



Fractional Order Techniques for Stiff Differential Equations Arising from Chemistry Kinetics

Rania Wannan¹, Muhammad Aslam², Muhammad Farman³, Ali Akgül⁴, Farhina Kouser⁵, Jihad Asad^{1,*}

¹ Faculty of Applied Science, Palestine Technical University - Kadoorie, Tulkarem, Palestine.

² Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of Ministry of Education, Department of Chemistry and Materials Science, Northwest University, Xi'an 710127, P.R China

³ Department of Mathematics, Khawaja Fareed University of Engineering and Information Technology, Rahim Yar Khan, Pakistan.

⁴ Department of Mathematics, Art and Science Faculty, Siirt University, 56100 Siirt, Turkey

⁵ Department of Mathematics and Statistics, The University of Lahore, Lahore, Pakistan

Abstract. In this paper, we consider the stiff systems of ordinary differential equations arising from chemistry kinetics. We develop the fractional order model for chemistry kinetics problems by using the Caputo Fabrizio and Atangana-Baleanu derivatives in Caputo sense. We apply the Sumudu transform to obtain the solutions of the models. Uniqueness and stability analysis of the problem are also established by using the fixed point theory results. Numerical results are obtained by using the proposed schemes which supports theoretical results. These concepts are very important for using the real-life problems like Brine tank cascade, Recycled Brine tank cascade, pond pollution, home heating and biomass transfer problem. These results are crucial for solving the nonlinear model in chemistry kinetics.

2020 Mathematics Subject Classifications: 65P40, 68M07

Key Words and Phrases: Chemistry kinetics, fractional technique, stability, uniqueness, Sumudu transform.

1. Introduction

Some problems with the fractional derivatives which include the trigonometric and exponential functions [3–8, 12, 14] show some related approaches for models of epidemic. Different fractional operator is used in literature to solve the real life problems [2, 9, 10, 13, 15]. The chemical reaction has been introduced by Robertson as [1]:

*Corresponding author.

DOI: <https://doi.org/10.29020/nybg.ejpam.v15i3.4406>

Email addresses: j.asad@ptuk.edu.ps (Jihad Asad)



The problem has three equations, where k_1, k_2 and k_3 describe the rate constants and A,B and C are the chemical species contained. By using the mass action law, the get

$$\begin{aligned} y_1' &= -M_1y_1 + M_3y_2y_3, \\ y_2' &= M_1y_1 - M_2y_2^2 - M_3y_2y_3, \\ y_3' &= M_2y_2^2. \end{aligned} \tag{4}$$

In this system $y_1(t), y_2(t)$ and $y_3(t)$ are the concentrations of the chemical species A,B and C. The initial time $t = 0$ can be given by $(y_{01}, y_{02}, y_{03})^T$. Where $M_1 = 0.04, M_2 = 3 \times 10^7$ and $M_3 = 10^4$, and the initial concentrations were $y_{01} = 1/100000, y_{02} = 0$ and $y_{03} = 0$. Our new Caputo–Fabrizio fractional model for Robertson problem can therefore be written as follows:

$$\begin{aligned} {}_0^{CF}D_t^\rho y_1 &= -M_1y_1 + M_3y_2y_3, \\ {}_0^{CF}D_t^\rho y_2 &= M_1y_1 - M_2y_2^2 - M_3y_2y_3, \\ {}_0^{CF}D_t^\rho y_3 &= M_2y_2^2. \end{aligned} \tag{5}$$

2. Basic Definitions

Some basic definitions are given in this section [3–5, 12].

Definition 1. Sumudu transform for any function $\phi(t)$ over a set is given as, $A = \{\phi(t) : \text{there exist } \Lambda, \tau_1, \tau_2 > 0, |\phi(t)| < \Lambda \exp(|t|/\tau_i), \text{ if } t \in (-1)^i \times [0, \infty)\}$ is described by

$$F(u) = ST[\phi(t)] = \int_0^\infty \exp(-t)\phi(ut)dt, u \in (-\tau_1, \tau_2). \tag{6}$$

Definition 2. Atangana-Baleanu derivative in Caputo sense is described as [13] :

$${}_a^{ABC}D_\tau^\alpha \phi(t) = \frac{AB(\alpha)}{n - \alpha} \int_a^t \frac{d^n}{dw^n} \phi(w) E_\alpha \frac{-\alpha(t - w)^\alpha}{(n - \alpha)} dw, n - 1 < \alpha < n. \tag{7}$$

The Laplace transform of equation (7) is acquired as:

$$L[{}_a^{ABC}D_\tau^\alpha \phi(t)](s) = \frac{AB(\alpha)}{1 - \alpha} \frac{(s^\alpha L[\phi(t)](s) - s^{\alpha-1}\phi(0))}{s^\alpha + \frac{\alpha}{1-\alpha}}. \tag{8}$$

By using Sumudu transform (ST) for equation (7), we obtain

$$ST[{}_0^{ABC}D_\tau^\alpha \phi(t)](s) = \frac{B(\alpha)}{1 - \alpha} \alpha \Gamma(\alpha + 1) E_\alpha \left(\frac{-1}{1 - \alpha} w^\alpha\right) [ST(\phi(t)) - \phi(0)]. \tag{9}$$

