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Complexity Analysis to Fractional Order Enzyme Model

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ABSTRACT

This study examines a discrete-time enzyme model with Caputo fractional order. We look into the existence and uniqueness of fixed points in the discrete dynamic model and discover parametric criteria for their local asymptotic stability. Additionally, it is demonstrated using bifurcation theory that the system experiences Period-Doubling and Neimark-Sacker bifurcation in a constrained area around the singular positive fixed point and that an invariant circle would result. It has been determined that the parameter values and the initial conditions have a significant impact on the dynamical behavior of the fractional order enzyme model. Additionally, with the use of Matlab tools, numerical analysis is offered to illustrate the theoretical debates. Therefore, numerical simulations are used to support the key theoretical findings.

KEYWORDS: Fractional order Enzyme model, Period-Doubling (PD) and Neimark-Sacker (NS) Bifurcations, Phase portraits.

1. INTRODUCTION

Fractional calculus is a branch of mathematical analysis that studies the many definitions of real number powers or complex number powers of the differentiation operator. Fractional calculus is a notion that has been around since the 17th century.

Numerous epidemiological models with mathematical specifications have been created over time [1, 2], but the majority of these models are only compatible with differential equations of integer order (IDEs). Fractional-order differential equations have been successfully analyzed during the past 30 years in a variety of disciplines, including science, engineering, money and finance, economics, and epidemiology [3–7]. FDEs can be used to model some phenomena that IDEs are insufficient to capture [8]. Since biological systems inherently relate to memory-based systems, FDEs are commonly applied to them. The study of chaos in fractional-order dynamical systems is an intriguing and alluring subject [9-13].

Michaelis and Menten [14] are credited with pioneering work in the realm of enzyme processes. They described a model that is thought to be the cornerstone for the research of enzyme kinetics. The steady-state approximation, which has been extensively employed in the analysis of complicated biochemical networks [15], was used by Briggs and Haldane [16] to quantify the rate function of an enzyme one-substrate reaction. To determine the numerical solutions to the enzyme-substrate reaction model, Iqbal et al. [18] used the modified wavelets method. The PD and NS bifurcations was investigated in a 3D system in [18]. Curiosity about the numerous Caputo fractional order discrete systems has been sparked by the NS and PD bifurcations, stable orbits, and chaotic attractors [19,20].

The planar set of non-linear differential equations shown below governs a two-dimensional form of the enzyme model [17]:

$$\begin{aligned} \dot{x} &= -x + (\beta-\alpha)y + xy \\ \dot{y} &= \frac{1}{\gamma}(x - \beta y - xy) \end{aligned} \tag{1}$$

where α, β, γ are assumed to be three positive constants.

The Caputo fractional derivative on the system (1) is used to provide the discretized form in this case.

$$\begin{aligned} x_{n+1} &= x_n + \frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)}(-x_n + (\beta-\alpha)y_n + x_n y_n), \\ y_{n+1} &= y_n + \frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)}\left(\frac{1}{\gamma}(x_n - \beta y_n - x_n y_n\right), \end{aligned} \tag{2}$$

The remaining section of this paper is structured as follows: Sect. 2 investigates the topological divisions of fixed points. In Section 3, we demonstrate analytically that, given a particular parametric condition, the system (2), suffers a PD or NS bifurcation. To support our analytical conclusions, in Section 4, we quantitatively illustrate system dynamics, including bifurcation diagrams and phase portraits. The conclusion was delivered in Section 5.

2. STABILITY ANALYSIS

The system(2)'s trivial equilibrium point is $O = (0,0)$, which is the only solution to equation (2).
The Variation matrix of system (2) evaluated at $O(x^*, y^*)$ are

$$J(x^*,y^*) = \begin{pmatrix} 1+(-1+y^*)\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} & (x^*+\beta-\alpha)\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} \\ \frac{(1-y^*)}{\gamma}\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} & (1-x^{*2})\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} \end{pmatrix} \tag{3}$$

Now at $O(0,0)$

$$J_O = \begin{pmatrix} 1-\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} & (\beta-\alpha)\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} \\ \frac{1}{\gamma}\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} & 1-\frac{\beta}{\gamma}\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} \end{pmatrix} \tag{4}$$

