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Research Article

Fractional Numerical Treatment for Biochemical Reaction Networks

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Abstract: Nowadays, numerical models have great importance in every field of science, especially for solving the nonlinear differential equations, partial differential equations, biochemical reactions, etc. In this article, we familiarize fractional-order into a model of Michaelis-Menten. We learned the influence of the changing of different values of fractional order. We display that the model familiarize in this article has nonnegative elucidations. We have checked the stability of the system. Numerical replications are also offered to confirm the attained results.

Keywords: Michaelis-Menten model, NSFD method, fractional order differential equation

1. INTRODUCTION

The enzyme kinetics model is a chemical model which includes a nonlinear reaction. The model consists of the binding/unbinding of enzyme and substrate, and production of the product. The model mechanism is described as follows:

$$E + S \rightleftharpoons_{k_{-1}}^{k_1} ES \overset{k_2}{\rightarrow} E + P \tag{1}$$

where E, S, ES and P denote enzyme, substrate, enzyme-substrate complex and product, respectively, and k_1, k_{-1} and k_2 denote the rates of reactions. If we denote the concentrations of E, S, ES, P by y_1, y_2, y_3, y_4, respectively, and $\boldsymbol{y} = (y_1, y_2, y_3, y_4)^T$, we write the governing equation as

$$\frac{d\boldsymbol{y}}{dt} = \begin{bmatrix} -1 & 1 & 1 \\ -1 & 1 & 0 \\ 1 & -1 & -1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} k_1 y_1 y_2 \\ k_{-1} y_3 \\ k_2 y_3 \end{bmatrix} = \begin{bmatrix} -k_1 y_1 y_2 + k_{-1} y_3 + k_2 y_3 \\ -k_1 y_1 y_2 + k_{-1} y_3 \\ k_1 y_1 y_2 - k_{-1} y_3 - k_2 y_3 \\ k_2 y_3 \end{bmatrix}, \tag{2}$$

We assume a typical initial condition $(y_1, y_2, y_3, y_4) = (e_0, s_0, 0, 0)$. Since the substrate is exhausted and it produces the product P at the equilibrium, the equilibrium of the model can be founded easily as $(y_1, y_2, y_3, y_4) = (e_0, 0, 0, s_0)$. Since the conserved quantities for the model are $y_1 + y_3 + y_4 = s_0$ and $y_2 + y_3 = e_0$, one can reduce the above system (2) into

$$\begin{aligned} \frac{dy_1}{dt} &= -k_1 e_0 y_1 + k_1 y_1 y_3 + k_{-1} y_3 \\ \frac{dy_3}{dt} &= k_1 e_0 y_1 - k_1 y_1 y_3 - (k_{-1} + k_2) y_3 \end{aligned} \tag{3}$$

with the initial condition $(y_1, y_3) = (s_0, 0)$.

As in [1], to obtain the system of the non-dimensional variables from the above system (3) we define the following variables.

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$$u(\tau) = \frac{y_1(t)}{s_0},\ v(\tau) = \frac{(s_0+K_m)y_3(t)}{s_0 e_0},\ \tau = k_1(s_0+K_m)t,$$
$$K_m = \frac{(k_{-1}+k_2)}{k_1},\ \rho = \frac{k_{-1}}{k_2},\ \epsilon = \frac{e_0}{s_0+K_m},\ \sigma = \frac{s_0}{K_m} \tag{4}$$

And

$$T = \epsilon(1+\rho)k_2 t = \frac{\epsilon(1+\rho)k_2}{k_1(s_0+K_m)}\tau$$

Then the system of (3) can be represented in dimensionless form as follows:

$$\frac{du}{dt} = -(1+\sigma)u + \sigma uv + \frac{\rho}{1+\rho}v$$
$$\epsilon\frac{dv}{dt} = (1+\sigma)u - \sigma uv - v \tag{5}$$

subject to the initial condition $u(0) = 1$ and $v(0) = 0$ determined by (4).

2. OPENINGS AND CYPHERS

In this section, some elementary descriptions and things of the fractional calculus theory and nonstandard discretization are discussed.