3. Caputo Fabrizio Derivative

By using Sumudu Transform on system (5), we have

$$\begin{aligned}
 M(\rho) \frac{ST(y_1(t)) - y_1(0)}{1 - \rho + \rho u} &= ST[-M_1 y_1 + M_3 y_2 y_3], \\
 M(\rho) \frac{ST(y_2(t)) - y_2(0)}{1 - \rho + \rho u} &= ST[M_1 y_1 - M_2 y_2^2 - M_3 y_2 y_3], \\
 M(\rho) \frac{ST(y_3(t)) - y_3(0)}{1 - \rho + \rho u} &= ST[M_2 y_2^2].
 \end{aligned}
 \tag{10}$$

Rearranging the above equations yields:

$$\begin{aligned}
 ST(y_1(t)) &= y_1(0) + \frac{1 - \rho + \rho u}{M(\rho)} ST[-M_1 y_1 + M_3 y_2 y_3], \\
 ST(y_2(t)) &= y_2(0) + \frac{1 - \rho + \rho u}{M(\rho)} ST[M_1 y_1 - M_2 y_2^2 - M_3 y_2 y_3], \\
 ST(y_3(t)) &= y_3(0) + \frac{1 - \rho + \rho u}{M(\rho)} ST[M_2 y_2^2].
 \end{aligned}
 \tag{11}$$

Taking inverse transform for system (11) gives:

$$\begin{aligned}
 y_1(t) &= y_1(0) + ST^{-1} \left[\frac{1 - \rho + \rho u}{M(\rho)} ST(-M_1 y_1 + M_3 y_2 y_3) \right], \\
 y_2(t) &= y_2(0) + ST^{-1} \left[\frac{1 - \rho + \rho u}{M(\rho)} ST(M_1 y_1 - M_2 y_2^2 - M_3 y_2 y_3) \right], \\
 y_3(t) &= y_3(0) + ST^{-1} \left[\frac{1 - \rho + \rho u}{M(\rho)} ST(M_2 y_2^2) \right].
 \end{aligned}
 \tag{12}$$

We get this recursive form as:

$$\begin{aligned}
 y_{1(n+1)}(t) &= y_{1(n)}(0) + ST^{-1} \left[\frac{1 - \rho + \rho u}{M(\rho)} ST(-M_1 y_{1(n)} + M_3 y_{2(n)} y_{3(n)}) \right], \\
 y_{2(n+1)}(t) &= y_{2(n)}(0) + ST^{-1} \left[\frac{1 - \rho + \rho u}{M(\rho)} ST(M_1 y_{1(n)} - M_2 y_{2(n)}^2 - M_3 y_{2(n)} y_{3(n)}) \right], \\
 y_{3(n+1)}(t) &= y_{3(n)}(0) + ST^{-1} \left[\frac{1 - \rho + \rho u}{M(\rho)} ST(M_2 y_{2(n)}^2) \right].
 \end{aligned}
 \tag{13}$$

And the solution of system (13) is obtained as:

$$y_1(t) = \lim_{n \rightarrow \infty} y_{1(n)}(t), \quad y_2(t) = \lim_{n \rightarrow \infty} y_{2(n)}(t), \quad y_3(t) = \lim_{n \rightarrow \infty} y_{3(n)}(t).
 \tag{14}$$

3.1. Stability Analysis of the Problem

Theorem 1. *Let $(X_1, .)$ be a Banach space and P be a self-map of X_1 satisfying*

$$\|P_x - P_y\| \leq C\|x - P_x\| + c\|x - y\|$$

for all $x, y \in X_1$, where $0 \leq C, 0 \leq c < 1$. Consider that P is a P -Stable. We have

$$\begin{aligned} y_{1(n+1)}(t) &= y_{1(n)}(0) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(-M_1y_{1(n)} + M_3y_{2(n)}y_{3(n)})\right], \\ y_{2(n+1)}(t) &= y_{2(n)}(0) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(M_1y_{1(n)} - M_2y_{2(n)}^2 - M_3y_{2(n)}y_{3(n)})\right], \\ y_{3(n+1)}(t) &= y_{3(n)}(0) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(M_2y_{2(n)}^2)\right]. \end{aligned} \tag{15}$$

Where $\frac{1-\rho+\rho u}{M(\rho)}$ is the fractional Lagrange multiplier.

Theorem 2. Let us describe a self-map P as

$$\begin{aligned} P(y_{1(n)}(t)) &= y_{1(n+1)}(t) = y_{1(n)}(0) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(-M_1y_{1(n)} + M_3y_{2(n)}y_{3(n)})\right], \\ P(y_{2(n)}(t)) &= y_{2(n+1)}(t) = y_{2(n)}(0) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(M_1y_{1(n)} - M_2y_{2(n)}^2 - M_3y_{2(n)}y_{3(n)})\right], \\ P(y_{3(n)}(t)) &= y_{3(n+1)}(t) = y_{3(n)}(0) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(M_2y_{2(n)}^2)\right]. \end{aligned} \tag{16}$$

is P -Stable in $L^1(a, b)$ if

$$\begin{aligned} C &= ([1 - M_1f(\gamma) + M_3(K + L)h(\gamma)], [1 + M_1f(\gamma) - M_2g(\gamma) - M_3(K + L)h(\gamma)], \\ &[1 + M_2g(\gamma)]), \\ c &= (0, 0, 0). \end{aligned} \tag{17}$$