Additionally, the characteristic polynomial for the variational matrix J_O is calculated in the manner described below:

$$F_a(\lambda) := \lambda^2 - Tr(J_O)\lambda + Det(J_O) = 0 \tag{5}$$

where $Tr(J_O)$ and $Det(J_O)$ are given by

$$Tr(J_O) = 2 - \frac{\beta+\gamma}{\gamma}\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)}$$

$$Det(J_O) = 1 - \frac{\beta+\gamma}{\gamma}\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)} + \frac{\alpha}{\gamma}\left(\frac{\rho^{\vartheta}}{\Gamma(1+\vartheta)}\right)^2 \tag{6}$$

You may express the eigenvalues of (6) as $\lambda_{1,2} = \frac{Tr(J_O)\pm\sqrt{(Tr(J_O))^2-4Det(J_O)}}{2}$.

Jury Criterion: *The condition for reaching the equilibrium point $O(x^*, y^*)$ stability is given as follows $F_a(1) > 0, F_a(-1) > 0, F_a(0) - 1 < 0$.*

Let,

$$PDB_O = \left\{(\alpha,\beta,\gamma,\rho,\vartheta): \rho = \left(\Gamma(1+\vartheta).\frac{\ddot{B_{2a}} \pm \sqrt{L_a}}{\ddot{B_{1a}}}\right)^{\frac{1}{\vartheta}} = \rho_{\pm}, L_a \geq 0\right\}.$$

where,

$$\ddot{B_{1a}} = \alpha; \ddot{B_{2a}} = \beta+\gamma; \ddot{B_{3a}} = 4\gamma$$

$$L_a = \ddot{B_{2a}}^2 - \ddot{B_{3a}} * \ddot{B_{1a}}$$

The system (2) undergoes a PD bifurcation at O when $(\alpha,\beta,\gamma,\rho,\vartheta)$ changes around PDB_O.

Also let

$$NSB_O = \left\{(\alpha,\beta,\gamma,\rho,\vartheta): \rho = \left(\Gamma(1+\vartheta).\frac{\ddot{B_{2a}}}{\ddot{B_{1a}}}\right)^{\frac{1}{\vartheta}} = \rho_N, L_a < 0\right\}$$

The system (2) undergoes a NS bifurcation at O when $(\alpha,\beta,\gamma,\rho,\vartheta)$ changes around NSB_O.

For the stability stipulation of the fixed point O, we offer the subsequent Lemma.

Lemma 1. *For any random selection of parameter values, the fixed point O is a*

sink if

(i) $L_a \geq 0, \rho < \rho_-(stable\ node)$,

(ii) $L_a < 0, \rho < \rho_N(stable\ focus)$,

source if

(i) $L_a \geq 0, \rho < \rho_+(unstable\ node)$,

(ii) $L_a < 0, \rho > \rho_N(unstable\ focus)$,

non-hyperbolic

(i) $L_a \geq 0, \rho = \rho_-\ or\ \rho = \rho_+(saddle\ with\ PD)$,

(ii) $L_a < 0, \rho = \rho_N(\ focus)$,

saddle: otherwise

3. BIFURCATION ANALYSIS

The presence, direction, and stability analysis of PD and NS bifurcations close to the fixed point O will be investigated in this part using center-manifold and bifurcation theory.

3.1 PD Bifurcation

PD bifurcation in the system (2) can be worked out by defining the parameters lie in PDB_O.

Let,

$$\rho = \left(\Gamma(1+\vartheta).\frac{\ddot{B_{2a}}-\sqrt{L_a}}{\ddot{B_{1a}}}\right)^{\frac{1}{\vartheta}} = \rho_-, L_a \geq 0.$$

Also the eigenvalues are

$$\lambda_1 = -1 \text{ and } \lambda_2 = 1 + \ddot{B_{2a}}\rho_-$$

$$\text{For } |\lambda_2| \neq 1 \text{ gives } \ddot{B_{2a}}\rho_- \neq 0, -2 \tag{7}$$

