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Dynamics and Hopf Bifurcation of a Chaotic Chemical Reaction Model

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Abstract

Taking into account an ideal mixture and a well-stirred reactor, some dynamical aspects for a 3-dimensional chaotic system are carried out. Positivity and boundedness of solutions are discussed. Equilibria are investigated and method of linearization is implemented for asymptotic behavior of system about these equilibria. Lyapunov function is constructed to prove the global stability of positive equilibrium point. Moreover, it is proved that system undergoes Hopf bifurcation about its interior (positive) equilibrium. An explicit criterion of Hopf bifurcation without finding the eigenvalues is used for the existence of Hopf bifurcation. Numerical simulation is presented for the illustration of theoretical discussion. Lyapunov dimension is approximated and maximum Lyapunov characteristic exponents are plotted to ensure the chaotic behavior of the model.

1 Introduction

There is an increasing concern in the microscopic theoretical investigation and numerical simulation of fluctuating behavior originating in the nonlinear dynamical systems operating in the situations far from equilibrium. In addition to the basic appeal of how coordinated macroscopic behavior can be generated by molecular motion at the molecular level, such approaches provide the possibility to test theoretical hypotheses on phenomenological equations, and even direct experimental studies to deal with accessible situations.

The chemical dynamics in a well-ignited reactor provides the clearest example of a complex imbalance, as it can lead to deterministic chaos with internal dynamics rather than local degrees of freedom. Since this form of chaos is acceptable for a small number of macro variables, one can reasonably expect it to form an ideal case of study and to understand the transition from microscopic to macroscopic behavior [1].

In order to investigate some dynamical behavior for the microscopic aspects of a system demonstrating chaotic and bifurcating nature at the macroscopic level, it is necessary to take into account model systems in which the balance equations are transformable to an explicit chemical mechanism possessing an accurately stated microscopic counterpart. In the systems related to chemical reactions such requirements can be achieved by considering the chemical reactions obeying mass action kinetics. For this, the following chemical reactions model is considered [1-2]:

$$\begin{gathered} \mathrm{A}_1 + \mathrm{X} \underset{\mathrm{k}_{-1}}{\overset{\mathrm{k}_1}{\rightleftarrows}} 2\,\mathrm{X},\ \mathrm{X} + \mathrm{Y} \underset{\mathrm{k}_{-2}}{\overset{\mathrm{k}_2}{\rightleftarrows}} 2\,\mathrm{Y}, \\ \mathrm{A}_5 + \mathrm{Y} \underset{\mathrm{k}_{-3}}{\overset{\mathrm{k}_3}{\rightleftarrows}} \mathrm{A}_2\,,\ \mathrm{X} + \mathrm{Z} \underset{\mathrm{k}_{-4}}{\overset{\mathrm{k}_4}{\rightleftarrows}} \mathrm{A}_3, \\ \mathrm{A}_4 + \mathrm{Z} \underset{\mathrm{k}_{-5}}{\overset{\mathrm{k}_5}{\rightleftarrows}} 2\mathrm{Z}\,. \end{gathered} \tag{1}$$

In model (1) two autocatalytic steps concerning ingredients X and Z are linked via three other steps consisting of X and Z, and the third ingredient Y. On the other hand, the initial product concentrations, that is, A_1, A_4 and A_5 and the final product concentrations, that is, A_2 and A_3 are kept fixed. Moreover, $k_{\pm 1}$, $k_{\pm 2}$, $k_{\pm 3}$, $k_{\pm 4}$ and $k_{\pm 5}$ are rate constants. Taking into account the simplicity of model (1), one may assume that $k_{-2} = k_{-3} = k_{-4} = 0$. Furthermore, we assume that A_2 and A_3 are continuously eliminated from the reactor. Next, taking into account a well-stirred reactor and an ideal mixture, the rate equations for model (1) are given as follows:

$$\begin{cases} \dfrac{dx}{dt} = ax - b\,x^2 - xy - xz, \\ \dfrac{dy}{dt} = x\,y - c\,y, \\ \dfrac{dz}{dt} = d\,z - x\,z - \alpha\,z^2, \end{cases} \tag{2}$$

where $a = k_1[\mathrm{A}_1]$, $b = k_{-1}$, $c = k_5[\mathrm{A}_5]$, $d = k_4[\mathrm{A}_4]$, and $\alpha = k_{-5}$. Moreover, it is also assumed that $k_2 = k_4 = 1$. All parametric values related to system (2) are positive, and the initial conditions associated to system (2) are given as follows:

$$\begin{cases} x(0) = x_0 > 0, \\ y(0) = y_0 > 0, \\ z(0) = z_0 > 0. \end{cases} \tag{3}$$

Huang [2] studied chaotic behavior of system with some numerical simulation. Furthermore, it is also interesting to discuss stability, bifurcation analysis, discretization, and chaos control for such chemical reaction models. Din *et al.* [3] considered the 2-dimensional rate equations related to chlorine dioxide– iodine–malonic acid reaction system, and studied discretization, stability, various types of bifurcation, and chaos control. In [4], taking into account two discrete versions of glycolysis model, bifurcating and chaotic behaviors have been discussed. An exponential type chaos control methodology was proposed in [5] for discrete-time Brusselator models. Din and Haider [6] studied discretization, stability, flip bifurcation, Hopf bifurcation, and chaos control for Schnakenberg model. Kol'tsov [7] reported a four-step chemical reaction model. Moreover, chaotic behavior of the model is confirmed through numerical simulation. Vikhansky and Cox [8] investigated two chemical reduced models in a laminar chaotic flow. Numerical methods are implemented to explore the chaotic dynamics of the models. Bodale and Oancea [9] studied synchronization and chaos control for Willamowski–Rössler type chemical reaction model. Poland [10] studied catalysis and chaos for a cooperative chemical reaction model for the Lorenz equations. Monwanou et al. [11] discussed reactions between four molecules for an amplitude-modulated excitation on the nonlinear dynamics. Furthermore, analysis of steady-states, Hopf bifurcation and routes to chaos have been studied. Cramer and Booksh [12] reviewed some concepts of chaos theory in chemometrics and chemistry. Kim and Chang [13] reported a chaotic model incorporating measurable state variables less than the degrees of freedom of the model and the system was identified with the artificial neural networks.