2.1 Essentials of Fractional-order

Fractional differential equations (FDEs) have gained the considerable prominence owing to their submissions in various sciences, like mechanics, physics, engineering and chemistry [13]. In current years, the dynamic comportments of fractional-order differential systems have established increasing consideration. Although the concept of the fractional calculus was discussed in the same time interval of integer-order calculus, the complexity and the lack of applications postponed its progress till a few decades ago. Recently most of the dynamical systems based on the integer-order calculus have been modified into the fractional order domain due to the extra degrees of freedom and the flexibility which can be used to precisely fit the experimental data much better than the integer order modeling.

2.2 Grunwald-Letnikov (GL) Technique

The GL technique of guesstimate for the 1-D fractional derivative is as follows [13].

$$D^{\beta}\, x(t) = f\big(t, x(\tau)\big),\ \ x(0) = x_0,\ \tau \in [0, \tau_f], \tag{6}$$
$$D^{\beta}x(t) = \lim_{h\to 0} h^{-\beta}\ \sum_{\boldsymbol{j=0}}^{\left[\frac{\tau_f}{h}\right]}(-1)^i \binom{\beta}{i}\ x(\tau - ih),$$

where $0 < \beta < 1$, D^{β} denotes the fractional derivative, h is the step size and $\left[\frac{\tau_f}{\boldsymbol{h}}\right]$ represents the integer part of $\frac{\tau_f}{\boldsymbol{h}}$. Therefore, Eq. (4) is discretized in the next form,

$$\sum_{i=0}^{n} C_j^{\beta}\ x_{n-j} = f(\tau_n, x_n), \qquad n = 1,2,3,\ldots$$

where $\tau_n = n\,h$ and C_j^{β} are the GL coefficients demarcated as

$$C_i^{\beta} = \left(1 - \frac{1+\beta}{i}\right) C_{i-1}^{\beta}, \qquad C_0^{\beta} = h^{-\beta}, \qquad i = 1,2,3\ldots$$

The Micken's paper [15] provides a common route for determining $\psi(h)$ for the ODEs.

A case of the NSFD discretization procedure is its submission to the decay equation

$$X' = -\xi\, X$$

where ξ is constant. The discretization scheme [15] is

$$\frac{X_{n+1}-X_n}{\psi} = -\xi\, X_n, \qquad \psi(h,\xi\,) = \frac{1-e^{-\xi\, h}}{\xi}$$

Let us take another application given by

$$X' = \lambda_1\, X - \lambda_2\, X^2$$

where the NSFD scheme is

$$\frac{X_{n+1} - X_n}{\psi} = \xi_1\, X_n - \xi_2 X_n X_{n+1}$$

$$\psi(h,\xi_1\,) = \frac{e^{\xi_1\, h} - 1}{\xi_1}$$

It ought to be noted that the NSFD schemes for both ODEs are exact in the logic that $X_n = X(\tau_n)$ for every pertinent values of $h > 0$.

3. FRACTIONAL ORDER CHEMICAL MODEL

The fractional order above said chemical model can be written as

$$\frac{d^{\gamma_1} X}{dt^{\gamma_1}} = -(1+\sigma)X + \left(\frac{\rho}{1+\rho}\right) Y + \sigma XY, \tag{7}$$

$$\frac{d^{\gamma_2} Y}{dt^{\gamma_2}} = \frac{1}{\epsilon}((1+\sigma)X - \ Y - \sigma XY), \tag{8}$$

with initial conditions

$$X(0) \ = \ 1\ , Y(0) \ = \ 0 \text{ and } 0 < \gamma_i \leq 1, \text{ i=1,2.}$$

Theorem 1. [14] Consider the fractional order system given below:

$$D^{\beta}\, U(t) = F(U), \ \ U(0) = U_0 \tag{9}$$

where $0 < \beta \leq 1$ and $u \in R^n$. Equilibrium points of system (9) should be determined by cracking the equation $F(U) = 0$. These points will be locally asymptotically steady if all eigenvalues η matrix of the jacobian $J = \frac{\partial F}{\partial U}$ evaluated at the equilibrium point satisfy:

$$|\arg(\eta)| > \frac{\beta\, \pi}{2}.$$

The jacobian matrix J system Eqtions (7) and (8) of the equilibrium point $E = (X^*, Y^*)$

$$J(F^*) = \begin{bmatrix} -1-\sigma+\sigma Y^* & \dfrac{\rho}{1+\rho} + \sigma X^* \\ \dfrac{1}{\epsilon}(1+\sigma+\sigma Y^*) & \dfrac{\sigma X^* - 1}{\epsilon} \end{bmatrix}$$