Proof. We prove that P has a fixed point. For this, we evaluate the following for all $(m, n) \in \mathbb{N} \times \mathbb{N}$.

$$\begin{aligned} P(y_{1(n)}(t)) - P(y_{1(m)}(t)) &= y_{1(n)}(t) - y_{1(m)}(t) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(-M_1y_{1(n)} + M_3y_{2(n)}y_{3(n)})\right] \\ &- ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(-M_1y_{1(m)} + M_3y_{2(m)}y_{3(m)})\right], \\ P(y_{2(n)}(t)) - P(y_{2(m)}(t)) &= y_{2(n)}(t) - y_{2(m)}(t) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(M_1y_{1(n)} - M_2y_{2(n)}^2 - M_3y_{2(n)}y_{3(n)})\right] \\ &- ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(M_1y_{1(m)} - M_2y_{2(m)}^2 - M_3y_{2(m)}y_{3(m)})\right], \\ P(y_{3(n)}(t)) - P(y_{3(m)}(t)) &= y_{3(n)}(t) - y_{3(m)}(t) + ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(M_2y_{2(n)}^2)\right] \\ &- ST^{-1}\left[\frac{1-\rho+\rho u}{M(\rho)}ST(M_2y_{2(m)}^2)\right] \end{aligned} \tag{18}$$

Considering equation (18) , we get

$$\begin{aligned} \|P(y_{1(n)}(t)) - P(y_{1(m)}(t))\| &= \|y_{1(n)}(t) - y_{1(m)}(t)\| \\ &+ ST^{-1}\left[\frac{1 - \rho + \rho u}{M(\rho)} ST(-M_1 y_{1(n)} + M_3 y_{2(n)} y_{3(n)})\right] \\ &- ST^{-1}\left[\frac{1 - \rho + \rho u}{M(\rho)} ST(-M_1 y_{1(m)} + M_3 y_{2(m)} y_{3(m)})\right]\|. \end{aligned} \tag{19}$$

Using triangular inequality for equation (19), we get

$$\begin{aligned} \|P(y_{1(n)}(t)) - P(y_{1(m)}(t))\| &= \|y_{1(n)}(t) - y_{1(m)}(t)\| \\ &+ \|ST^{-1}\left[\frac{1 - \rho + \rho u}{M(\rho)} ST(-M_1 y_{1(n)} + M_3 y_{2(n)} y_{3(n)})\right]\| \\ &- \|ST^{-1}\left[\frac{1 - \rho + \rho u}{M(\rho)} ST(-M_1 y_{1(m)} + M_3 y_{2(m)} y_{3(m)})\right]\|. \end{aligned} \tag{20}$$

Upon further simplification gives:

$$\begin{aligned} \|P(y_{1(n)}(t)) - P(y_{1(m)}(t))\| &= \|y_{1(n)}(t) - y_{1(m)}(t)\| \\ &+ \|ST^{-1}\left[\frac{1 - \rho + \rho u}{M(\rho)} ST(-M_1 y_{1(n)} + M_3 y_{2(n)} y_{3(n)} + M_1 y_{1(m)} \right. \\ &\left. - M_3 y_{2(m)} y_{3(m)})\right]\|. \end{aligned} \tag{21}$$

$$\begin{aligned} \|P(y_{1(n)}(t)) - P(y_{1(m)}(t))\| &= \|y_{1(n)}(t) - y_{1(m)}(t)\| \\ &+ ST^{-1}\left[\frac{1 - \rho + \rho u}{M(\rho)} ST(\| - M_1 (y_{1(n)} - y_{1(m)})\| + \|M_3 y_{2(n)} (y_{3(n)} - y_{3(m)})\| \right. \\ &\left. + \|M_3 y_{3(m)} (y_{2(n)} - y_{2(m)})\|)\right]. \end{aligned} \tag{22}$$

$$\begin{aligned} \|y_{1(n)}(t) - y_{1(m)}(t)\| &\approx \|y_{2(n)}(t) - y_{2(m)}(t)\| \\ \|y_{1(n)}(t) - y_{1(m)}(t)\| &\approx \|y_{3(n)}(t) - y_{3(m)}(t)\| \end{aligned}$$

Replacing this in equation (22) gives:

$$\begin{aligned} \|P(y_{1(n)}(t)) - P(y_{1(m)}(t))\| &= \|y_{1(n)}(t) - y_{1(m)}(t)\| \\ &+ ST^{-1}\left[\frac{1 - \rho + \rho u}{M(\rho)} ST(\| - M_1 (y_{1(n)} - y_{1(m)})\| + \|M_3 y_{2(n)} (y_{1(n)} - y_{1(m)})\| \right. \\ &\left. + \|M_3 y_{3(m)} (y_{1(n)} - y_{1(m)})\|)\right] \tag{23} \\ \|P(y_{1(n)}(t)) - P(y_{1(m)}(t))\| &= \|y_{1(n)} - y_{1(m)}\| \left[1 + ST^{-1} ST\left(\frac{1 - \rho + \rho u}{M(\rho)}\right)\| - M_1\| + \right. \\ &\left. ST^{-1}\left(ST\frac{1 - \rho + \rho u}{M(\rho)}\right)\|M_3(y_{2(n)} + y_{3(m)})\|\right] \end{aligned}$$

