MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **90** (2023) 151–174
ISSN: 0340–6253
doi: 10.46793/match.90-1.151D

Stability, Discretization, and Bifurcation Analysis for a Chemical Reaction System

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(Received January 7, 2023)

Abstract

Chemical reactions reveal all types of exotic behavior, that is, multistability, oscillation, chaos, or multistationarity. The mathematical framework of rate equations enables us to discuss steady-states, stability and oscillatory behavior of a chemical reaction. A planar cubic dynamical system governed by nonlinear differential equations induced by kinetic differential equations for a two-species chemical reaction is studied. It is investigated that system has unique positive steady state. Moreover, local dynamics of system is studied around its positive steady state. Existence and direction of Hopf bifurcation about positive equilibrium are carried out. In order to modify the bifurcating behavior, bifurcation control is investigated. Keeping in mind, a consistency preserving discretization for continuous chemical reaction system, a discrete counterpart is proposed, and its qualitative behavior is investigated. Numerical simulation along with bifurcation diagrams are provided to illustrate the mathematical investigations.

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1 Introduction

The qualitative analysis of chemical reactions is an interesting topic of study for both mathematicians and biologists due to the investigation of the oscillatory behavior of chemical reactions. Existence of the limit cycles and Hopf bifurcation analysis are topics of great interest and many authors have studied chemical reaction systems. Schnakenberg [1] investigated limit cycle analysis for a two-component chemical system of autocatalytic type involving at least three reactions. Csaszar et al. [2] proposed some chemical reaction systems yielding limit cycle behavior. Di Cera et al. [3] studied oscillatory behavior for a 4–dimensional chemical reaction model including limit cycle analysis, and chaotic behavior. Forbes and Holmes [4] discussed the limit cycle behavior for a cubic autocatalator type chemical reaction system. Vance and Ross [5] explored fluctuating behavior around limit cycle for a chemical reaction system of homogeneous type by applying a master equation approach. Shabunin et al. [6] discussed limit cycle analysis and chaotic behavior for a chemical reaction system under an external periodic force. Nagy et al. [7] reported two nested type limit cycles for a two-species chemical reaction model.

Nielsen et al. [8] investigated supercritical Hopf bifurcation for Belousov–Zhabotinsky type chemical reaction models. Olsen [9] addressed codimension one and codimension two Hopf bifurcation for some variants of Citri–Epstein type chlorite–iodide chemical reactions. Errami et al. [10] explored emergence of Hopf bifurcation in a chemical reaction of networks. Fercec et al. [11] studied supercritical Hopf bifurcation for two reaction systems related to biochemistry. Din et al. [12] studied a cubic autocatalator chemical reaction model incorporating limit cycle analysis, Hopf bifurcation and discretization. Din [13] discussed a chaotic 3–dimensional chemical reaction model with local, global behaviors and Hopf bifurcation analysis. Discretization, bifurcation analysis and chaos control for some chemical reaction models have been investigated in [14–17]. Wilhelm and Heinrich [18] proposed a bimolecular chemical reaction model with the smallest possible reaction system for appearance of Hopf bifurcation. Wang et al. [19] studied Gierer–Meinhardt type chemical reaction system incorporating pattern formation mechanism and emergence of Hopf bifurcation. Dutt [20] reported oscillatory behavior for a diffusion type chemical reaction model.

Two-species chemical reaction systems involve the interaction between only two different chemical species. They are important because they can exhibit a wide range of dynamic behaviors, such as periodic oscillations, chaos, and fixed points. Understanding these systems can provide insight into the behavior of more complex reaction systems and can help in the design of chemical processes and the development of new materials. For example, two-species reaction systems are used in the study of chemical oscillators, which are chemical reactions that exhibit periodic changes in concentration over time. These oscillators are used in a variety of applications, including clocks, sensors, and biological systems. Another example is the study of bistable chemical reactions, which are reactions that have two stable states, separated by an unstable intermediate state. These systems can be used to create chemical switches and memory devices, where the state of the reaction can be controlled and maintained by an external stimulus. In other words, two-species chemical reaction systems are important because they provide a simple and well-understood model system for the study of chemical dynamics, which can be applied to a wide range of real-world problems.

Two-species chemical reaction systems are also important in systems biology, where they are used to model the interactions between different components of biological systems such as protein-protein interactions or gene regulation. In chemical engineering, two-species reaction systems are used to model and optimize the behavior of chemical reactors, where the goal is to achieve a desired product yield with a minimum of waste.