Utilizing the transformation $\hat{x} = x - x^+, \hat{y} = y - y^+$ and set $A(\rho) = J(x^*, y^*)$. So, the system (2) rewritten as

$$\begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix} \to A(\rho_-)\begin{pmatrix}\hat{x}\\ \hat{y}\end{pmatrix} + \begin{pmatrix}F_1(\hat{x},\hat{y},\rho_-)\\ F_2(\hat{x},\hat{y},\rho_-)\end{pmatrix} \tag{8}$$

where $X = (\hat{x},\hat{y})^T$ and

$$F_1(\hat{x},\hat{y},\rho_-) = \hat{x}\hat{y}\rho_-$$

$$F_2(\hat{x},\hat{y},\rho_-) = -\frac{\hat{x}\hat{y}\rho_-}{\gamma} \tag{9}$$

So (8) becomes

$$X_{n+1} = AX_n + \frac{1}{2}B(X_n, X_n) + \frac{1}{6}C(X_n, X_n, X_n) + O(\|X_n\|^4)$$

where $B(x,y) = \begin{pmatrix}B_1(x,y)\\ B_2(x,y\end{pmatrix}$ and $C(x,y,v) = \begin{pmatrix}C_1(x,y,v)\\ C_2(x,y,v)\end{pmatrix}$are multi-linear vector functions of $x, y, v \in \mathbb{R}^2$ that are symmetric and defined as follows:

$$B_1(x,y) = \sum_{j,k=1}^{2} \frac{\delta^2 F_1(\varepsilon,\rho)}{\delta\varepsilon_j \delta\varepsilon_k}\Bigg|_{\varepsilon=0} x_j y_k = (x_2y_1 + x_1y_2)\rho_-$$

$$B_2(x,y) = \sum_{j,k=1}^{2} \frac{\delta^2 F_2(\varepsilon,\rho)}{\delta\varepsilon_j \delta\varepsilon_k}\Bigg|_{\varepsilon=0} x_j y_k = \frac{-(x_2y_1 + x_1y_2)\rho_-}{\gamma}$$

and

$$C_1(x,y,v) = \sum_{j,k,l=1}^{2} \frac{\delta^2 F_1(\varepsilon,\rho)}{\delta\varepsilon_j \delta\varepsilon_k \delta\varepsilon_l}\Bigg|_{\varepsilon=0} x_j y_k v_l = 0$$

$$C_2(x,y,v) = \sum_{j,k,l=1}^{2} \frac{\delta^2 F_1(\varepsilon,\rho)}{\delta\varepsilon_j \delta\varepsilon_k \delta\varepsilon_l}\Bigg|_{\varepsilon=0} x_j y_k v_l = 0$$

Let, the two eigenvectors of A and A^T for eigenvalue $\lambda_1(\rho_-) = -1$ be $s_1, s_2 \in \mathbb{R}^2$ such that $A(\rho_-)s_1 = -s_1$ and $A^T(\rho_-)s_2 = -s_2$.

Using a rigorous calculation, we get,

$$s_1 = \begin{pmatrix}\beta - \gamma - \sqrt{L_a}\\ 1\end{pmatrix} = \begin{pmatrix}s_{11}\\ 1\end{pmatrix};$$

$$s_2 = \begin{pmatrix}\dfrac{\gamma - \beta + \sqrt{L_a}}{2\alpha\gamma - 2\beta\gamma}\\ 1\end{pmatrix} = \begin{pmatrix}s_{21}\\ 1\end{pmatrix}$$

In order to get, $< s_1, s_2 > = 1$, where $< s_1, s_2 > = s_{11}s_{21} + s_{12}s_{22}$, use of the normalized vector is required as $s_2 = \gamma_F s_2$, with $\gamma_F = \frac{1}{1+s_{11}s_{21}}$.

The coefficient $l_1(\rho_F)$ must not be zero in order for the system (2) to undergo Period-Doubling bifurcation. The coefficient is

$$l_1(\rho_-) = \frac{1}{6} < s_2, C(s_1, s_1, s_1) > -\frac{1}{2} < s_2, B(s_2, (A - I)^{-1}B(s_1, s_1)) > \tag{10}$$

As a result, the following theorem concerning Period-Doubling bifurcation exists:

Theorem 1. *System (2) will experience PD bifurcation at fixed point O if* ρ *changes its value in a small region around* PDB_O *with (7) is true and* $l_1(\rho_-) \neq 0$. *Additionally, a smooth closed invariant curve that bifurcates from the equation O exists and is attractive (or repulsive), and the bifurcation is sub-critical (or super-critical) if* $l_1(\rho_-) < 0$*(resp.* $l_1(\rho_-) > 0$).