Taking into account previous investigation related to system (2), it is worthwhile to point out that in [1] the master rate equations were presented. Moreover, chaotic behavior of proposed model was illustrated through numerical simulation. On the other hand, entropy method and numerical simulation were carried out in [2] to ensure the chaotic behavior of system (2). According to the best of our knowledge, global stability of system (2) and parametric conditions for the occurrence of Hopf bifurcation about its coexistence is remaining a topic for further investigation.

The novelty of present manuscript is emphasized as follows:

- The positivity and boundedness of solutions for system (2) are carried out. Existence of constant solutions (equilibria) is studied, and local asymptotic behavior of system (2) is investigated about these equilibria.
- Lyapunov function is constructed to show that system (2) is globally asymptotically stable about its coexistence.

- An efficient and explicit criterion is implemented to show that system (2) undergoes Hopf bifurcation around its unique positive steady-state.
- Theoretical investigation is well illustrated through numerical simulation including bifurcation diagrams, phase portraits, computation of Lyapunov dimension, depiction of Lyapunov characteristic exponents, and validation of global stability of positive equilibrium.

The rest of the discussion for this paper is summarized as follows. The positivity of solutions for system (2) and their boundedness are discussed in Section 2. In Section 3, we explore existence of steady-states for system (2), and local asymptotic stability analysis of system about these equilibria is also carried out. In Section 4, global stability of positive equilibrium point is carried out. In Section 5, bifurcation theory is used to study the Hopf bifurcation for the system (2) about its interior (positive) equilibrium. Some numerical simulation is presented in Section 6 for the illustration of theoretical discussion.

2 Positivity and boundedness of solutions

In this section, we discuss positivity of solutions and boundedness of the solutions for system (2). Taking into account system (2), we consider

$$X = \begin{bmatrix} x \\ y \\ z \end{bmatrix}, F(X) = \begin{bmatrix} ax - b\,x^2 - xy - xz \\ x\,y - c\,y \\ d\,z - x\,z - \alpha\,z^2 \end{bmatrix}.$$

Then, it is easy to see that F has continuous partial derivatives on $\mathbb{R}^3$, and therefore it is locally Lipschitz in $\mathbb{R}^3$. Consequently, system (2) has unique solution. Next, considering first equation of the system (2) and assume that (3) holds true, then it follows that:

$$x(t) = x(0)\, exp\left(\int_0^t (a - b\,x(s) - y(s) - z(s))ds \right) > 0.$$

Similarly, from second and third equations of the system (2), and (3), it follows that:

$$y(t) = y(0)\, exp\left(\int_0^t (\,x(s) - c)ds \right) > 0,$$

and

$$z(t) = z(0)\, exp\left(\int_0^t (d - x(s) - \,\alpha\, z(s))ds \right) > 0.$$

Therefore, assuming that the initial conditions satisfy $x(0) > 0$, $y(0) > 0$ and $z(0) > 0$, one has $x(t) > 0$, $y(t) > 0$ and $z(t) > 0$ for all $t > 0$, where $(x(t), y(t), z(t)) \equiv (x(t, x_0), y(t, y_0), z(t, z_0))$ be any arbitrary solution of system (2) subject to initial conditions given in (3).

Next, the following Theorem shows that any arbitrary solution $(x(t), y(t), z(t))$ with initial conditions (3) is ultimately bounded.

Theorem 1. Assume that (3) holds true, then every positive solution of system (2) is ultimately bounded.

Proof. Keeping in mind the positivity of solutions and considering the first equation of the system (2), we have $\frac{dx}{dt} = ax - b\,x^2 - xy - xz \le a\,x - b\,x^2$. Then, standard comparison principle yields that $\lim_{t\to\infty} sup\; x(t) \le M_1$, where $M_1 := max\left\{x_0, \frac{a}{b}\right\}$. Similarly, it follows from third equation of the system (2) that $\frac{dz}{dt} = d\,z - x\,z - \alpha\,z^2 \le d\,z - \alpha\,z^2$, and again standard comparison result gives that $\lim_{t\to\infty} sup\; z(t) \le M_2$, where $M_2 := max\left\{z_0, \frac{d}{\alpha}\right\}$. Next, we define $w(t) := x(t) + y(t) + z(t)$, then it follows that:

$$
\begin{aligned}
\frac{dw}{dt} &= \frac{dx}{dt} + \frac{dy}{dt} + \frac{dz}{dt} \\
&= ax - b\,x^2 - 2\,xz - c\,y + d\,z - \alpha\,z^2 \\
&\le a\,x - cy + d\,z \\
&= -a\,x - c\,y - d\,z + 2ax + 2dz \\
&\le -\delta(x + y + z) + M,
\end{aligned}
$$

where $\delta := min\{a, c, d\}$ and $M := 2a\,M_1 + 2\,d\,M_2$. Consequently, the differential inequality $\frac{dw}{dt} + \delta\,w \le M$ yields that $w(t) \le M/\delta + w(0)\,e^{-\delta\,t}$. Thus, one has $\lim_{t\to\infty} sup\; w(t) \le M/\delta$, and consequently $w(t) = (x + y + z)(t)$ is bounded. Therefore, $x(t)$, $y(t)$ and $z(t)$ are ultimately bounded, and all solutions of the system (2) enter the region Ω defined by:

$$\Omega := \{(x(t), y(t), z(t)) \in \mathbb{R}^3_+ : x(t) + y(t) + z(t) \le M/\delta\}.$$