Overall, two-species chemical reaction systems provide a simple yet powerful framework for studying a wide range of phenomena in chemical kinetics, systems biology, and chemical engineering.

Arguing as in [2], a two-species chemical reaction described by A and B is given as follows:

$$O \xrightarrow{k_1} B, \quad A \xrightarrow{k_2} O, \quad B \xrightarrow{k_3} A, \quad 2A \xrightarrow{k_4} B, \quad 2A + B \xrightarrow{k_5} 3A, \tag{1}$$

where O represents the environment and $k_1, \cdots, k_5$ are positive numbers representing reaction rate coefficients. Moreover, the schematic diagram of two-species chemical reaction (1) is depicted in Fig. 1.

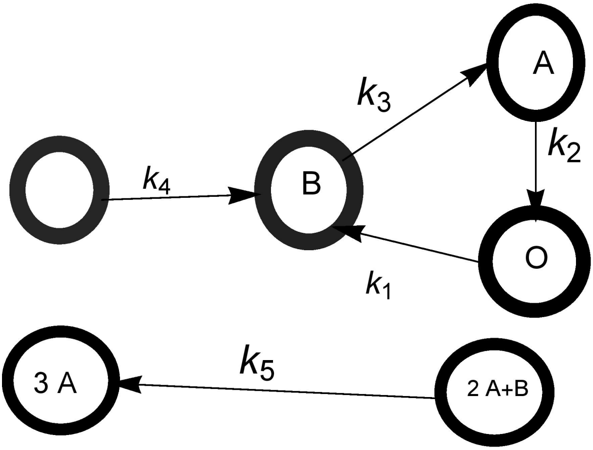


Figure 1. Schematic diagram of reaction (1).

Taking into account the reaction (1), one has the following two-dimensional induced dynamical system:

$$\begin{aligned} \frac{dx}{dt} &= -k_2x - 2k_4x^2 + k_3y + k_5x^2y, \\ \frac{dy}{dt} &= k_1 + k_4x^2 - k_3y - k_5x^2y, \end{aligned} \tag{2}$$

where x and y are concentrations of species A and B, respectively. Keeping in mind the simplicity for further computation, we assume that $k_4{=}k_5{=}\,1$, $k_2{=}a$, $k_3{=}b$ and $k_1{=}c$. Then system (2) can be rewritten as follows:

$$\begin{aligned} \frac{dx}{dt} &= -ax - 2x^2 + by + x^2y, \\ \frac{dy}{dt} &= c + x^2 - by - x^2y. \end{aligned} \tag{3}$$

The novelty of present study is described as follows:

- The existence and direction of Hopf bifurcation about positive equilibrium of the system (3) are investigated.

- The bifurcating behavior of the system (3) is controlled through implementation of a chaos control method.
- Taking into account the consistency preserving discretization for the system (3), a discrete counterpart is proposed, and its qualitative behavior is studied.

The rest of the discussion for this paper is summarized as follows. In Section 2, existence of interior (positive) equilibrium point is discussed. Moreover, the parametric conditions are analyzed for which coexistence is a sink and a source. In Section 3, it is investigated that system (3) undergoes Hopf bifurcation about its coexistence. Moreover, bifurcation theory of normal forms is implemented to explore direction of Hopf bifurcation and the Lyapunov first exponent is also computed. The bifurcating behavior of the model is controlled in Section 4. A consistency preserving discretization is implemented to system (3) in Section 5. Moreover, stability about fixed point, and bifurcation analysis are studied for discrete counterpart of system (3). In Section 6, numerical simulation is presented for illustration of theoretical investigation.

2 Local stability analysis

In order to find equilibria of system (3), we solve the following system:

$$\begin{aligned} -ax-2x^2+by+x^2y &= 0, \\ c+x^2-by-x^2y &= 0. \end{aligned} \tag{4}$$

Then, it is easy to see that unique positive equilibrium (x^*, y^*) of system (3) is given as follows:

$$(x^*, y^*) = \left(\frac{-a+\sqrt{a^2+4c}}{2}, \frac{(b+c)(a^2+4c)+\sqrt{a^2+4c}(c-b)}{2\left(a^2b+(b+c)^2\right)} \right).$$