The existence and local stability conditions of this equilibrium point E is as follows. Suppose that $H(P)$ denotes the discriminant of a polynomial P

$$P(\eta) = \eta^2 + b_1\, \eta + b_2 = 0$$

where $b_1 = -trace\ (J)$, $b_2 = det(J)$.

$$H(P) = b_1^2 - 4b_2 < 0 \quad \text{or} \quad b_1^2 < 4b_2$$

and $\left|\tan^{-1}(\sqrt{-b_1^2 + 4b_2})/\, b_1\right| > \frac{\beta\, \pi}{2}$

In simple words, stability holds if and only if $b_1 > 0$ and $b_2 > 0$.

Now we evaluate the equilibrium points of the system (7) and (8).

3.1 Equilibrium Point

Equate (7) and (8) equal to zero i.e.

$$-(1+\sigma)X + \left(\frac{\rho}{1+\rho}\right)Y + \sigma XY = 0 \tag{10}$$

$$\frac{1}{\epsilon}((1+\sigma)X - Y - \sigma XY) = 0 \tag{11}$$

we obtain $(X^*, Y^*) = (0,0)$, that is the equilibrium point.

The Jacobian matrix J of system (7) and (8) at the equilibrium point $E(X^*, Y^*) = (0,0)$ we have

$$J = \begin{bmatrix} -1-\sigma & \dfrac{\rho}{1+\rho} \\ \dfrac{1}{\epsilon}(1+\sigma) & \dfrac{-1}{\epsilon} \end{bmatrix}$$

$b_1 = -tace(J) = -(-1-\sigma-\frac{1}{\epsilon}) > 0$, $b_2 = det(J) = \left(\frac{1+\sigma}{\epsilon(1+\rho)}\right) > 0.$

Since $b_1 > 0$ and $b_2 > 0$, so stability holds.

3.2 Numerical Experiments

Numerical experiments are performed using values of parameters given in Table 1.

Table 1. Different parameters & values.

Parameters	Value
ϵ	1
ρ	0.1
σ	0.1

4. NSFD DISCRETIZATION

In this section we shall construct Non Standard Finite Difference Scheme proposed by Mickens [6, 7], for the equations (7) and (8) and swapping the step size h by a function $\psi(h)$ and using GL discretization technique, it can be seen that

$$\sum_{j=0}^{n+1} C_j^{\gamma_1} X^{n+1-j} = \sigma X^n Y^n + \left(\frac{\rho}{1+\rho}\right)Y^n - (1+\sigma)X^{n+1} \tag{12}$$

$$\sum_{j=0}^{n+1} C_j^{\gamma_2} Y^{n+1-j} = \frac{1}{\epsilon}((1+\sigma)X^n - Y^{n+1} - \sigma X^{n+1}Y^{n+1}) \tag{13}$$

$$(12) \implies X^{n+1} = \frac{\sigma X^n Y^n + \left(\frac{\rho}{1+\rho}\right)Y^n - \sum_{j=1}^{n+1} C_j^{\gamma_1} X^{n+1-j}}{(C_0^{\gamma_1} + 1 + \sigma)} \tag{14}$$

$$(13) \implies Y^{n+1} = \frac{\frac{(1+\sigma)}{\epsilon}X^{n+1} - \sum_{j=1}^{n+1} C_j^{\gamma_2} Y^{n+1-j}}{C_0^{\gamma_2} + \frac{1}{\epsilon}(1+\sigma X^{n+1})} \tag{15}$$

with $\boldsymbol{C_0^{\gamma_1}} = \left(\frac{e^{(1+\sigma)h}-1}{(1+\sigma)}\right)^{-\gamma_1}$, $\boldsymbol{C_0^{\gamma_2}} = \left(\frac{e^{\frac{1}{\epsilon}h}-1}{\frac{1}{\epsilon}}\right)^{-\gamma_2}$

4.1 Numerical Experiments

Analytical studies permanently remain unfinished without numerical authentication of the outcomes. In this unit, we present numerical simulation to exemplify the outcomes attained in previous sections. Now we solve the fractional-order Michaelis-Menten biochemical reaction model in two cases. The guestimate elucidations are revealed in Fig. 1-4, for various values of $0 < \gamma_i \leq 1$, $i = 1,2$.