3 Existence of equilibria and stability

In this section, we start our discussion with the existence of equilibria for system (2). For this, the equilibria of system (2) solve the following system:

$$
\begin{cases}
ax - b\,x^2 - xy - xz = 0, \\
x\,y - c\,y = 0, \\
d\,z - x\,z - \alpha\,z^2 = 0.
\end{cases}
\tag{4}
$$

Then, it is easy to see that non-negative solutions of system (4) or equivalently equilibria of system (2) are given as follows: $O = (0,0,0)$ a trivial equilibrium, $E1 = \left(0,0,\frac{d}{\alpha}\right)$, $E2 = \left(\frac{a}{b},0,0\right)$, $E3 = (c, a-bc, 0)$, and $E4 = \left(\frac{d-a\alpha}{1-b\alpha}, 0, \frac{a-bd}{1-b\alpha}\right)$ are semi-trivial equilibria, and $P = \left(c, a-bc+\frac{c-d}{\alpha}, \frac{d-c}{\alpha}\right)$ be interior equilibrium. Moreover, $E3$ exists if $a > bc$, $E4$ exists if $0 < b < \frac{1}{\alpha}$, $a\,\alpha < d < \frac{a}{b}$ or $b > \frac{1}{\alpha}$, $\frac{a}{b} < d < a\,\alpha$. On the other hand, P is unique positive equilibrium of system if $c < d$, and $d + \alpha\, b\, c < \alpha\, a + c$.

Moreover, for $(a,b,c) \in [0,10\ ]^3$, $d = 8$, and $\alpha = 5.5$ the 3-dimensional existence region for positive equilibrium of system (2) is shown in Fig. 1.

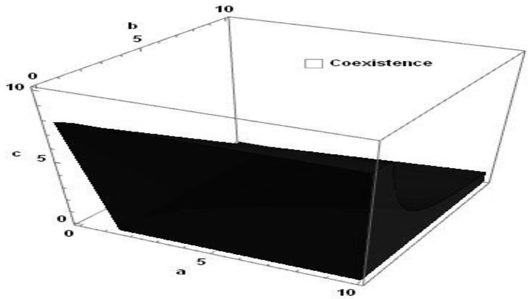

Figure 1: Coexistence region for system (2).

To see the qualitative behaviors of system (2) about its trivial and semi-trivial equilibria, the Jacobian matrices about these equilibria are given as follows:

$$J(O) = \begin{bmatrix} a & 0 & 0 \\ 0 & -b & 0 \\ 0 & 0 & d \end{bmatrix}, J(E1) = \begin{bmatrix} a-\frac{d}{\alpha} & 0 & 0 \\ 0 & -c & 0 \\ -\frac{d}{\alpha} & 0 & -d \end{bmatrix}, \text{J(E2)}= \begin{bmatrix} -a & -\frac{a}{b} & -\frac{a}{b} \\ 0 & \frac{a}{b}-c & 0 \\ 0 & 0 & d-\frac{a}{b} \end{bmatrix},$$

$$J(E3) = \begin{bmatrix} -bc & -c & -c \\ a-bc & 0 & 0 \\ 0 & 0 & d-c \end{bmatrix}, \text{and } J(E4) = \begin{bmatrix} \frac{b(d-a\alpha)}{b\alpha-1} & \frac{d-a\alpha}{b\alpha-1} & \frac{d-a\alpha}{b\alpha-1} \\ 0 & \frac{d-a\alpha}{1-b\alpha}-c & 0 \\ \frac{a-bd}{b\alpha-1} & 0 & \frac{(a-bd)\alpha}{b\alpha-1} \end{bmatrix}.$$

Then, it is easy to see that a, $-b$ and d are eigenvalues of $J(O)$, and thus trivial equilibrium is unstable. Similarly, $a-\frac{d}{\alpha}$, $-c$ and $-d$ are eigenvalues of $J(E1)$, which shows that $E1$ is a sink if $\alpha\, a < d$ and it is unstable if $\alpha\, a > d$. On the other hand, $-a, \frac{a-bc}{b}, \frac{b\,d-a}{b}$ are eigenvalues for

Jacobian $J(E2)$, and consequently $E2$ is a sink if $b\,d < a < b\,c$. Moreover, $E2$ is unstable if $a > b\,c$ or $b\,d > a$. Furthermore, the characteristic polynomial for $J(E3)$ is given as follows:

$$P(\lambda) = (\lambda - d + c)(\lambda^2 + b\,c\,\lambda + a\,c - bc^2),$$

showing that $E3$ is a sink if $d < c$ and it is unstable if $d > c$. Similarly, the characteristic polynomial for $J(E4)$ is given as follows:

$$Q(\lambda) = \left(\lambda + c - \frac{d - a\alpha}{1 - b\alpha}\right)\left(\lambda^2 - \left(\frac{bd + a\alpha - b(a + d)\alpha}{b\alpha - 1}\right)\lambda + \frac{(a - bd)(d - a\alpha)}{b\alpha - 1}\right).$$

Then, $E4$ is a sink if $\frac{d-a\alpha}{1-b\alpha} < c$, and it is unstable if $\frac{d-a\alpha}{1-b\alpha} > c$.