Since $y_{2(n)}, y_{3(m)}$ are bounded as they are convergent sequence, therefore, we can obtain two different constants K, L for all “ t ” such that

$$\|y_{2(n)}\| < K, \quad \|y_{3(m)}\| < L, \quad (m, n) \in \mathbb{N} \times \mathbb{N}. \tag{24}$$

Now considering equation (22) with equation (23), we get

$$\|P(y_{1(n)}(t)) - P(y_{1(m)}(t))\| = (1 - M_1f(\gamma) + M_3(K + L)h(\gamma))\|y_{1(n)} - y_{1(m)}\| \tag{25}$$

Where f, g and h are functions from $ST^{-1}ST(\frac{1-\rho+\rho u}{M(\rho)})$. Similarly we get

$$\|P(y_{2(n)}(t)) - P(y_{2(m)}(t))\| = (1 + M_1f(\gamma) - M_2g(\gamma) - M_3(K + L)h(\gamma))\|y_{2(n)} - y_{2(m)}\| \tag{26}$$

$$\|P(y_{3(n)}(t)) - P(y_{3(m)}(t))\| = (1 + M_2g(\gamma))\|y_{3(n)} - y_{3(m)}\| \tag{27}$$

Where

$$\begin{aligned} 1 - M_1f(\gamma) + M_3(K + L)h(\gamma) &< 1, \\ 1 + M_1f(\gamma) - M_2g(\gamma) - M_3(K + L)h(\gamma) &< 1, \\ 1 + M_2g(\gamma) &< 1, \end{aligned}$$

Then, we get $c = (0, 0, 0)$,
 $C = (1 - M_1f(\gamma) + M_3(K + L)h(\gamma),$
 $1 + M_1f(\gamma) - M_2g(\gamma) - M_3(K + L)h(\gamma),$
 $1 + M_2g(\gamma)).$

4. Atangana-Baleanu Derivative in Caputo Sense

We consider

$$\begin{aligned} {}_0^{ABC}D_t^\alpha y_1 &= -M_1y_1 + M_3y_2y_3, \\ {}_0^{ABC}D_t^\alpha y_2 &= M_1y_1 - M_2y_2^2 - M_3y_2y_3, \\ {}_0^{ABC}D_t^\alpha y_3 &= M_2y_2^2. \end{aligned} \tag{28}$$

By using Sumudu transform, we have

$$\begin{aligned} \frac{B(\alpha)\alpha\Gamma(\alpha + 1)}{(1 - \alpha)} E_\alpha(-\frac{1}{(1 - \alpha)}w^\alpha)ST(y_1(t) - y_1(0)) &= ST[-M_1y_1 + M_3y_2y_3], \\ \frac{B(\alpha)\alpha\Gamma(\alpha + 1)}{(1 - \alpha)} E_\alpha(-\frac{1}{(1 - \alpha)}w^\alpha)ST(y_2(t) - y_2(0)) &= ST[M_1y_1 - M_2y_2^2 - M_3y_2y_3], \\ \frac{B(\alpha)\alpha\Gamma(\alpha + 1)}{(1 - \alpha)} E_\alpha(-\frac{1}{(1 - \alpha)}w^\alpha)ST(y_3(t) - y_3(0)) &= ST[M_2y_2^2]. \end{aligned} \tag{29}$$

Rearranging the above equations gives:

$$\begin{aligned}
 ST(y_1(t)) &= y_1(0) + \frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times ST[-M_1y_1 + M_3y_2y_3], \\
 ST(y_2(t)) &= y_2(0) + \frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times ST[M_1y_1 - M_2y_2^2 - M_3y_2y_3], \quad (30) \\
 ST(y_3(t)) &= y_3(0) + \frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times ST[M_2y_2^2]. \\
 \\
 y_1(t) &= y_1(0) + ST^{-1}\left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times ST(-M_1y_1 + M_3y_2y_3)\right], \\
 y_2(t) &= y_2(0) + ST^{-1}\left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times ST(M_1y_1 - M_2y_2^2 - M_3y_2y_3)\right], \\
 y_3(t) &= y_3(0) + ST^{-1}\left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times ST(M_2y_2^2)\right].
 \end{aligned}
 \tag{31}$$

Then, we get

$$\begin{aligned}
 y_{1(n+1)}(t) &= y_{1(n)}(0) + ST^{-1}\left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times \right. \\
 &\quad \left. ST(-M_1y_{1(n)} + M_3y_{2(n)}y_{3(n)})\right], \\
 y_{2(n+1)}(t) &= y_{2(n)}(0) + ST^{-1}\left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times \right. \\
 &\quad \left. ST(M_1y_{1(n)} - M_2y_{2(n)}^2 - M_3y_{2(n)}y_{3(n)})\right], \quad (32) \\
 y_{3(n+1)}(t) &= y_{3(n)}(0) + ST^{-1}\left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \times ST(M_2y_{2(n)}^2)\right].
 \end{aligned}$$

And the solution of system (32) is obtained as:

$$y_1(t) = \lim_{n \rightarrow \infty} y_{1(n)}(t), \quad y_2(t) = \lim_{n \rightarrow \infty} y_{2(n)}(t), \quad y_3(t) = \lim_{n \rightarrow \infty} y_{3(n)}(t). \tag{33}$$

4.1. Stability and Uniqueness of the Proposed Scheme

Assume that $(X, |\cdot|)$ is a Banach space and H a self-map of X . Let $r_{n+1} = f(Hr_n)$ be specific recursive procedure. The following condition must be fulfilled for $r_{n+1} = Hr_n$

- The fixed point set of H possesses at least one element.
- r_n converges to a point $p \in F(H)$.
- $\lim_{n \rightarrow \infty} x_n(t) = p$.

