ and $R^k(x)$ have the following Fourier series expansions

$$e^k(x)=\sum_{l=-\infty}^{\infty}\eta_k(l)e^{\frac{i2\pi lx}{L}}, \qquad k=0,1,\ldots,N,$$

$$R^k(x)=\sum_{l=-\infty}^{\infty}\xi_k(l)e^{\frac{i2\pi lx}{L}}, \qquad k=0,1,\ldots,N,$$

where

$$\eta_k(l)=\frac{1}{L}\int_0^L e^k(x)e^{\frac{-i2\pi lx}{L}}dx, \qquad k=0,1,\ldots,N,$$

$$\xi_k(l)=\frac{1}{L}\int_0^L R^k(x)e^{\frac{-i2\pi lx}{L}}dx, \qquad k=0,1,\ldots,N.$$

Now, we define the following notations [3]

$$\begin{gathered} e_j^k=u(x_j,t_k)-U_j^k=\bar{u}_j^k-U_j^k, \\ k=1,2,\ldots,N, \qquad j=1,2,\ldots,M, \end{gathered} \tag{4.3}$$

$$e^k=\left[e_1^k,e_2^k,\ldots,e_{M-1}^k\right], \ R^k=\left[R_1^k,R_2^k,\ldots,R_{M-1}^k\right], \ k=1,2,\ldots,N,$$

and introduce the following norms

$$\|e\|_2=\left(\sum_{j=1}^{M-1}h\left|e_j^k\right|^2\right)^{\frac{1}{2}}=\left[\int_0^L\left|e^k(x)\right|^2dx\right]^{\frac{1}{2}}, \quad k=0,1,\ldots,N, \tag{4.4}$$

$$\|R\|_2 = \left(\sum_{j=1}^{M-1} h \left| R_j^k \right|^2 \right)^{\frac{1}{2}} = \left[\int_0^L \left| R^k(x) \right|^2 dx \right]^{\frac{1}{2}}, \quad k = 0,1,\ldots,N . \tag{4.5}$$

Using the Parseval equality

$$\int_0^L \left| e^k(x) \right|^2 d_x = \sum_{l=-\infty}^{\infty} \left| \eta_k(l) \right|^2 , \quad k = 0,1,\ldots,N,$$

and

$$\int_0^L \left| R^k(x) \right|^2 dx = \sum_{l=-\infty}^{\infty} \left| \xi_k(l) \right|^2, \quad k = 0,1,\ldots,N ,$$

we also have

$$\left\| e^k \right\|_2^2 = \sum_{l=-\infty}^{\infty} \left| \eta_k(l) \right|^2, \quad k = 0,1,\ldots,N , \tag{4.6}$$

$$\left\| R^k \right\|_2^2 = \sum_{l=-\infty}^{\infty} \left| \xi_k(l) \right|^2, \quad k = 0,1,\ldots,N . \tag{4.7}$$

From (2.6), we obtain that

$$\left(1+\frac{1}{12}\delta_x^2\right)\bar{u}_j^k = \left(1+\frac{1}{12}\delta_x^2\right)\bar{u}_j^{k-1} + \mu_1 \sum_{l=0}^{k} \lambda_l \delta_x^2 \bar{u}_j^{k-l}$$

$$+\mu_2 \sum_{l=0}^{k} \lambda_l \left(1+\frac{1}{12}\delta_x^2\right)\bar{u}_j^{k-l} + \tau\left(1+\frac{1}{12}\delta_x^2\right)\bar{f}_j^{k-1} + R_j^k \tag{4.8}$$

$$k = 1,2,\ldots,N , \quad j = 1,2,\ldots,M ,$$

where $\bar{u}_j^k = u(x_j, t_k)$ and $\bar{f}_j^{k-1} = f(\bar{u}_j^{k-1}, x_j, t_{k-1})$. Subtracting (2.7) from (4.8), leads to

$$\begin{cases} \left(1+\frac{1}{12}\delta_x^2\right)e_j^k = \left(1+\frac{1}{12}\delta_x^2\right)e_j^{k-1} + \mu_1 \sum_{l=0}^{k} \lambda_l \delta_x^2 e_j^{k-l} \\ \quad + \mu_2 \sum_{l=0}^{k} \lambda_l \left(1+\frac{1}{12}\delta_x^2\right) e_j^{k-l} + \tau\left(1+\frac{1}{12}\delta_x^2\right)\bar{f}_j^{k-1} + R_j^k \\ e_0^k = e_M^k = 0, \quad e_j^0 = 0, \quad k = 1,2,\ldots,,N, \quad j = 1,2,\ldots,M. \end{cases} \tag{4.9}$$