Next, we assume that $c < d$ and $d + \alpha\,b\,c < \alpha\,a + c$, then Jacobian matrix of system (2) about unique positive equilibrium P is given by:

$$J(P) = \begin{bmatrix} -bc & -c & -c \\ a - bc + \dfrac{c-d}{\alpha} & 0 & 0 \\ \dfrac{c-d}{\alpha} & 0 & c-d \end{bmatrix}.$$

Simple computation yields the following characteristic polynomial for the Jacobian matrix $J(P)$:

$$F(\lambda) = \lambda^3 + (c(b-1) + d)\lambda^2 + \left(\frac{c\big(2c - 2d + a\alpha + \alpha b(d - 2c)\big)}{\alpha}\right)\lambda + \frac{c(c-d)(d - a\alpha + c(b\alpha - 1))}{\alpha}. \quad (5)$$

Taking into account the Routh-Hurwitz criterion [14], positive equilibrium of system (2) is asymptotically stable if the following conditions are satisfied:

$$\begin{cases} c < b\,c + d, \qquad 2(d + b\,c) < a\,\alpha + 2c + b\,d, \\ (d - c)(c\,(2\,b - 1) + d) < \alpha\,b(c(a + c - 2bc) + c\,d(b - 2) + d^2). \end{cases} \quad (6)$$

In order to visualize the 3-dimensional stability region (feasible region of (6)) of system (2) about its positive equilibrium Fig. 2 is presented.

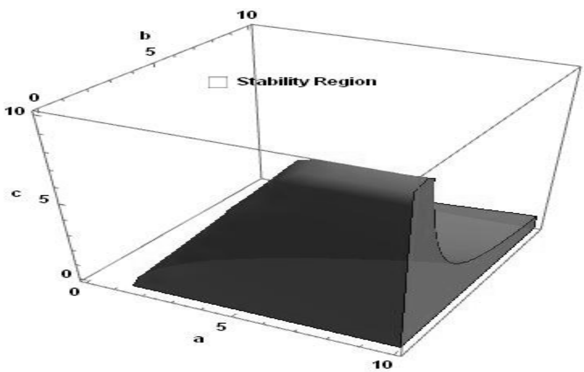

Figure 2: Stability region of (2) about P at $d = 9.5$, $\alpha = 7.8$

4 Global stability analysis

In this section, we investigate global stability analysis of system (2) about its positive equilibrium $P(x^*, y^*, z^*) = \left(c, a - bc + \frac{c-d}{\alpha}, \frac{d-c}{\alpha}\right)$. For this, we assume that $c < d$, and $d + \alpha\, b\, c < \alpha\, a + c$. Moreover, we consider the following Lyapunov function:

$$V(x,y,z) = \left(x - x^* - ln\frac{x}{x^*}\right) + \left(y - y^* - ln\frac{y}{y^*}\right) + \left(z - z^* - ln\frac{z}{z^*}\right).$$

Then, it is easy to see that $V(x^*, y^*, z^*) = 0$, and $V(x,y,z) > 0$ for all

$$(x,y,z) \in \Omega = \{(x,y,z) \in \mathbb{R}_+^3 : x(t) + y(t) + z(t) \leq M/\delta\}.$$

Taking into account system (2), and differentiation of V with respect to t yields that

$$\begin{aligned}\frac{d\,V}{d\,t} &= \left(\frac{x - x^*}{x}\right)\frac{d\,x}{d\,t} + \left(\frac{y - y^*}{y}\right)\frac{d\,y}{d\,t} + \left(\frac{z - z^*}{z}\right)\frac{d\,z}{d\,t} \\ &= (x - x^*)(a - b\,x\, - y - z) + (y - y^*)(x - x^*) + (z - z^*)(d\, - \,x - \alpha\,z).\end{aligned}$$

After some simple calculation and simplification, one has that:

$$(a - b\,x\, - y - z) = (y^* - y - b(x - x^*) + z^* - z),$$

and

$$(d\, - \,x - \alpha\,z) = \alpha\left(z^* - z - \frac{x - x^*}{\alpha}\right).$$

Consequently, we have the following expression for $\frac{d\,V}{d\,t}$:

$$\begin{aligned}\frac{d\,V}{d\,t} &= (x - x^*)(y^* - y - b(x - x^*) + z^* - z) + (y - y^*)(x - x^*) \\ &\quad + (z - z^*)\alpha\left(z^* - z - \frac{x - x^*}{\alpha}\right) \\ &= -b(x - x^*)^2 - \alpha(z - z^*)^2 - 2(x - x^*)(z - z^*).\end{aligned}$$

Then, it follows that $\frac{d\,V}{d\,t} < 0$ in the region S defined by:

$$S = \{(x,y,z) \in \mathbb{R}_+^3 : x > x^* \text{ and } z > z^* \text{ or } x < x^* \text{ and } z < z^*\}.$$

Next, the following Theorem gives the conditions for global asymptotic stability of system (2) about its positive equilibrium point.

Theorem 2. Assume that $c < d$, $d + \alpha\, b\, c < \alpha\, a + c$, and conditions (6) hold true, then positive equilibrium P is globally asymptotically stable in the region S defined by:

$$S = \{(x,y,z) \in \mathbb{R}_+^3 : x > x^* \text{ and } z > z^* \text{ or } x < x^* \text{ and } z < z^*\}.$$

5 Explicit criterion of Hopf bifurcation

In this section, we investigate that system (2) undergoes Hopf bifurcation around its positive equilibrium. For this, an explicit criterion for existence of Hopf bifurcation without finding the eigenvalues of Jacobian matrix is implemented. First, we need the following Theorem [15]:

Theorem 3. Considering the following n-dimensional autonomous system of differential equations:

$$\frac{d\,X}{d\,t} = F(X,\theta), \tag{7}$$

where $x \in \mathbb{R}^n$, $\theta \in \mathbb{R}$, and $F \in C^{\infty}$. Moreover, assume that (X^*,θ^*) be an equilibrium point for system (7), and $P(\lambda,\theta)$ is characteristic polynomial of the Jacobian matrix of system (7) given as follows:

$$P(\lambda,\theta) = a_n(\theta)\,\lambda^n + a_{n-1}(\theta)\,\lambda^{n-1} + \cdots + a_1(\theta)\,\lambda + a_0(\theta)\,. \tag{8}$$