Theorem 3. Suppose that $(X, |\cdot|)$ is a Banach space and H a self-map of X satisfying

$$\|Hx - Hr\| \leq \Theta \|x - Hx\| + \theta \|x - r\|$$

for all $x, r \in X$, where $0 \leq \Theta, 0 \leq \theta < 1$. Then H is Picard H -Stable.

Theorem 4. Describe H as a self-map:

$$\begin{aligned} H[y_{1(n+1)}(t)] &= y_{1(n+1)}(t) = y_{1(n)}(t) + ST^{-1} \left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \right. \\ &\quad \left. \times ST(-M_1y_{1(n)} + M_3y_{2(n)}y_{3(n)}) \right], \\ H[y_{2(n+1)}(t)] &= y_{2(n+1)}(t) = y_{2(n)}(0) + ST^{-1} \left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \right. \\ &\quad \left. \times ST(M_1y_{1(n)} - M_2y_2^2(n) - M_3y_{2(n)}y_{3(n)}) \right], \\ H[y_{3(n+1)}(t)] &= y_{3(n+1)}(t) = y_{3(n)}(0) + ST^{-1} \left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \right. \\ &\quad \left. \times ST(M_2y_2^2(n)) \right]. \end{aligned} \tag{34}$$

Proof. By using norm properties, then the iteration is H-Stable

$$\begin{aligned} \|H[y_{1(n)}(t)] - H[y_{1(m)}(t)]\| &\leq \|y_{1(n)}(t) - y_{1(m)}(t)\| + ST^{-1} \left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \right. \\ &\quad \left. \times ST(-M_1\|y_{1(n)} - y_{1(m)}\| + M_3\|y_{2(n)}y_{3(n)} - y_{2(m)}y_{3(m)}\|) \right], \\ \|H[y_{2(n)}(t)] - H[y_{2(m)}(t)]\| &\leq \|y_{2(n)}(t) - y_{2(m)}(t)\| + ST^{-1} \left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \right. \\ &\quad \left. \times ST(M_1\|y_{1(n)} - y_{1(m)}\| - M_2\|y_2^2(n) - y_2^2(m)\| - M_3\|y_{2(n)}y_{3(n)} - y_{2(m)}y_{3(m)}\|) \right], \\ \|H[y_{3(n)}(t)] - H[y_{3(m)}(t)]\| &\leq \|y_{3(n)}(t) - y_{3(m)}(t)\| + ST^{-1} \left[\frac{1 - \alpha}{B(\alpha)\alpha\Gamma(\alpha + 1)E_\alpha(-\frac{1}{(1-\alpha)}w^\alpha)} \right. \\ &\quad \left. \times ST(M_2\|y_2^2(n) - y_2^2(m)\|) \right]. \end{aligned} \tag{35}$$

Its satisfied in theorem 3, when

$$\begin{aligned} \theta = (0, 0, 0), \quad \Theta = & (\|y_{1(n)}(t) - y_{1(m)}(t)\| \times \|-(y_{1(n)}(t) + y_{1(m)}(t))\| - M_1\|y_{1(n)} - y_{1(m)}\| + \\ & M_3\|y_{2(n)}y_{3(n)} - y_{2(m)}y_{3(m)}\| \times \|y_{2(n)}(t) - y_{2(m)}(t)\| \times \|-(y_{2(n)}(t) + y_{2(m)}(t))\| + \\ & M_1\|y_{1(n)} - y_{1(m)}\| - M_2\|y_2^2(n) - y_2^2(m)\| - M_3\|y_{2(n)}y_{3(n)} - y_{2(m)}y_{3(m)}\| \times \\ & \|y_{3(n)}(t) - y_{3(m)}(t)\| \times \|-(y_{3(n)}(t) + y_{3(m)}(t))\| + M_2\|y_2^2(n) - y_2^2(m)\|) \end{aligned} \tag{36}$$

Theorem 5. *The special solution of system (28) using the iteration method is unique singular solution.*

Proof. By using Hilbert space $H = L^2((p, q) \times (0, r))$ which can be described as

$$h : (p, q) \times (0, T) \rightarrow \mathbb{R}$$

Considering $\theta = (0, 0, 0)$, $\Theta = (-M_1y_1 + M_3y_2y_3, M_1y_1 - M_2y_2^2 - M_3y_2y_3, M_2y_2^2)$. We have

$$T((y_{1(11)}(t) - y_{1(12)}(t), y_{2(21)}(t) - y_{2(22)}(t), y_{3(31)}(t) - y_{3(32)}(t)), (V_1, V_2, V_3)). \tag{37}$$