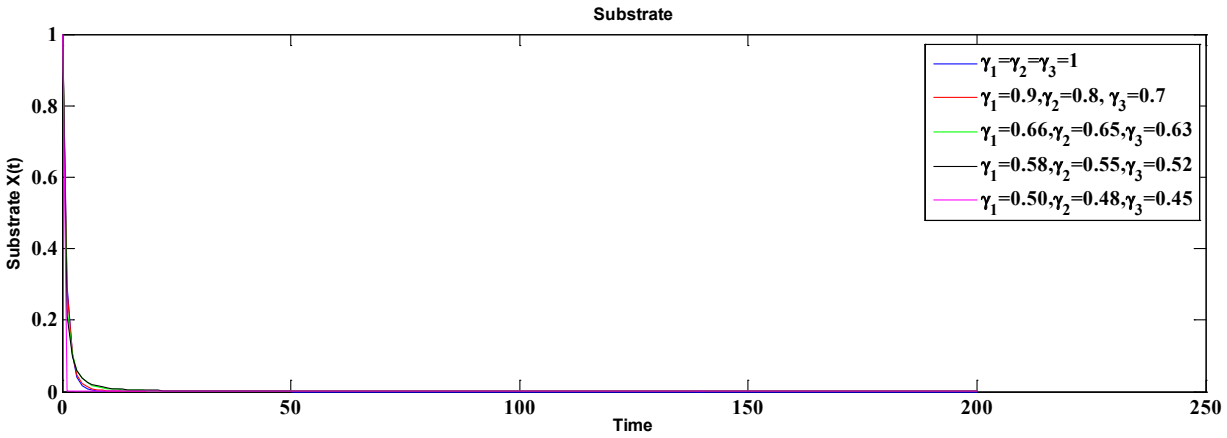

Fig 1. The concentration of Substrate at $N = 200$ with step size $h = 1.1$.

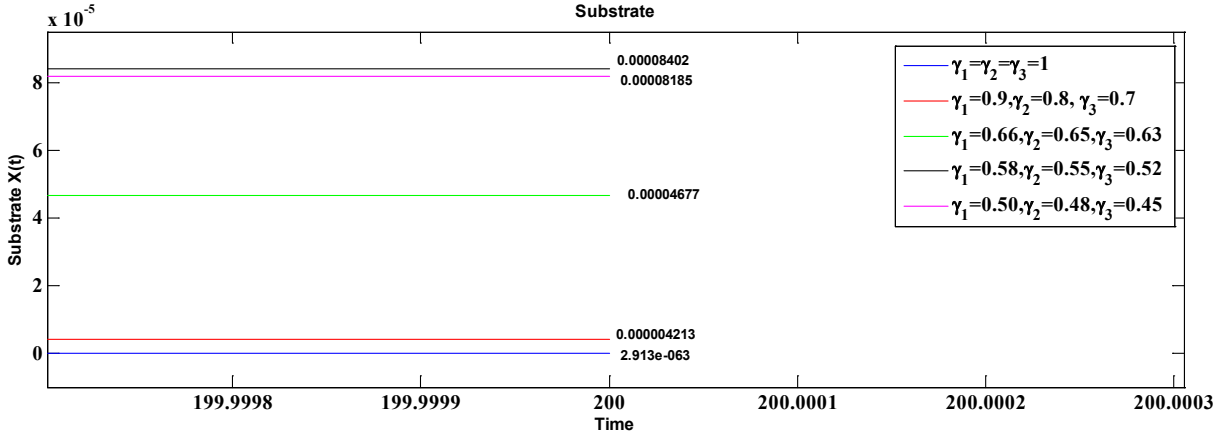

Fig. 1. In zoom.