Then, system (7) undergoes Hopf bifurcation about (X^*,θ^*) if the following conditions hold true:

(i) $a_0(\theta^*) > 0, D_1(\theta^*) > 0, \cdots, D_{n-2}(\theta^*) > 0, D_{n-1}(\theta^*) = 0,$

(ii) $\frac{d\,D_{n-1}(\theta^*)}{d\,\theta} \neq 0,$

where

$$D_n(\theta) = det\begin{pmatrix} a_1(\theta) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ a_{2n-1}(\theta) & \cdots & a_n(\theta) \end{pmatrix}.$$

Lemma 1. For $n = 3$, conditions (i) and (ii) reduce to the following:

$$a_0(\theta^*) > 0, D_1(\theta^*) = a_1(\theta^*) > 0, D_2(\theta^*) = a_1(\theta^*)\,a_2(\theta^*) - a_0(\theta^*) = 0,$$

and

$$\frac{d\,D_2(\theta^*)}{d\,\theta} \neq 0.$$

Taking into account system (2) and its characteristic polynomial (5), one may take α as bifurcation parameter, then a simple application of Lemma 1 gives the following result related to existence of Hopf bifurcation in system (2) about its positive equilibrium.

Lemma 2. Assume that $c < d$ and $d + \alpha\,b\,c < \alpha\,a + c$, then system (2) undergoes Hopf bifurcation about its positive equilibrium $\left(c, a - bc + \frac{c-d}{\alpha}, \frac{d-c}{\alpha}\right)$ as α varies in a small neighborhood of $\alpha^* = \frac{1+\frac{-ac+bcd}{c(a+c-2bc)+(-2+b)cd+d^2}}{b}$, if the following hold true:

$$\begin{cases} c < b\,c + d, & 2(d + b\,c) < a\,\alpha + 2c\, + b\,d, \\ (d - c)(c\,(2\,b - 1) + d) = \alpha\,b(c(a + c - 2bc) + c\,d(b - 2) + d^2). \end{cases} \tag{9}$$

and

$$\frac{b^2c(c(a+c-2bc)+(-2+b)cd+d^2)^2}{(c-d)((-1+2b)c+d)} \neq 0. \tag{10}$$

6 Numerical simulation and discussion

This section is dedicated to verification of our theoretical discussion. For this some parametric values are chosen for the system (2) for illustration of its dynamical and chaotic behavior. Mainly, we discuss stability analysis and bifurcating behavior of system (2) about its positive equilibrium. Mathematica packages are used for various plots, phase portraits, bifurcation diagrams, Lyapunov dimension and maximum Lyapunov characteristic exponents related to system (2).

First, we select the parametric values for the system (2) as follows: $a = 2.2$, $b = 0.3$, $c = 1.3$, $d = 3.2$, and $\alpha = 2.65$, then system (2) has unique positive equilibrium given by $(1.3, 1.093, 0.71698)$. Moreover, system (2) is asymptotically stable about this equilibrium, and plots of state variables and 3-dimensional phase portrait are depicted in Fig. 3, Fig. 4, Fig. 5, and Fig. 6.

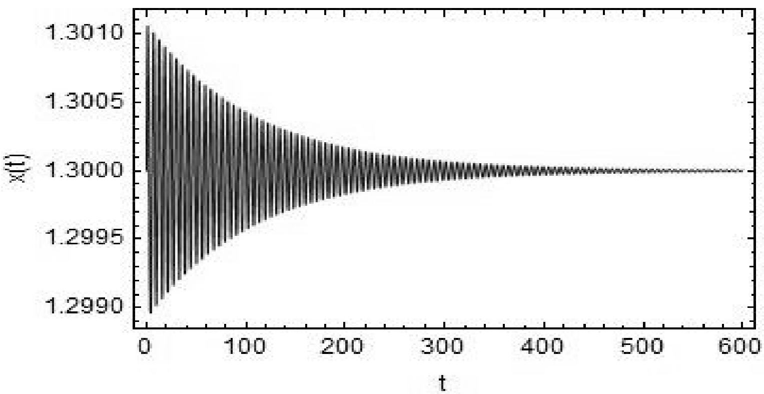

Figure 3: Plot of $x(t)$ for system (2)

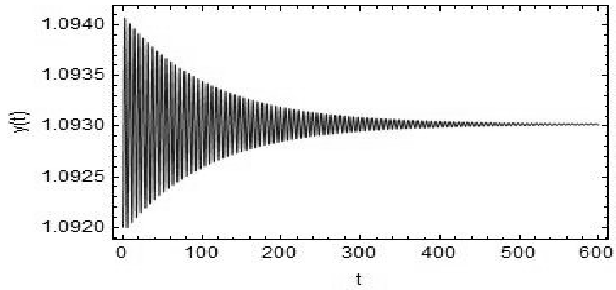

Figure 4: Plot of $y(t)$ for system (2)

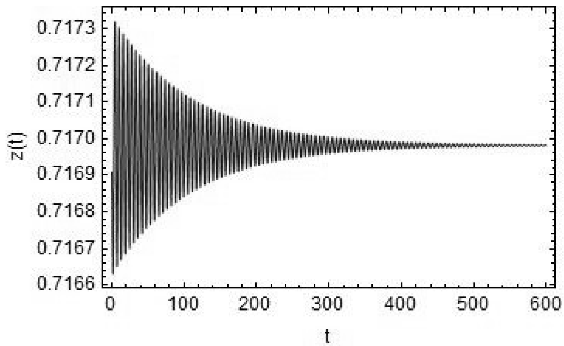

Figure 5: Plot for $z(t)$ of system (2)