we get

$$\begin{aligned} &(-M_1(y_{1(11)} - y_{1(12)}) + M_3(y_{2(21)} - y_{2(22)})(y_{3(31)} - y_{3(32)}), V_1) \leq M_1\|y_{1(11)} - y_{1(12)}\| \\ &\|V_1\| + M_3\|y_{2(21)} - y_{2(22)}\|\|y_{3(31)} - y_{3(32)}\|\|V_1\|, \\ &(M_1(y_{1(11)} - y_{1(12)}) - M_2(y_{2(21)}^2 - y_{2(22)}^2) - M_3(y_{2(21)} - y_{2(22)})(y_{3(31)} - y_{3(32)}), V_2) \\ &\leq M_1\|y_{1(11)} - y_{1(12)}\|\|V_2\| + M_2\|(y_{2(21)}^2 - y_{2(22)}^2)\| \\ &\|V_2\| + \| + M_3\|y_{2(21)} - y_{2(22)}\|\|y_{3(31)} - y_{3(32)}\|\|V_2\|, \\ &(M_2(y_{2(21)}^2 - y_{2(22)}^2), V_3) \leq M_2\|(y_{2(21)}^2 - y_{2(22)}^2)\|\|V_3\|. \end{aligned} \tag{38}$$

By using conditions, we get

$$\begin{aligned} \|y_1 - y_{1(11)}\|, \|y_1 - y_{1(12)}\| &\leq \frac{\chi e_1}{\omega}, \\ \|y_2 - y_{2(21)}\|, \|y_2 - y_{2(22)}\| &\leq \frac{\chi e_2}{\varsigma}, \\ \|y_3 - y_{3(31)}\|, \|y_3 - y_{3(32)}\| &\leq \frac{\chi e_3}{\upsilon}. \end{aligned} \tag{39}$$

where

$$\begin{aligned} \omega &= 3(M_1\|y_{1(11)} - y_{1(12)}\| + M_3\|y_{2(21)} - y_{2(22)}\|\|y_{3(31)} - y_{3(32)}\|)\|V_1\|, \\ \varsigma &= 3(M_1\|y_{1(11)} - y_{1(12)}\| + M_2\|(y_{2(21)}^2 - y_{2(22)}^2)\| + M_3\|y_{2(21)} - y_{2(22)}\| \\ &\|y_{3(31)} - y_{3(32)}\|)\|V_2\|, \\ \upsilon &= 3(M_2\|(y_{2(21)}^2 - y_{2(22)}^2)\|)\|V_3\|. \end{aligned} \tag{40}$$

But, it is obvious that

$$\begin{aligned} &(M_1\|y_{1(11)} - y_{1(12)}\| + M_3\|y_{2(21)} - y_{2(22)}\|\|y_{3(31)} - y_{3(32)}\|) \neq 0 \\ &(M_1\|y_{1(11)} - y_{1(12)}\| + M_2\|(y_{2(21)}^2 - y_{2(22)}^2)\| + M_3\|y_{2(21)} - y_{2(22)}\|\|y_{3(31)} - y_{3(32)}\|) \neq 0 \\ &(M_2\|(y_{2(21)}^2 - y_{2(22)}^2)\|) \neq 0 \\ &\text{Where } \|V_1\|, \|V_2\|, \|V_3\| \neq 0 \end{aligned} \tag{41}$$

Therefore, we have

$$\|y_{1(11)} - y_{1(12)}\| = 0, \quad \|y_{2(21)} - y_{2(22)}\| = 0, \quad \|y_{3(31)} - y_{3(32)}\| = 0, \quad (42)$$

Which yields that

$$y_{1(11)} = y_{1(12)}, \quad y_{2(21)} = y_{2(22)}, \quad y_{3(31)} = y_{3(32)} \quad (43)$$

This completes the proof of uniqueness.

5. Results and Discussion

The mathematical analysis of chemistry kinetics model with non-linear occurrence has been offered. Some convergence of theoretical results with some numerical method is also given in [11]. In Figures 1, 2, 3, 4, 5, 6 the memory effect of fractional order technique for Robertson problem has been demonstrated. Figures 1, 2, 3 represent the results by using Caputo-Fabrizio derivative and Figures 4, 5, 6 are obtained with ABC derivative. We can get better concentration of the components by using the fractional derivative which are very important for chemical problem to check the actual behavior of the concentration of the chemical with smallest changes in derivative with respect to time.

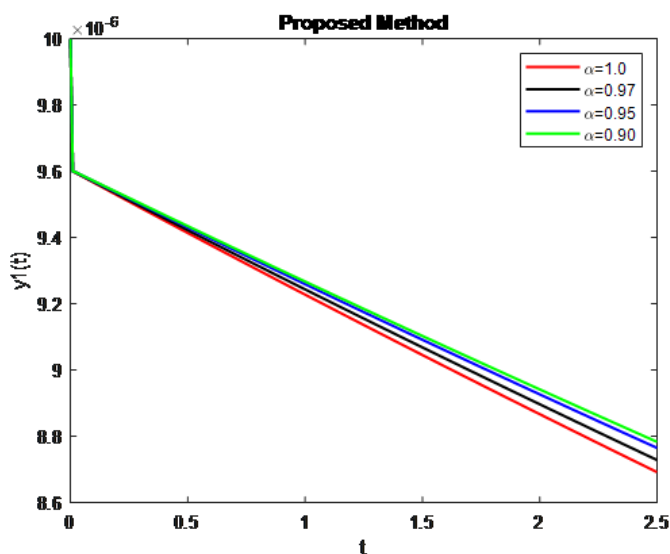


Figure 1: Concentration results of $y_1(t)$ with CF operator at different fractional order .