Now we assume that e_j^k and R_j^k are

$$e_j^k = \eta_k e^{i(\sigma j h)},$$

$$R_j^k = \xi_k e^{i(\sigma j h)},$$

where $\sigma = \frac{2l\pi}{L}$. Substituting the above relations into (4.9) results

$$\eta_k = \frac{1}{\mu}\left[\hat{\mu} + \varpi \sum_{l=2}^{k} \lambda_l \eta_{k-l} + \tau\left(1+\frac{1}{12}\delta_x^2\right)e^{-ij\theta}\left(f_j^k - \bar{f}_j^k\right) + \xi_k\right],$$
$$k = 1,2,\ldots,N. \tag{4.10}$$

Notice that $e^0 = 0$ and we have

$$\eta_0 \equiv \eta_0(l) = 0.$$

In addition, from the left hand equality of (4.5) and (4.2), we obtain [3]

$$\left\|R^k\right\|_2 \le \sqrt{Mh}C_1\left(\tau^2 + \tau h^4\right) = C_1\sqrt{L}\left(\tau^2 + \tau h^4\right). \tag{4.11}$$

Also from convergence of the series in the right hand side of (4.7), there is a positive constant C_2 such that [3]

$$|\xi_k| \equiv |\xi_k(n)| \le C_2 L\tau |\xi_1| \equiv C_2 L\tau |\xi_1(n)|, \qquad k = 1,2,\ldots,N. \tag{4.12}$$

Proposition 2. If η_k $(k = 1,2,\ldots,N)$ be the solutions of equation (4.10), then there is a positive constant C_2 such that

$$|\eta_k| \le C_2 k\left(1+3L\tau\right)^k |\xi_1|, \qquad k = 1,2,\ldots,N.$$

Proof. We use the mathematical induction for proof. Firstly, from (4.10) and (4.12) we have

$$\left|\eta_1\right| \le \frac{1}{\mu}\left|\xi_1\right| \le \frac{\tau}{\mu} C_2\, L\left|\xi_1\right| \le 3C_2\, L\,\tau\left|\xi_1\right| \le 3C_2\, L\,\tau\left|\xi_1\right| \le C_2\,(1+3L\,\tau)\left|\xi_1\right|.$$

Now, suppose that

$$|\,\eta_n| \le C_2\, n\,(1+3L\,\tau)^n\,|\,\xi_1|, \qquad n=1,2,\dots,k-1$$

From Lemma 2 and noticing that $\hat{\mu}>0$ we have,

$$\begin{aligned}
|\,\eta_k| \le{} & \frac{C_2\,(k-1)}{\mu}(1+3L\,\tau)^{k-1}\left\{\hat{\mu}+|\,\varpi\,|\sum_{l=0}^{k-2}|\,\lambda_{k-l}\,|\right\}|\,\xi_1\,| \\
& +\frac{1}{\mu}\left\{\tau\, e^{-ij\theta}\left(1+\frac{1}{12}\delta_x^2\right)\left[\left|\,f_j^k-\overline{f}_j^k\right|\right]+\tau\, C_2\, L|\,\xi_1|\right\} \\
\le{} & \frac{C_2\,(k-1)}{\mu}(1+3L\,\tau)^{k-1}\left\{\hat{\mu}+|\,\varpi\,|\left(\sum_{l=0}^{k-1}|\,\lambda_{k-l}\,|-|\,\lambda_1|\right)+\tau\, L\right\}|\,\xi_1\,|+3C_2\,\tau\, L|\,\xi_1\,| \\
\le{} & \frac{C_2\,(k-1)}{\mu}(1+3L\,\tau)^{k-1}\left\{\hat{\mu}+|\,\varpi\,|\left(-\sum_{l=1}^{k}|\,\lambda_l\,|-|\,\lambda_1|\right)+\tau\, L\right\}|\,\xi_1\,|+(1+3L\,\tau)^k\, C_2\,|\,\xi_1\,| \\
\le{} & \frac{C_2\,(k-1)}{\mu}(1+3L\,\tau)^{k-1}\left\{\hat{\mu}+|\,\varpi\,|\,\gamma+\tau\, L\right\}|\,\xi_1\,|+(1+3L\,\tau)^k\, C_2\,|\,\xi_1\,| \\
\le{} & C_2\,(k-1)(1+3L\tau)^{k-1}\left(\frac{\hat{\mu}+\tau\, L}{\mu}\right)|\,\xi_1\,|+(1+3L\,\tau)^k\, C_2\,|\,\xi_1\,| \\
={} & k\, C_2\,(1+3L\,\tau)^k\left|\xi_1\right|.
\end{aligned}$$

Theorem 3. Suppose $u(x,t)$ is the exact solution of the Eq. (1.6), then the compact finite difference scheme (2.7) is L_2-convergent with convergence order $\mathrm{O}(\tau+h^4)$.