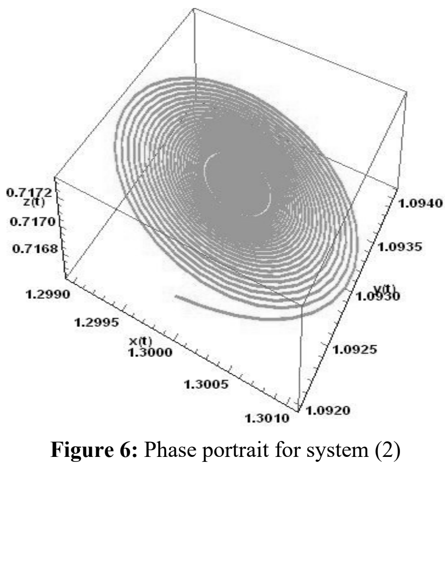

Figure 6: Phase portrait for system (2)

In order to see the bifurcating behavior of system (2), we take $a = 2.2$, $b = 0.3$, $c = 1.3$, and $d = 3.2$. Considering α as bifurcation parameter such that $\alpha \in [2,\ 3]$, then system (2) undergoes Hopf bifurcation about $\alpha^* = 2.53182$. On the other hand, for the parametric values $a = 2.2$, $b = 0.3$, $c = 1.3$, $d = 3.2$, and $\alpha = 2.53182$, the positive equilibrium of system (2) is given by $(1.3, 1.05955, 0.750448)$. For these parametric values, conditions (9) and (10) are satisfied as follows: $1.3 = c < bc + d = 3.59$, $7.18 = 2(d + b\,c) < a\,\alpha + 2c\ + b\,d = 9.13008$, $5.09694 = (d - c)(c\,(2\,b - 1) + d) = \alpha\,b(c(a + c - 2bc) + c\,d(b - 2) + d^2) = 5.09694$, and $\frac{b^2c(c(a+c-2bc)+(-2+b)cd+d^2)^2}{(c-d)((-1+2b)c+d)} = 1.032679315003928 \neq 0$.

On the other hand, bifurcation diagrams for system (2) are depicted in Fig. 7, Fig. 8 and Fig. 9.

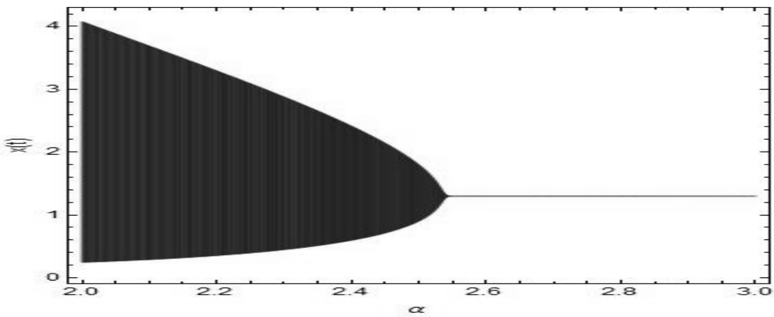

Figure 7: Bifurcation diagram of $x(t)$ for system (2)

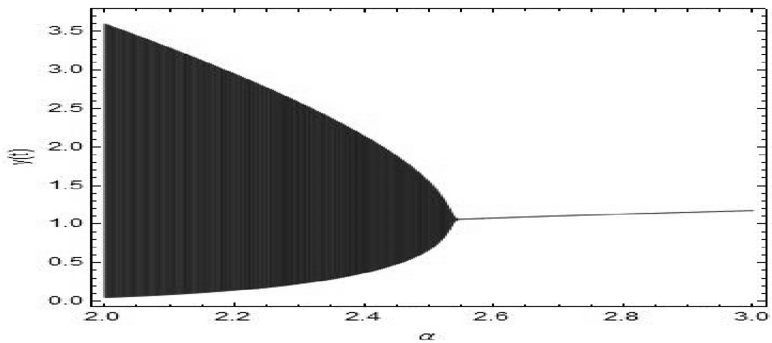

Figure 8: Bifurcation diagram of $y(t)$ for system (2)

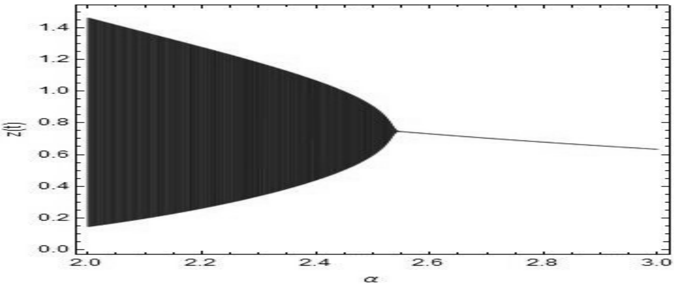

Figure 9: Bifurcation diagram of $z(t)$ for system (2)

In order to see the chaotic behavior of the system (2) in the chaotic region $[2, 2.53182]$, some phase portraits of this system must be depicted in chaotic region. For this, some 3-dimensional phase portraits of system (2) are shown in Fig. 10, Fig. 11, Fig. 12, and Fig. 13.