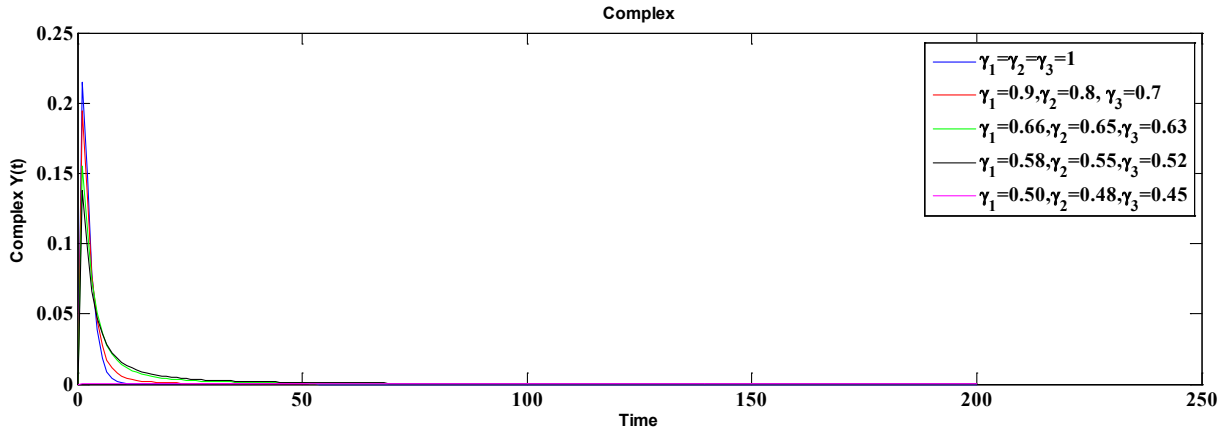

Fig. 2. The concentration of Complex at $N = 200$ with step size $h = 1.1$.

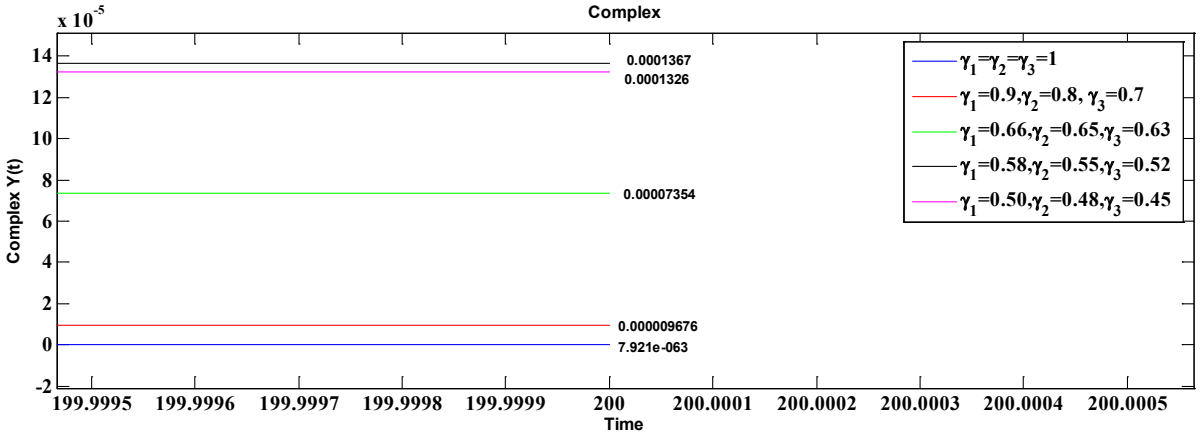

Fig. 2. In Zoom.