Proof. By considering Proposition 2 and noticing (4.6), (4.7) and (4.11), we can obtain

$$\left\|e^k\right\|_2 \le C_2\, k\,(1+3L\,\tau)^k\left\|R^1\right\|_2 \le C_1\,\tau\sqrt{L}\, C_2\, k\, e^{3kL\,\tau}(\tau+h^4).$$

Since $k\tau \le T$, we have

$$\left\|e^k\right\|_2 \le \mathrm{C}\left(\tau + h^4\right)$$

in which

$$\mathrm{C} = C_1 C_2 T\sqrt{L}e^{3\mathrm{L}T},$$

and this completes the proof.

5. NUMERICAL RESULTS

In this section we present the numerical results of the new method on several test problems. We tested the accuracy and stability of the method described in this paper by performing the mentioned scheme for different values of h and τ. We performed our computations using Matlab 7 software on a Pentium IV, 2800 MHz CPU machine with 2 Gbyte of memory. We calculated the computational orders of the method presented in this article in time variable with [17, 24]

$$\mathrm{C}_1\text{-order} = \log_2\left(\frac{\left\|L_\infty(2\tau, h)\right\|}{\left\|L_\infty(\tau, h)\right\|}\right),$$

and in space variables with [4]

$$\mathrm{C}_2\text{-order} = \log_2\left(\frac{\left\|L_\infty(16\tau, 2h)\right\|}{\left\|L_\infty(\tau, h)\right\|}\right).$$

5.1 Test problem 1.

We consider the fractional linear PDE

$$\frac{\partial u(x,t)}{\partial t} = {}_0D_t^{1-\gamma}\left[\frac{\partial^2 u(x,t)}{\partial x^2} - u(x,t)\right] + (1+\gamma)e^x t^\gamma, \tag{5.1}$$

with boundary and initial conditions

$$u_0^k = t^{1+\gamma}, \quad u_M^k = e^L t^{1+\gamma}, \quad k = 1,2,\dots,N,$$
$$u_j^0 = 0, \quad j = 1,2,\dots,M. \tag{5.2}$$

Then, the exact solution of (5.1), (5.2) is

$$u(x,t) = e^x t^{1+\gamma}.$$

We solve this problem with the method presented in this article with several values of h, τ and γ for $L = 1$ at final time $T = 1$. The L_∞ error, C_1-order, C_2-order and CPU time (s) of applied method are shown in Tables 1,2.

Table 1. Errors and computational orders obtained for test problem 1 with $h = \frac{1}{20}$.

	$\gamma = 0.25$		$\gamma = 0.65$		
τ	L_∞	$C_1 - order$	L_∞	$C_1 - order$	CPU time(s)
1/10	1.3470×10^{-2}	_	1.4174×10^{-2}	_	00.1570
1/20	6.4528×10^{-3}	1.0617	6.9994×10^{-3}	1.0179	00.2029
1/40	3.1118×10^{-3}	1.0522	3.4728×10^{-3}	1.0111	00.3599
1/80	1.5086×10^{-3}	1.0445	1.7280×10^{-3}	1.0070	01.0000
1/160	7.3457×10^{-4}	1.0382	8.6135×10^{-4}	1.0044	03.5620
1/320	3.5902×10^{-4}	1.0328	4.2982×10^{-4}	1.0029	12.9840
1/640	1.7404×10^{-4}	1.0281	2.1446×10^{-4}	1.0011	49.2340

Tables 1,2 show that the computational orders are close to theoretical orders, i.e the order of method is $O(\tau)$ in time variable and $O(h^4)$ in space variables. Figure 1 shows the plots of error and approximate solution of this test problem with $h = 1/50$, $\tau = 1/100$ and $\gamma = 0.55$.