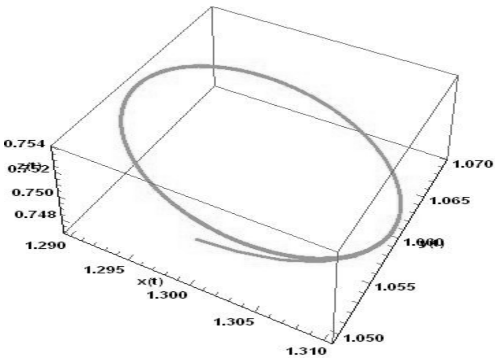

Figure 10: Phase portrait at $\alpha = 2.53182$

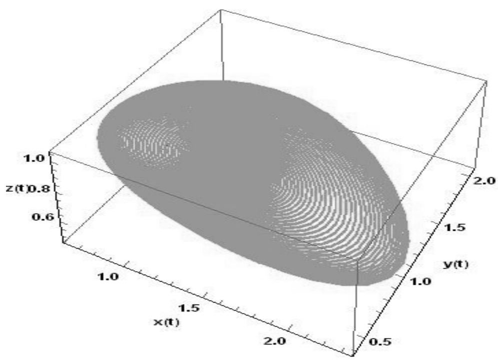

Figure 11: *Phase portrait at* $\alpha = 2.4$

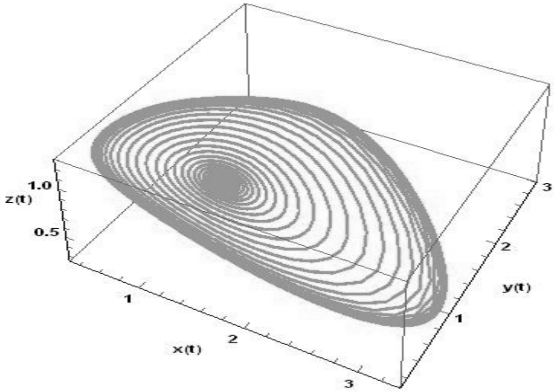

Figure 12: Phase portrait at $\alpha = 2.2$

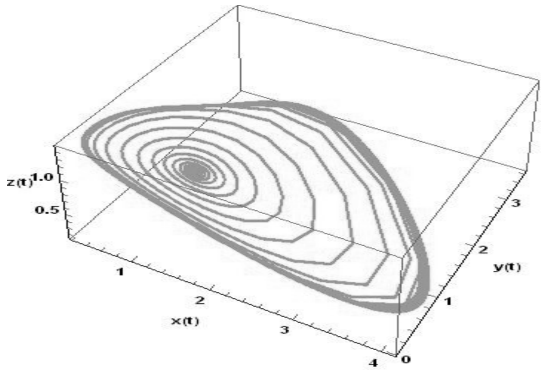

Figure 13: Phase portrait at $\alpha = 2$

Next, we investigate Lyapunov dimension for the system (2). The concept of Lyapunov dimension was first presented by Kaplan and Yorke [16]. The Lyapunov dimension is an approximation for Hausdorff dimension of strange attractors. Furthermore, it must be noted that an attractor with non-integer Hausdorff dimension is known as a strange attractor [17]. The numerical computation of Hausdorff dimension is a complex task and alternatively Lyapunov dimension is used widely for its approximation. Moreover, Lyapunov dimension is an upper bound for Hausdorff dimension. For an n dimensional autonomous dynamical system $x' = f(x)$, the formula of Lyapunov dimension is given as follows:

$$L_d = s + \frac{\sum_{i=1}^{s} \mu_i}{|\mu_{s+1}|},$$

where μ_i are Lyapunov exponents, and s is the largest value of i for which $\sum_{i=1}^{s} \mu_i > 0$.
For the computation of Lyapunov dimension related to system (2), we take $a = 2.2$, $b = 0.3$, $c = 1.3$, $d = 3.2$, and $\alpha = 2$ in system (2). For these parametric values, a 3-dimensional attractor of system (2) is depicted in Fig. 13. Moreover, applying Mathematica package we have the following Lyapunov exponents: $\mu_1 = 0.0560005$, $\mu_2 = -0.044475$ and $\mu_3 = -2.310523399$. Moreover, $\mu_1 + \mu_2 = 0.01152535 > 0$ implies that $s = 2$, therefore $L_d = 2.004988$.
Moreover, the Lyapunov characteristic exponents (LCEs) related to these parametric values are depicted in Fig. 14.

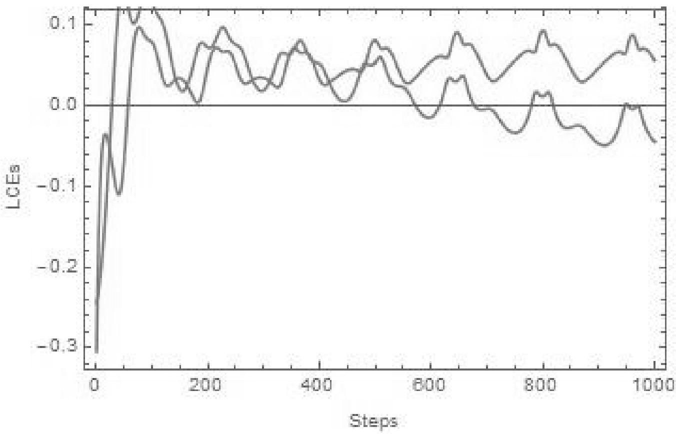

Figure 14: LCEs for system (2) at $a = 2.2$, $b = 0.3$, $c = 1.3$, $d = 3.2$, and $\alpha = 2$.