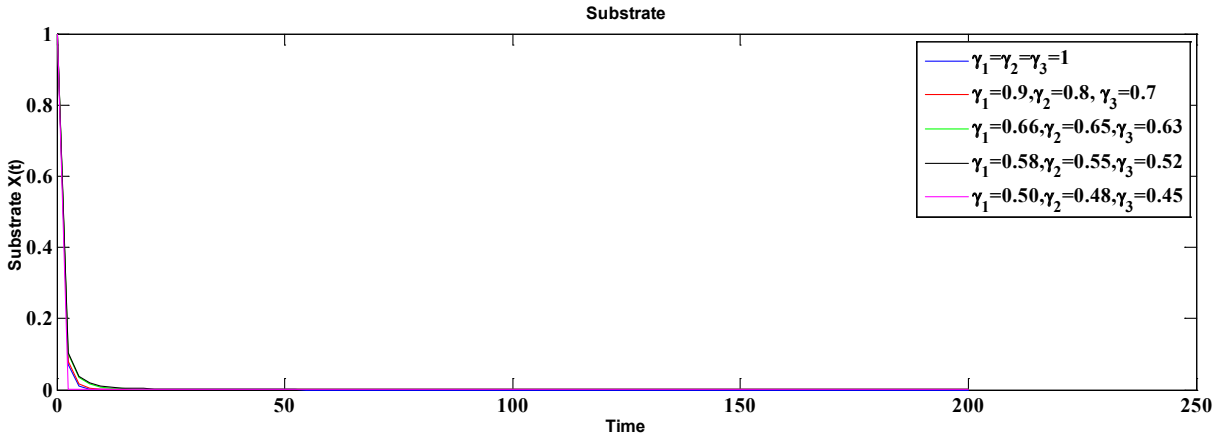

Fig. 3. The concentration of Substrate at $N = 200$ with step size $h = 2.4$.