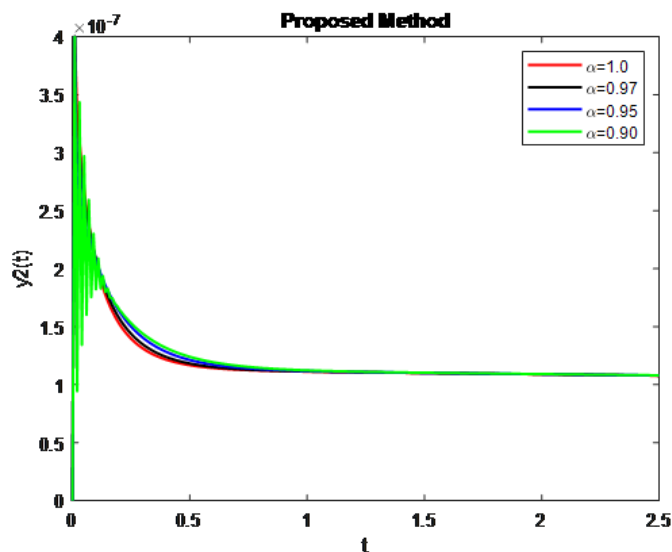


Figure 2: Concentration results of $y_2(t)$ with CF operator at different fractional order .

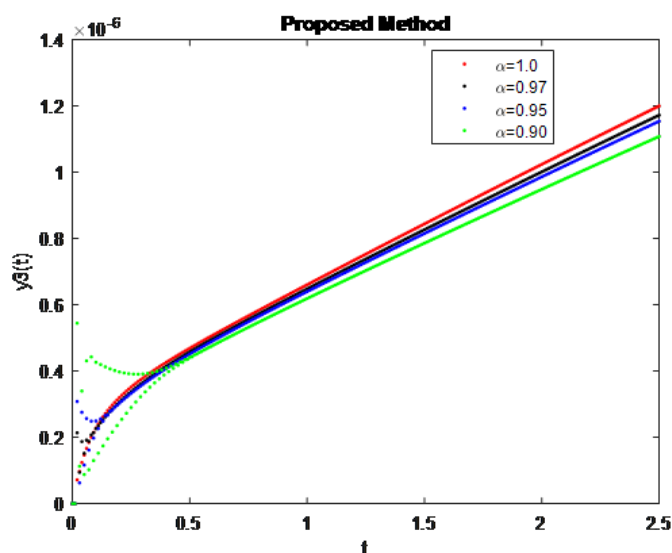


Figure 3: Concentration results of $y_3(t)$ with CF operator at different fractional order .

6. Conclusion

In this paper, we considered the stiff systems of nonlinear ordinary equations which are depend on time t with given initial conditions. The new fractional operator has been implemented to several initial value problems arising from chemical reactions composed of large systems of stiff ordinary differential equations. By using the fixed point theory results, stability and uniqueness of the chemistry kinetic model have been researched. The arbitrary derivative of fractional order has been taken in the Caputo-Fabrizio sense

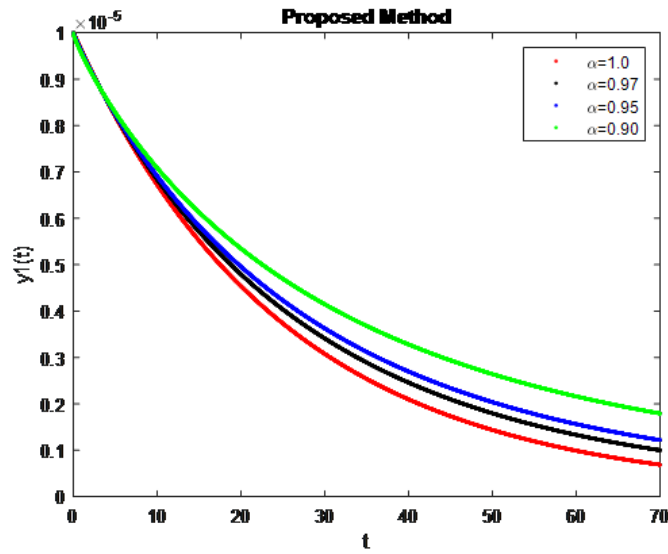


Figure 4: Concentration results of $y_1(t)$ with ABC operator at different fractional order .

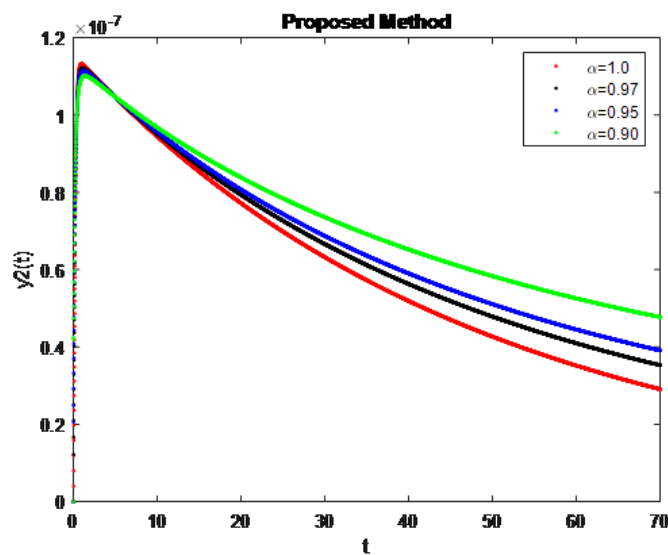


Figure 5: Concentration results of $y_2(t)$ with ABC operator at different fractional order .

with no singular kernel and Atangana-Baleanu in caputo sense with Mittag-Leffler kernel respectively. Sumudu transform is used to obtain the results for proposed schemes. These concepts are very important to use real life problems like Brine tank cascade, Recycled Brine tank cascade, pond pollution, home heating and biomass transfer problem.