3.2 Neimark-Sacker Bifurcation

NS bifurcation in the system (2) can be worked out by defining the parameters lie in NSB_O.

Let,
$$\rho = \rho_N = \left(\Gamma(1+\vartheta).\frac{\ddot{B_{2a}}}{\ddot{B_{1a}}}\right)^{\frac{1}{\vartheta}}$$

Also,
$$\left.\frac{d|\lambda_i(\rho)|}{d\rho}\right|_{\rho=\rho_{NS}} = \frac{\ddot{B_{2a}}}{2\ddot{B_{3a}}} \neq 0$$
$$-(Tr(J_O))|_{\rho=\rho_N} \neq 0 \Rightarrow \frac{\ddot{B_{2a}}^2}{\ddot{B_{1a}}\ddot{B_{3a}}} \neq 2,3 \quad (11)$$

Suppose the two eigenvectors $s_1, s_2 \in \mathbb{C}^2$ satisfy the following conditions
$$A(\rho_N)s_1 = \lambda(\rho_N)s_1, A(\rho_N)\overline{s_1} = \bar{\lambda}(\rho_N)\overline{s_1}$$
And
$$A^T(\rho_N)s_2 = \bar{\lambda}(\rho_N)s_2,\ A^T(\rho_N)\overline{s_2} = \lambda(\rho_N)\overline{s_2} \quad (12)$$
We construe $W \in \mathbb{R}^2$as $W = vs_1 + \bar{v}\overline{s_1}$ by choosing ρ vary near to ρ_N and for $v \in \mathbb{C}$. Then v is $v = \langle s_2, W\rangle$. Consequently,
$$v \to \lambda(\rho)v + \hat{k}(v, \bar{v}, \rho) \quad (13)$$
where $\lambda(\rho) = (1+\tau(\rho))e^{i\theta\rho}$ with $\tau(\rho_N) = 0$ and $\hat{k}(v, \bar{v}, \rho)$is a smooth function of complex value.
Using Taylor expansion to $\hat{k}$, we get
$\hat{k}(v, \bar{v}, \rho) = \sum_{j+l\geq 2}\frac{1}{j!l!}\widehat{k_{jl}}(\rho)v^j v^{-l}$, with $\widehat{k_{jl}} \in \mathbb{C}, j, l = 0,1, \ldots$
The coefficients $k_{jl}$are
$$\widehat{k_{20}}(\rho_N) = \langle s_2, B(s_1, s_1)\rangle, \widehat{k_{11}}(\rho_N) = \langle s_2, B(s_1, \overline{s_1})\rangle$$
$$\widehat{k_{02}}(\rho_N) = \langle s_2, B(\overline{s_1}, \overline{s_1})\rangle, \widehat{k_{21}}(\rho_N) = \langle s_2, C(s_1, s_1, \overline{s_1})\rangle \quad (14)$$
The coefficient $l_2(\rho_N)$ must not be zero in order for the system (2) to undergo Neimark-Sacker bifurcation. The coefficient is
$$l_2(\rho_N) = Re\left(\frac{\lambda_2\widehat{k_{21}}}{2}\right) - Re\left(\frac{(1-2\lambda_1)\lambda_2{}^2\widehat{k_{20}}\widehat{k_{11}}}{2(1-\lambda_1)}\right) - \frac{1}{2}\left|\widehat{k_{11}}\right|^2 - \frac{1}{2}\left|\widehat{k_{02}}\right|^2 \quad (15)$$
As a result, the following theorem concerning NS bifurcation exists:

Theorem 2. *System (2) will experience NS bifurcation at fixed point O if* ρ *changes its value in a small region around* PDB_O *with (11) is true and* $l_2(\rho_N) \neq 0$. *Additionally, a smooth closed invariant curve that bifurcates from the equation O exists and is attractive (or repulsive), and the bifurcation is sub-critical (or super-critical) if* $l_2(\rho_N) < 0$*(resp.* $l_2(\rho_N) > 0$).