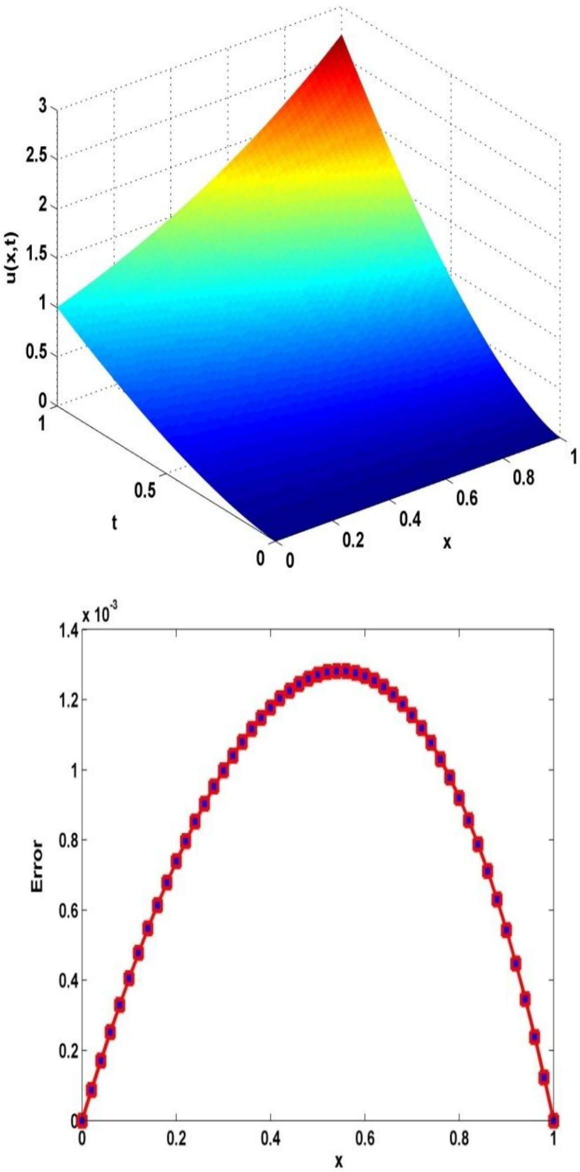

Figure 1. Error (Right Panel) and Approximate Solution (Left Panel) Obtained for Test Problem 1 with $h = 1/50$, $\tau = 1/100$ and $\gamma = 0.55$.

Table 2. Errors and computational orders obtained for test problem 1.

	$\gamma = 0.1$		$\gamma = 0.9$	
	$C_2 - order$	L_∞	$C_2 - order$	L_∞
$h = \tau = \frac{1}{4}$	3.9584×10^{-2}	_	4.3139×10^{-2}	_
$h = \frac{1}{8},\ \tau = \frac{1}{64}$	2.2060×10^{-3}	4.1652	2.6889×10^{-3}	4.0044
$h = \frac{1}{16},\ \tau = \frac{1}{1024}$	1.2716×10^{-4}	4.1167	1.6913×10^{-4}	3.9903
$h = \tau = \frac{1}{8}$	1.9148×10^{-2}	_	2.1539×10^{-2}	_
$h = \frac{1}{16},\ \tau = \frac{1}{128}$	1.0859×10^{-3}	4.1402	1.3532×10^{-3}	3.9925
$h = \frac{1}{32},\ \tau = \frac{1}{2048}$	6.2336×10^{-5}	4.1227	8.4585×10^{-5}	4.0000

5.2 Test problem 2.

We consider the fractional PDE with the nonlinear source term

$$\frac{\partial u(x,t)}{\partial t} = {}_0D_t^{1-\gamma}\left[\frac{\partial^2 u(x,t)}{\partial x^2} - u(x,t)\right]$$

$$+u^3(x,t) + \cos(\pi x)\left[2t + (\pi^2+1)\frac{2t^{1+\gamma}}{\Gamma(2+\gamma)} - t^6\cos^2(\pi x)\right],$$

with boundary and initial conditions

$$u_0^k = t^2,\quad u_M^k = t^2\cos(\pi L),\ \ k = 1,2,\ldots,N,$$

$$u_j^0 = 0,\quad j = 1,2,\ldots,M.$$

where, the exact solution is

$$u(x,t) = t^2\cos(\pi x).$$

We solve this problem with the method presented in this article with several values of h, τ and γ for $L=1$ at final time $T=1$. The L_∞ error, C_1-order, C_2-order and CPU time (s) of applied method are shown in Tables 3, 4.

Table 3. Errors and computational orders obtained for test problem 2 with $h=\frac{1}{16}$.