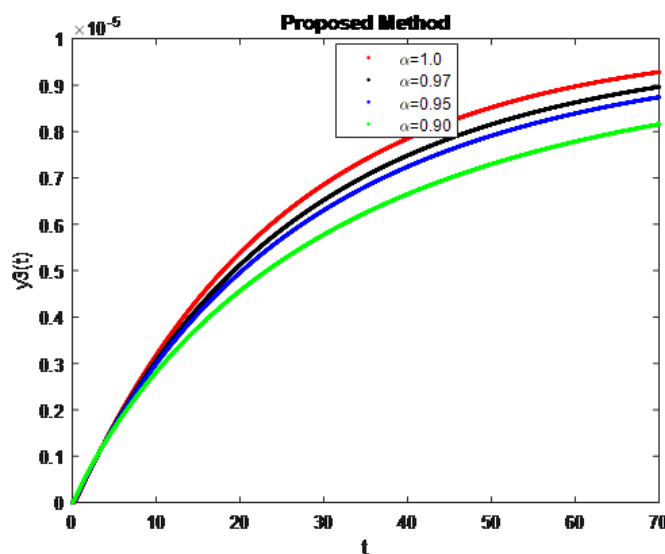


Figure 6: Concentration results of $y_3(t)$ with ABC operator at different fractional order.

Acknowledgements

Jihad Asad, and Rania Wannan would like to thank Palestine Technical University – Kadoorie for supporting this project financially.

References

- [1] Sergio Amat, María José Legaz, and Juan Ruiz-Álvarez. On a variational method for stiff differential equations arising from chemistry kinetics. *Mathematics*, 7(5):459, 2019.
- [2] A Atangana, E Bonyah, and AA Elsadany. A fractional order optimal 4d chaotic financial model with mittag-leffler law. *Chinese Journal of Physics*, 65:38–53, 2020.
- [3] Abdon Atangana and Badr Saad T Alkahtani. Analysis of the keller–segel model with a fractional derivative without singular kernel. *Entropy*, 17(6):4439–4453, 2015.
- [4] Abdon Atangana and Dumitru Baleanu. New fractional derivatives with nonlocal and non-singular kernel: theory and application to heat transfer model. *arXiv preprint arXiv:1602.03408*, 2016.
- [5] Michele Caputo and Mauro Fabrizio. A new definition of fractional derivative without singular kernel. *Progress in Fractional Differentiation & Applications*, 1(2):73–85, 2015.
- [6] Muhammad Farman, Ali Akgül, Dumitru Baleanu, Sumaiyah Imtiaz, and Aqeel Ahmad. Analysis of fractional order chaotic financial model with minimum interest rate impact. *Fractal and Fractional*, 4(3):43, 2020.

- [7] Muhammad Farman, Muhammad Umer Saleem, Aqeel Ahmad, Sumaiyah Imtiaz, Muhammad Farhan Tabassum, Sana Akram, and MO Ahmad. A control of glucose level in insulin therapies for the development of artificial pancreas by atangana baleanu derivative. *Alexandria Engineering Journal*, 59(4):2639–2648, 2020.
- [8] Muhammad Farman, Muhammad Umer Saleem, MF Tabassum, Aqeel Ahmad, and MO Ahmad. A linear control of composite model for glucose insulin glucagon pump. *Ain Shams Engineering Journal*, 10(4):867–872, 2019.
- [9] Hai-Feng Huo, Rui Chen, and Xun-Yang Wang. Modelling and stability of hiv/aids epidemic model with treatment. *Applied Mathematical Modelling*, 40(13-14):6550–6559, 2016.
- [10] Muhammad Altaf Khan and Abdon Atangana. Modeling the dynamics of novel coronavirus (2019-ncov) with fractional derivative. *Alexandria Engineering Journal*, 59(4):2379–2389, 2020.
- [11] MJ Legaz. Approximation of differential equations through a new variational technique and applications. 2012.
- [12] Jorge Losada and Juan J Nieto. Properties of a new fractional derivative without singular kernel. *Progr. Fract. Differ. Appl*, 1(2):87–92, 2015.
- [13] Sirisubtawee Moore and Koonprasert. A caputo–fabrizio fractional differential equation model for hiv/aids with treatment compartment. *Advances in Difference Equations*, 2019(200):1–20, 2019.
- [14] Muhammad Umer Saleem, Muhammad Farman, Aqeel Ahmad, Ehsan Ul Haque, and MO Ahmad. A caputo fabrizio fractional order model for control of glucose in insulin therapies for diabetes. *Ain Shams Engineering Journal*, 11(4):1309–1316, 2020.
- [15] Mekkaoui Toufik and Abdon Atangana. New numerical approximation of fractional derivative with non-local and non-singular kernel: application to chaotic models. *The European Physical Journal Plus*, 132(10):1–16, 2017.