4. NUMERICAL SIMULATIONS

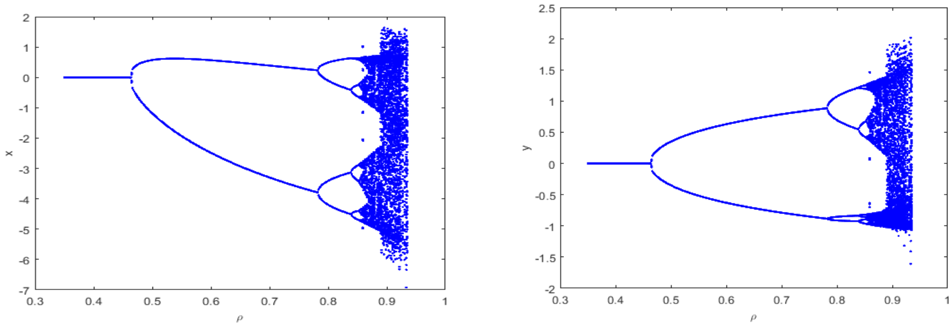
Utilizing Mathematica and MATLAB, the theoretical findings in this part are shown with graphics. These numerical simulations will feature phase portraits and bifurcation diagrams.

Example 1: The fixed parameter values are $\alpha = 2.45, \beta = 6.5, \gamma = 3.5, \vartheta = 0.4896$ and $,\rho$ fluctuates in $0.35 \leq \rho \leq 1.15$. The coexistence's idealized positive equilibrium is $(0.0002, 0.0002)$ and $\rho_F = 0.4618$. The eigenvalues are $\lambda_{1,2} = -1{,}0.790733$. The eigenvectors are
$s_1 \sim (-0.931108, 0.364743)^T$ and $s_2 \sim (-0.177239, 0.984168)^T$
To obtain $< s_1, s_2 > = 1$, the normalized vector are $\gamma_F = 1.98041$.
The crucial portion is calculated from (17) as $l_1(\rho_F) = 0.837982 > 0$. A subcritical PD bifurcation consequently takes place. Figure.1 display the system (2)'s bifurcation diagram. Different values of ρ are used to draw phase portraits in Figure.2.

Example 2: Consider the system with the following parameters $\alpha = 3.33, \beta = 1.8, \gamma = 0.4, \vartheta = 0.483$ and $,\rho$ fluctuates in $0.125 \leq \rho \leq 0.42$. The coexistence's idealized positive equilibrium is $(0.0002, 0.0002)$.

Also,
$$\left.\frac{d|\lambda_i(\rho)|}{d\rho}\right|_{\rho=\rho_N} = 2.75 \neq 0$$
$$-(Tr(J_O))|_{\rho=\rho_N} \neq 0 \Rightarrow 1.667 \neq 2,3$$

The eigenvalues are $\lambda, \bar{\lambda} = -0.833334 \pm 0.55277i$. The eigenvectors are
$s_1 \sim (0.553399 + 0.262202i, 0.790569)^T$ and $s_2 \sim (0.790569, -0.553399 - 0.262202i)^T$
To obtain $< s_1, s_2 > = 1$, the normalized vector are $\gamma_N = 2.41209i$.



(a) (b)

Figure 1. PD Bifurcation diagram by varying ρ.