Moreover, existence of unique positive equilibrium (x^*, y^*) is automatically satisfied under positivity conditions of parameters a, b and c. On the other hand, the Jacobian matrix $J(x^*, y^*)$ of system (3) about (x^*, y^*) is given as follows:

$$J(x^*,y^*)=\begin{pmatrix} \frac{a(b-c)^2-b\left(a^2+2(b+c)\right)\sqrt{a^2+4c}}{ba^2+(b+c)^2} & \frac{1}{4}\left(a-\sqrt{a^2+4c}\right)^2+b \\ \frac{(b-c)\left(a(c-b)+(b+c)\sqrt{a^2+4c}\right)}{ba^2+(b+c)^2} & -\frac{1}{4}\left(a-\sqrt{a^2+4c}\right)^2-b \end{pmatrix}.$$

Moreover, simple computation yields that the trace $TJ(x^*,y^*)$ of $J(x^*,y^*)$ and its determinant $\det J(x^*,y^*)$ are given by:

$$TJ(x^*,y^*):=\frac{a(b-c)^2-b\left(a^2+2(b+c)\right)\sqrt{a^2+4c}}{ba^2+(b+c)^2}-\frac{1}{4}\left(a-\sqrt{a^2+4c}\right)^2-b,$$

and

$$\det J(x^*,y^*):=-\frac{a^3}{2}+\sqrt{a^2+4c}(b+c)+\frac{1}{2}a^2\sqrt{a^2+4c}-2ac.$$

Taking into account the Routh–Hurwitz stability criterion, we have the following result.

Lemma 1. *The following hold true for positive equilibrium of system* (3)*:*

(i) (x^*,y^*) *is a sink if*

$$\frac{a(b-c)^2-b\left(a^2+2(b+c)\right)\sqrt{a^2+4c}}{ba^2+(b+c)^2}<\frac{1}{4}\left(a-\sqrt{a^2+4c}\right)^2+b,$$

and

$$\sqrt{a^2+4c}(b+c)+\frac{1}{2}a^2\sqrt{a^2+4c}>2ac+\frac{a^3}{2}.$$

(i) (x^*,y^*) *is a source if*

$$\frac{a(b-c)^2-b\left(a^2+2(b+c)\right)\sqrt{a^2+4c}}{ba^2+(b+c)^2}>\frac{1}{4}\left(a-\sqrt{a^2+4c}\right)^2+b,$$

and

$$\sqrt{a^2+4c}(b+c)+\frac{1}{2}a^2\sqrt{a^2+4c}>2ac+\frac{a^3}{2}.$$

Moreover, for $c=15.5$ the visualization counterpart of Lemma 2 is depicted in Fig. 2.

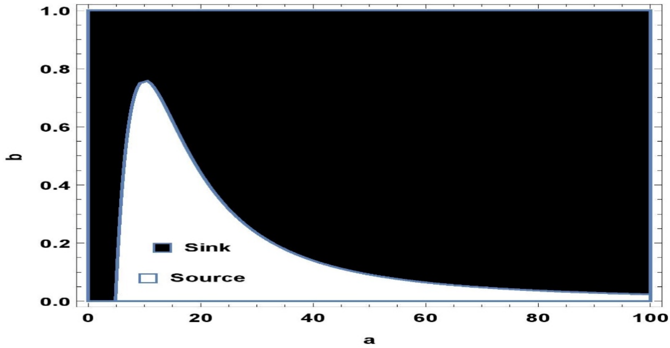


Figure 2. Dynamical classification of positive equilibrium of system (3).

3 Hopf bifurcation

In this section, emergence of Hopf bifurcation is discussed for system (3). For this, b is taken as bifurcation parameter, and we assume that $b{=}b_0$, where b_0 is possible positive root for the following cubic equation:

$$b^3 + A_1 b^2 + A_2 b + A_3 = 0,$$

where

$$A_1 = \frac{1}{2}\left(-a\left(\sqrt{a^2+4c}+2\right) + 4\sqrt{a^2+4c} + 3a^2 + 6c\right),$$

$$A_2 = \frac{a^4}{2} + a^2\left(\sqrt{a^2+4c}+2c\right) - ac\left(\sqrt{a^2+4c}-2\right) + c\left(2\sqrt{a^2+4c}+3c\right) - \frac{1}{2}a^3\sqrt{a^2+4c},$$

and

$$A_3 = \frac{1}{4}c^2\left(\left(a-\sqrt{a^2+4c}\right)^2 - 4a\right).$$

The following Theorem gives necessary and sufficient conditions for existence of Hopf bifurcation for system (3) about its positive equilibrium.