Finally, we check validity of global asymptotic stability of system (2) about its positive equilibrium by implementing numerical simulation. For this, we choose $a = 2.2$, $b = 0.3$, $c = 1.3$, $d = 3.2$, and $\alpha = 3.1$ in system (2). For these parametric values, system (2) has unique positive equilibrium given by $P = (1.3, 1.1971, 0.6129)$. Moreover, Jacobian matrix of system (2) has the following multipliers: $\mu_1 = -0.0373934 + 1.1547228041i$, $\mu_2 = -0.0373934 - 1.1547228041i$ and $\mu_3 = -2.215213252492716$ satisfying $Re\ (\mu_i) < 0$ for $i = 1,2,3$. Therefore, $P = (1.3, 1.1971, 0.6129)$ is locally asymptotically stable. In order to verify global stability of system (2) about $P = (1.3, 1.1971, 0.6129)$, initial conditions are kept away from the neighborhood of this equilibrium point. Indeed, in first case initial conditions are taken as $(x_0, y_0, z_0) = (40, 50, 60)$, secondly initial conditions are taken as $(x_0, y_0, z_0) = (45, 55, 65)$, thirdly we have taken $(x_0, y_0, z_0) = (50, 60, 70)$, and fourthly these initial conditions are chosen as $(x_0, y_0, z_0) = (60, 70, 80)$. In all these cases, the 3-dimensional phase portraits of system (2) are depicted in Fig. 15. All four trajectories starting from different initial conditions far away from neighborhood of equilibrium point are eventually converging to equilibrium solution of the system. Furthermore, the first portrait in first row is starting with $(x_0, y_0, z_0) = (40, 50, 60)$, the second phase portrait in first row is starting with $(x_0, y_0, z_0) = (45, 55, 65)$, the first phase portrait in second row is starting with $(x_0, y_0, z_0) = (50, 60, 70)$, and the second phase portrait in second row is starting with initial conditions $(x_0, y_0, z_0) = (60, 70, 80)$. Consequently, Fig. 15 shows that positive equilibrium is globally asymptotically stable.

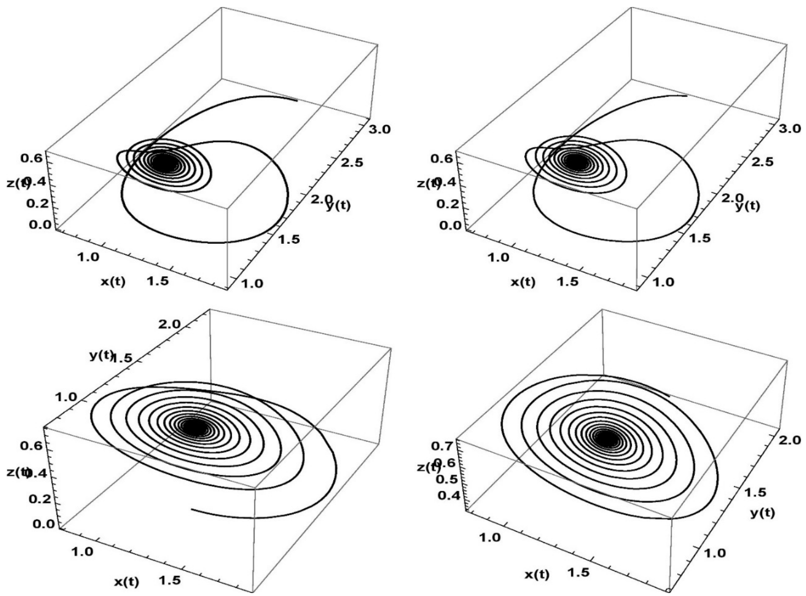

Figure 15: Phase portraits of system (2) with $a = 2.2$, $b = 0.3$, $c = 1.3$, $d = 3.2$, $\alpha = 3.1$ and various initial conditions for $40 \leq t \leq 200$.

Conclusion

Some dynamical aspects for a 3-dimesional autonomous chemical reaction system are studied. It is proved that system has six chemically feasible equilibria including a unique positive equilibrium. Local dynamical behavior of the system about these steady states is discussed. Particularly, Routh-Hurwitz criterion is implemented to obtain the parametric conditions for asymptotic stability of the system about its positive equilibrium. Moreover, an efficient criterion without using the eigenvalue is applied for existence of Hopf bifurcation in the chemical reaction model about is positive equilibrium. Taking into account α as bifurcation parameter, the following Hopf bifurcation curve is obtained:

$$\{(\alpha, a, b, c, d) \in \mathbb{R}_+^5 : c < b\,c + d, 2(d + b\,c) < a\,\alpha + 2c + b\,d, S_1 = 0, S_2 \neq 0\},$$

where

$$S_1 = (d - c)(c\,(2\,b - 1) + d) - \alpha\,b(c(a + c - 2bc) + c\,d(b - 2) + d^2),$$

and

$$S_2 = \frac{b^2 c(c(a + c - 2bc) + (-2 + b)cd + d^2)^2}{(c - d)((-1 + 2b)c + d)}.$$

Moreover, under the conditions of asymptotic stability P is globally asymptotically stable in the region S defined by:

$$S = \{(x, y, z) \in \mathbb{R}_+^3 : x > x^* \text{ and } z > z^* \text{ or } x < x^* \text{ and } z < z^*\}.$$

Bifurcation diagrams related to Hopf bifurcation are depicted for illustration of theoretical discussion (cf. Fig. 7, Fig. 8 and Fig. 9). Chaotic behavior of the system is explored by computing Lyapunov dimension and depicting the maximum Lyapunov characteristic exponents. Arguing as in [1], such chemical reactions mainly take place in thermodynamics where chaotic behavior can be observed up to certain volume size of system. Furthermore, our investigation reveals that chaotic and fluctuating behaviors can be observed up to certain range of parametric values, and on the other hand, global stability is also observed for such microscopic chemical reactions. This topic certainly deserves more attention in the future, especially in the context of dealing with spatiotemporal chaotic behavior and the evolution of turbulence [1].

Further rich dynamical behavior and chaos control can be discussed with implementation of some appropriate discretization of the system. Keeping in mind some recent dynamical study of discrete time models (cf. [18-23]), our future work will be focused on dynamical study of some discrete counterpart of this chemical reaction system.

For some other recent chemical reaction-based systems, neural network models, Hopf bifurcation and chaos control, we refer to [24-29] and references are therein.

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