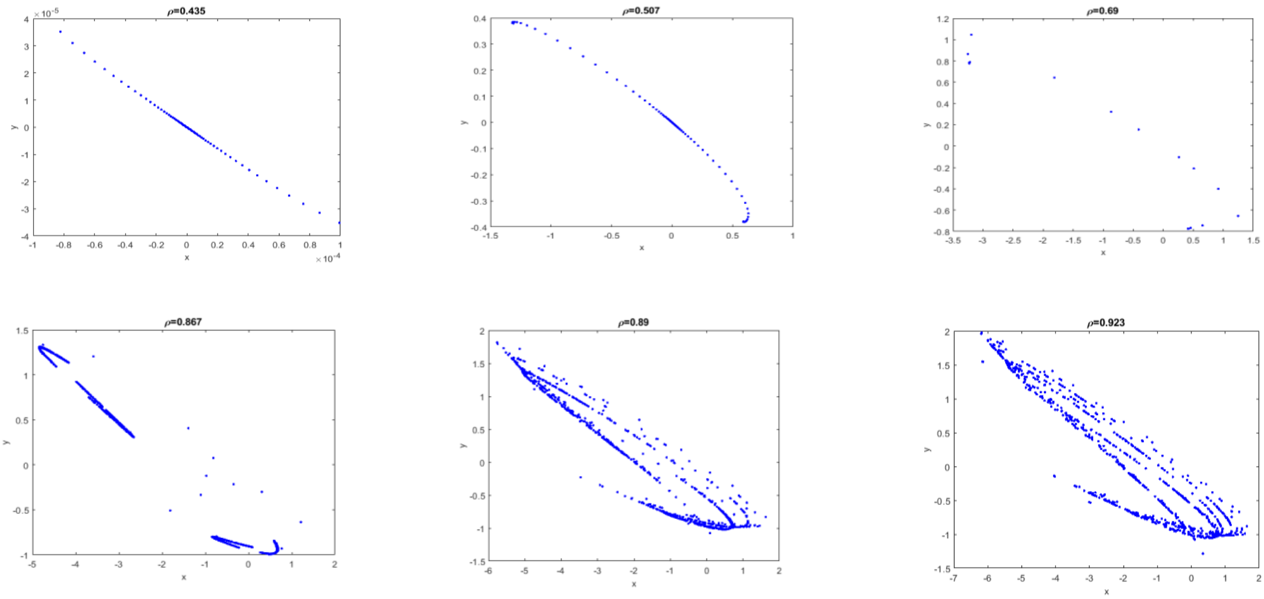
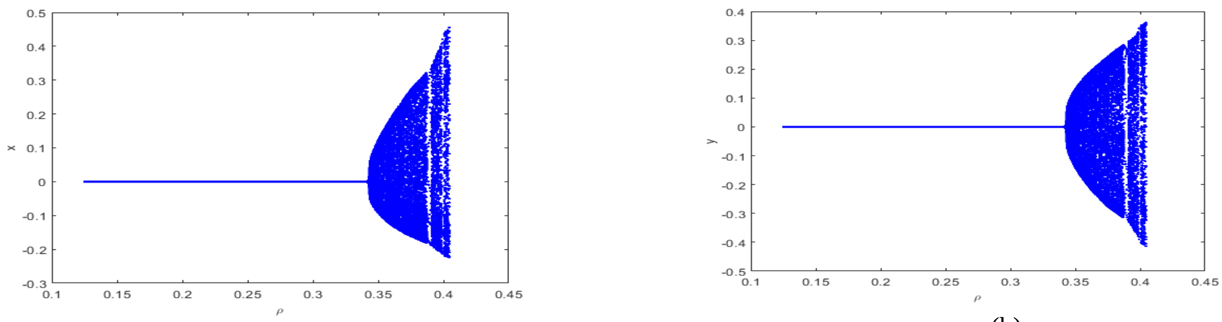


Figure 2. Phase portrait by varying ρ.

Also,

$$\widehat{K_{20}} = 0.527046 - 3.49603i$$
$$\widehat{k_{11}} = -0.922331 - 3.05903i$$
$$\widehat{k_{02}} = -2.37171 - 2.62202i$$
$$\widehat{k_{21}} = 26.0416 + 1.25632i$$

The crucial portion is calculated from (15) as $l_2(\rho_N) = -13.6285 < 0$. A supercritical NS bifurcation consequently takes place at $\rho_N = 0.336$. Figure.3 display the system (2)'s bifurcation diagram. Different values of ρ are used to draw phase portraits in Figure.4.



(a) (b)

Figure 3. NS Bifurcation diagram by varying ρ.