Theorem 1. *Assume that* $b{=}b_0$ *and* $\rho \neq 0$*, then system* (3) *undergoes*

Hopf bifurcation about its positive equilibrium (x^*, y^*), *where*

$$\rho = \frac{d}{db} T(b)|_{b=b_0},$$

$$T(b) := \frac{a(b-c)^2 - b\left(a^2 + 2(b+c)\right)\sqrt{a^2+4c}}{ba^2 + (b+c)^2} - \frac{1}{4}\left(a - \sqrt{a^2+4c}\right)^2 - b.$$

Proof. Taking into account analysis of Section 2, it is easy to see that the characteristic polynomial for $J(x^*, y^*)$ is given as follows:

$$P(\lambda) = \lambda^2 - T(b)\lambda + D(b), \tag{5}$$

where

$$D(b) := -\frac{a^3}{2} + \sqrt{a^2+4c}(b+c) + \frac{1}{2}a^2\sqrt{a^2+4c} - 2ac.$$

Furthermore, it is easy to see that $D(b) > 0$ for all $b > 0$, and $T(b_0) = 0$. Therefore, at $b = b_0$ characteristic equation (5) reduces to $P(\lambda) = \lambda^2 + D(b_0)$ yielding $\lambda_{1,2} = \pm i\sqrt{D(b_0)}$ as eigenvalues for $J(x^*, y^*)$. In order to verify transversality condition (that is, the eigenvalues must cross the imaginary axis with nonzero speed), we consider any point b in the neighborhood of b_0, and one has $\lambda_{1,2} = \alpha(b) \pm i\beta(b)$, where $\alpha(b) := T(b)/2$ and $\beta(b) := \sqrt{D(b) - \frac{T^2(b)}{4}}$. Therefore, if we assume that $\rho = \frac{d}{db}\alpha(b)|_{b=b_0} \neq 0$, then system (3) undergoes Hopf bifurcation about (x^*, y^*) when b varies in the neighborhood of b_0. ∎

Next, in order to investigate the direction of Hopf bifurcation, first we consider the translations $w_1 = x - x^*$ and $w_2 = y - y^*$, then under these translations system (3) is transformed into the following system with equilibrium at $(0, 0)$:

$$\begin{aligned} \frac{dw_1}{dt} &= -a(w_1 + x^*) - 2(w_1 + x^*)^2 + b(w_2 + y^*) + (w_1 + x^*)^2(w_2 + y^*), \\ \frac{dw_2}{dt} &= c + (w_1 + x^*)^2 - b(w_2 + y^*) - (w_1 + x^*)^2(w_2 + y^*). \end{aligned} \tag{6}$$

Applying Taylor series to system (6) about $(w_1, w_2) = (0, 0)$ yields the following system:

$$\begin{pmatrix} \frac{dw_1}{dt} \\ \frac{dw_2}{dt} \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} + \begin{pmatrix} f(w_1, w_2) \\ g(w_1, w_2) \end{pmatrix}, \tag{7}$$

where

$$m_{11} = \frac{a(b-c)^2 - b\left(a^2 + 2(b+c)\right)\sqrt{a^2+4c}}{ba^2 + (b+c)^2}, \quad m_{12} = \frac{1}{4}\left(a - \sqrt{a^2+4c}\right)^2 + b,$$

$$m_{21} = \frac{(b-c)\left(a(c-b) + (b+c)\sqrt{a^2+4c}\right)}{ba^2 + (b+c)^2}, \quad m_{22} = -\frac{1}{4}\left(a - \sqrt{a^2+4c}\right)^2 - b,$$

$$f(w_1, w_2) = (y^* - 2)w_1^2 + 2x^* w_1 w_2 + w_1^2 w_2,$$

and

$$g(w_1, w_2) = (1 - y^*)w_1^2 - 2x^* w_1 w_2 - w_1^2 w_2.$$

Assume that $b = b_0$, and the following transformation is considered:

$$\begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} m_{11} & 0 \\ -m_{12} & -\beta(b_0) \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}. \tag{8}$$