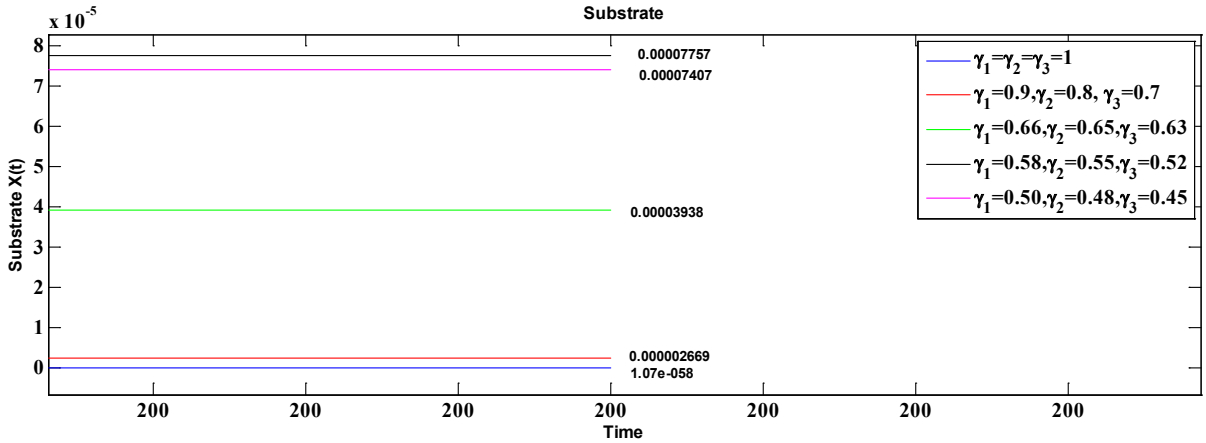

Fig. 3. In Zoom

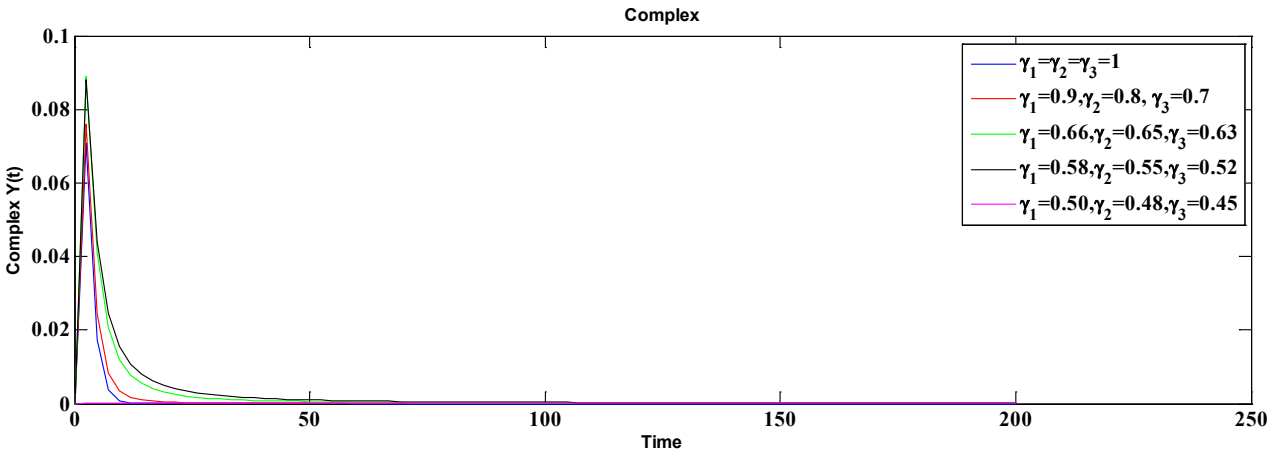

Fig. 4. The concentration of Complex at $N = 200$ with step size $h = 2.4$.

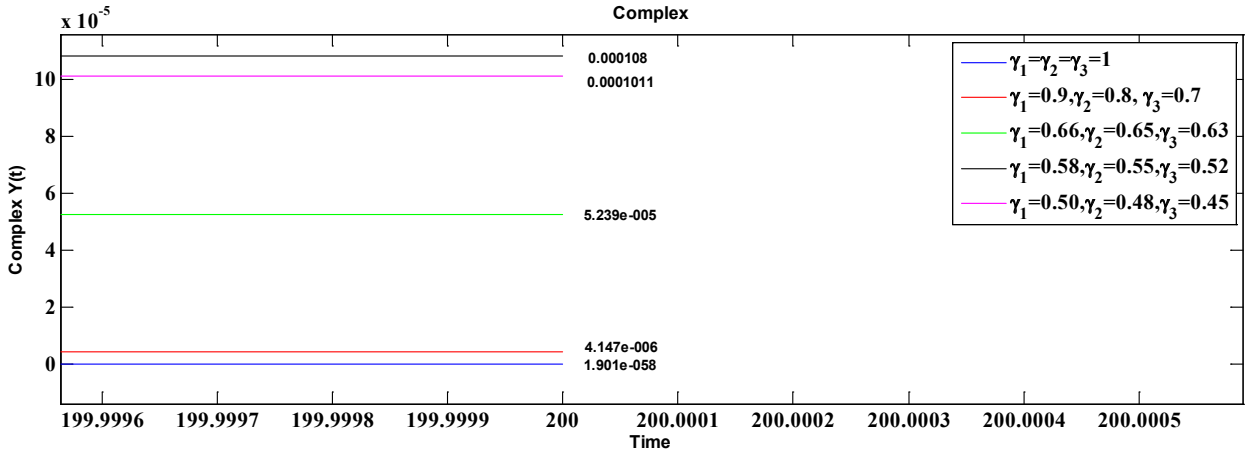

Fig. 4. In Zoom.

5. RESULTS AND DISCUSSION

The Fractional order modelling of well-known Michaelis-Menten non-linear reaction system has been analysed in this paper. An unconditionally convergent non-standard finite difference numerical model with inserting the GL Method, has been constructed for fractional order Michaelis-Menten model. Numerical experiments are performed for different values of fractions.

6. CONCLUSIONS

The present analysis revealed the applicability of the non-standard finite difference technique to crack systems of DEs of fractional order. The work accentuated our faith that the technique is a steadfast method to handle linear and nonlinear fractional order DEs. The goal for considering a fractional order system instead of its integer order counterpart is that fractional order DEs are generalization of integer order differential equations. Also, using fractional order DEs can help us to condense the errors arising from the neglecting parameters in modeling real life phenomenon. The proposed scheme is easy to implement and numerically stable.

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