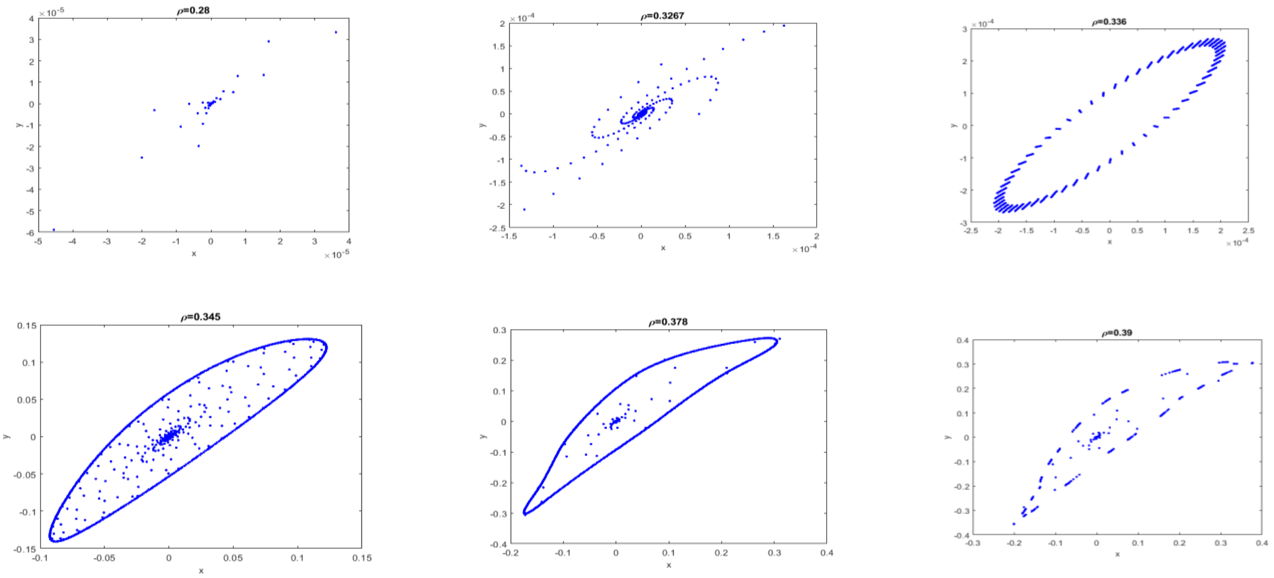


Figure 4. Phase portrait by varying ρ.

Example 3: The NS bifurcation diagram of the enzyme model may show more dynamic behavior when the values of γ, ϑ changes separately by fixing all the parameters as in Example 2. The bifurcation diagrams and phase portraits are shown in Figure 5&7 and Figure.6 respectively.

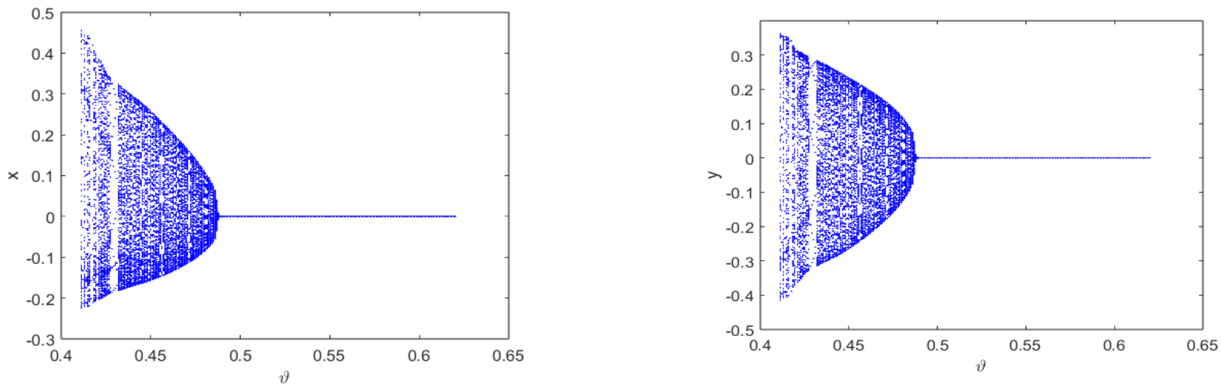
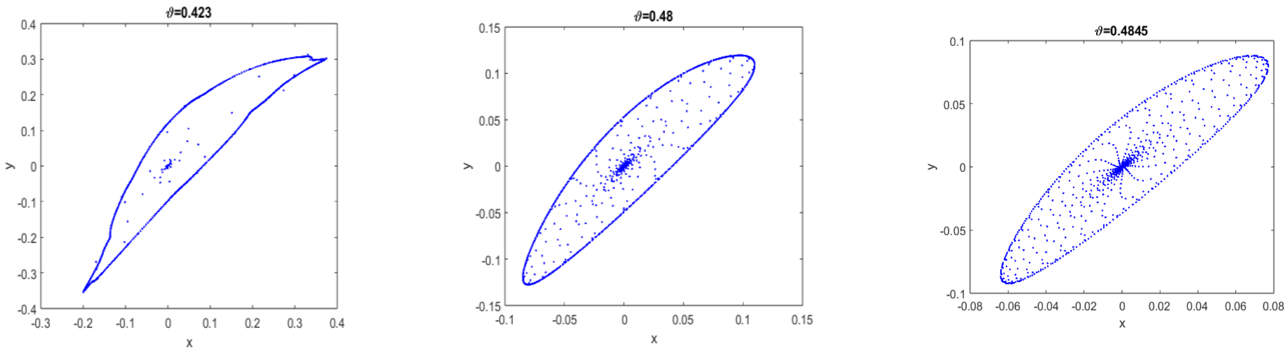