From (7) and (8), we obtain the following system in canonical form:

$$\begin{pmatrix} \frac{dz_1}{dt} \\ \frac{dz_2}{dt} \end{pmatrix} = \begin{pmatrix} 0 & -\beta(b_0) \\ \beta(b_0) & 0 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} + \begin{pmatrix} f^1(z_1, z_2) \\ g^1(z_1, z_2) \end{pmatrix}, \tag{9}$$

where

$$f^1(z_1, z_2) = \frac{1}{m_{11}} f(m_{11} z_1, \quad -m_{12} z_1 - \beta(b_0) z_2),$$

and

$$g^1(z_1,z_2) = -\frac{m_{12}}{\beta(b_0)m_{11}} f(m_{11}z_1, \quad -m_{12}z_1 - \beta(b_0)z_2) \\ - \frac{1}{\beta(b_0)} g(m_{11}z_1, \quad -m_{12}z_1 - \beta(b_0)z_2).$$

In order to discuss direction and stability of periodic orbits, the first Lyapunov exponent L_1 is computed at $(z_1, z_2, b) = (0, 0, b_0)$ as follows [21]:

$$L_1 = \frac{1}{16}[f^1_{z_1z_1z_1} + f^1_{z_1z_2z_2} + g^1_{z_1z_1z_2} + g^1_{z_2z_2z_2}] \\ + \frac{1}{16\beta(b_0)}\left[f^1_{z_1z_2}\left(f^1_{z_1z_1} + f^1_{z_2z_2}\right) - g^1_{z_1z_2}\left(g^1_{z_1z_1} + g^1_{z_2z_2}\right)\right] \\ - \frac{1}{16\beta(b_0)}\left[f^1_{z_1z_1}g^1_{z_1z_1} - f^1_{z_2z_2}g^1_{z_2z_2}\right].$$

Then, we have the following result.

Theorem 2. *Assume that $\rho \neq 0$, and $L_1 \neq 0$, then system* (3) *experiences Hopf bifurcation about (x^*, y^*) whenever b varies in a small neighborhood of b_0. Furthermore, bifurcation is subcritical if $L_1 > 0$, and it is supercritical if $L_1 < 0$.*

4 Bifurcation control

In order to achieve certain desired dynamical properties, controlling bifurcating behavior refers to the formulation of a controller that can modify the fluctuating behavior of a given nonlinear system. The Hopf bifurcation is associated with the appearance of a periodic solution. Such type of situation can lead to oscillations with large amplitude whenever the bifurcation (Hopf) point is approached. Consequently, it is appropriate to vary such fluctuating behavior, which can be accomplished due to the implementation of bifurcation control.

In this section, we apply a state feedback control method [22] to system

(3), and in a result the following controlled system is obtained:

$$\begin{aligned} \frac{dx}{dt} &= -ax - 2x^2 + (b_1 - k_1(x - x^*) - k_2(y - y^*))y + x^2y, \\ \frac{dy}{dt} &= c + x^2 - (b_1 - k_1(x - x^*) - k_2(y - y^*))y - x^2y, \end{aligned} \tag{10}$$

where (x^*, y^*) is positive equilibrium of system (3), k_1 and k_2 are control parameters, and b_1 is some appropriate value of bifurcation parameter b in the Hopf bifurcation region. On the other hand, the Jacobian matrix for system (10) about (x^*, y^*) is given as follows:

$$J(x^*, y^*) = \begin{pmatrix} 2x^*(y^* - 2) - a - k_1y^* & b + (x^*)^2 - k_2y^* \\ k_1y^* - 2x^*(y^* - 1) & k_2y^* - b - (x^*)^2 \\ & \end{pmatrix}.$$

A simple consequence of Routh–Hurwitz criterion gives that system (10) is controllable if the following conditions are satisfied:

$$\begin{aligned} y^*(k_2 - k_1 + 2x^*) &< a + b + x^*(x^* + 4), \\ b + (x^*)^2 &> k_2y^*. \end{aligned} \tag{11}$$

For $a = 2.5$, $b = 3.25$ and $c = 4.5$ the feasible region of (11), that is, controllable region for system (10) is depicted in Fig. 3.