	$\gamma=0.5$		$\gamma=0.8$		
τ	L_∞	$C_1-order$	L_∞	$C_1-order$	CPU time(s)
1/10	3.3534×10^{-2}	_	3.9372×10^{-2}	_	00.1250
1/20	1.7050×10^{-2}	0.9758	2.0125×10^{-2}	0.9682	00.1879
1/40	8.5963×10^{-3}	0.9880	1.0172×10^{-2}	0.9844	00.4070
1/80	4.3155×10^{-3}	0.9942	5.1132×10^{-3}	0.9923	00.8279
1/160	2.1616×10^{-3}	0.9974	2.5628×10^{-3}	0.9965	02.9059
1/320	1.0813×10^{-3}	0.9993	1.2825×10^{-3}	0.9988	10.5940
1/640	5.4035×10^{-4}	1.0008	6.4111×10^{-4}	1.0003	41.3440

Tables 3, 4 show that the computational orders are close to theoretical orders, i.e the order of method is $O(\tau)$ in time variable and $O(h^4)$ in space variables. Figure 1 shows the plots of error and approximate solution of this test problem with $h=1/32$, $\tau=1/100$ and $\gamma=0.45$

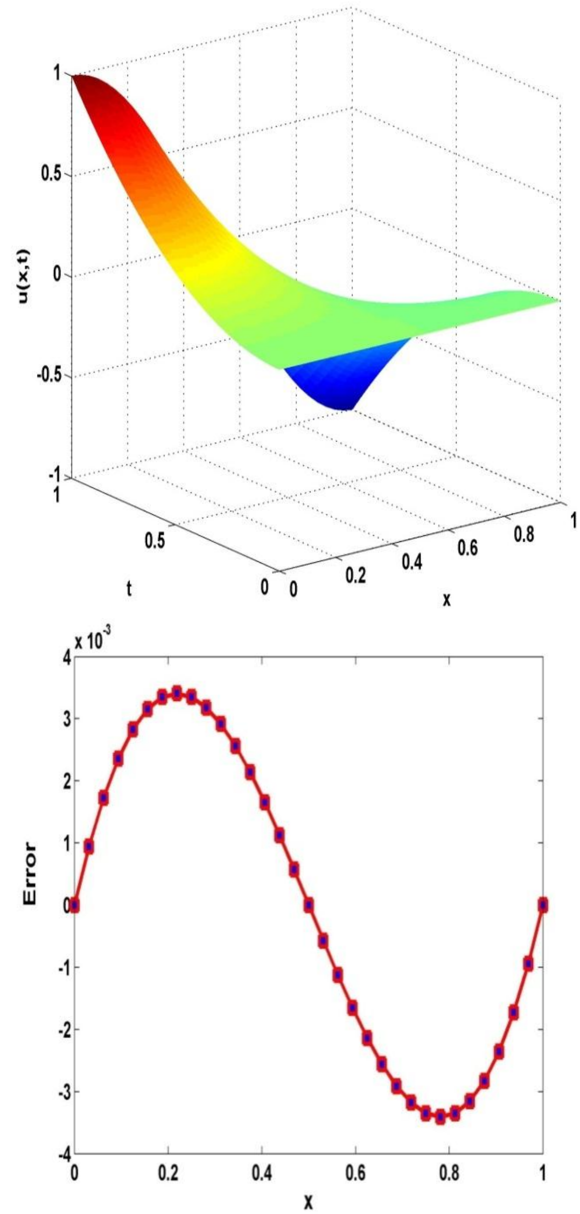

Figure 2. Error (Right Panel) and Approximate Solution (Left Panel) Obtained for Test Problem 2 with h = 1/32, τ = 1/100 and γ = 0.45.

Table 4. Errors and computational orders obtained for test problem 2.

	$\gamma = 0.35$		$\gamma = 0.75$	
	$C_2 - order$	L_∞	$C_2 - order$	L_∞
$h = \tau = \frac{1}{4}$	7.3142×10^{-2}	_	8.9651×10^{-2}	_
$h = \frac{1}{8},\ \tau = \frac{1}{64}$	4.8645×10^{-3}	3.9094	6.2011×10^{-3}	3.8537
$h = \frac{1}{16},\ \tau = \frac{1}{1024}$	3.0544×10^{-4}	3.9942	3.8992×10^{-4}	3.9913
$h = \tau = \frac{1}{8}$	3.7930×10^{-2}	_	4.7484×10^{-2}	_
$h = \frac{1}{16},\ \tau = \frac{1}{128}$	2.4473×10^{-3}	3.9540	3.1188×10^{-3}	3.9284
$h = \frac{1}{32},\ \tau = \frac{1}{2048}$	1.5600×10^{-4}	3.9716	1.9900×10^{-4}	3.9702

6. CONCLUSION

In this article, we constructed a compact difference scheme for the solution of a fractional nonlinear PDE in the electroanalytical chemistry. This compact difference scheme has the advantage of high accuracy and unconditional stability which we proved it using the Fourier analysis. Also we show that the proposed compact finite difference scheme converges with the spatial accuracy of fourth-order. Numerical results confirmed the theoretical results of proposed method.

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