Figure 5. Bifurcation diagram by varying ϑ.



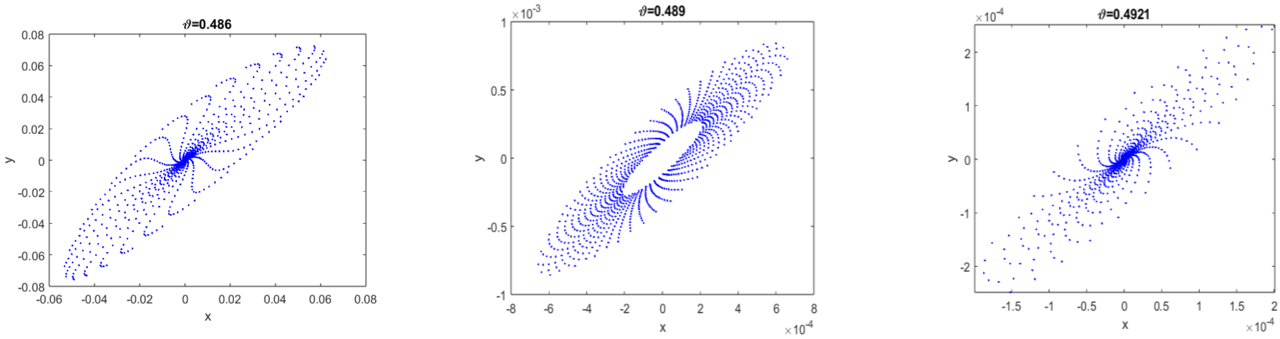


Figure 6. Phase portrait by varying ϑ

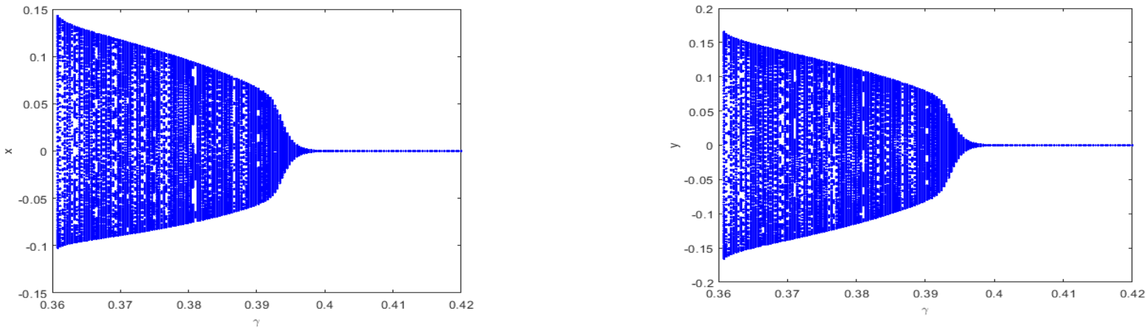


Figure 7. Bifurcation diagram by varying γ.

5. CONCLUSION

This work discusses a novel fractional order enzyme model. From the Caputo fractional derivative idea, such a fractional order model is created. We look into the equilibrium points of the system (2)'s stability conditions and demonstrate that the system (2) exhibits PD and NS bifurcations. Using the linearization method, we provide asymptotic stability requirements for the equilibria. Intricate dynamical characteristics such as the emergence of PD and NS bifurcations, orbits, quasi-periodic orbits, attracting invariant circles, and chaotic sets are all displayed by the model parameters are changed. Even yet, the problem of studying many parameter bifurcations in the system is still difficult. Future research is anticipated to yield additional analytical insights on this topic.

Conflict of Interest: There is no conflict of interest

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