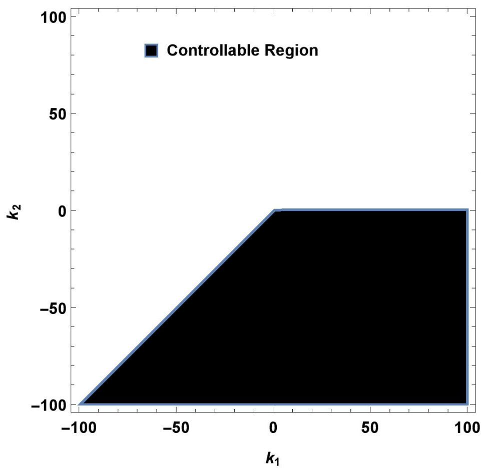


Figure 3. Controllable region of system (10) in k_1k_2-plane.

5 Discretization of system (3)

Discretization of chemical reaction systems is important because it allows the use of mathematical tools and techniques to study the dynamics of the system. The process of discretization converts the continuous-time dynamics of a chemical reaction system into a discrete-time dynamics, which is represented as a sequence of states. This discrete-time representation makes it possible to apply a wide range of mathematical and computational methods to study the system, such as numerical integration, stability analysis, and control theory.

Discretization can also help in the simplification of the system. For example, many chemical reaction systems are high-dimensional, and the discrete-time representation can reduce the dimensionality of the system, making it more tractable for analysis and control. Additionally, discretization can be used to identify and isolate important features of the system, such as steady states, limit cycles, and bifurcations.

Furthermore, discretization is also useful for the simulation of chemical reaction systems. It allows to use finite difference or finite element method, which is a common approach to simulate chemical reaction systems. This process helps to reduce the computational cost of solving the system and it allows the use of standard numerical integration techniques.

In summary, discretization is an important tool for studying chemical reaction systems, as it allows the application of mathematical and computational methods to analyze and control the system, and simplifying the system.

Consistency preserving discretization is a numerical method for approximating the solution of a continuous-time dynamical system, such as a chemical reaction system, in a discrete-time format. The main objective of this method is to ensure that important properties of the continuous-time system, such as stability and bifurcating behavior are preserved in the discrete-time approximation.

In this section, we propose a consistency preserving discretization for the system (3). For this, a nonstandard finite difference scheme is applied to system (3) as follows:

$$\begin{aligned}\frac{x_{n+1}-x_n}{h} &= -a\ x_{n+1}-2x_{n+1}x_n+by_n+(x_n)^2y_n,\\ \frac{y_{n+1}-y_n}{h} &= c+(x_n)^2-by_{n+1}-(x_n)^2y_{n+1},\end{aligned} \tag{12}$$

where $0<h<1$ is step size for discretization. Furthermore, some simplification of (12) yields the following 2-dimensional map:

$$\begin{pmatrix} x \\ y \end{pmatrix} \to \begin{pmatrix} \frac{x+b\ hy+hx^2y}{1+ah+2h\ x} \\ \frac{ch+y+h\ x^2}{1+bh+hx^2} \end{pmatrix}. \tag{13}$$

Furthermore, the Jacobian matrix $M(x^*,y^*)$ of system (13) about (x^*,y^*) is given as follows:

$$M\left(x^*,y^*\right)=\begin{pmatrix} \theta_{11} & \frac{\left(a^2+2(b+c)-a\sqrt{a^2+4c}\right)h}{2+2\sqrt{a^2+4c}h} \\ \theta_{21} & \frac{1}{1+bh+\frac{1}{4}\left(a-\sqrt{a^2+4c}\right)^2h} \end{pmatrix},$$

where

$$\theta_{11}=\frac{1+ah+2h\left(x^*+h\left(-b+x^*\left(a+x^*\right)\right)\right)y^*}{\left(1+ah+2hx^*\right)^2},$$

and

$$\theta_{21}=\frac{2hx^*\left(1+bh-ch-y^*\right)}{\left(1+h\left(b+x^{*2}\right)\right)^2}.$$

On the other hand, the characteristic equation for $M\left(x^*,y^*\right)$ is computed as follows:

$$F\left(X\right)=X^2-\left(\frac{1}{1+bh+\frac{1}{4}\left(a-\sqrt{a^2+4c}\right)^2h}+\theta_{11}\right)X+\det M\left(x^*,y^*\right).$$

With some tedious calculations, one can show that $F\left(\pm1\right)>0$, and $\det M\left(x^*,y^*\right)\ <1$ if the following inequality holds true:

$$\begin{aligned}&h\theta_{21}\left(a^4h+a^2(2bh+4ch+1)-a^3h\sqrt{a^2+4c}\right)\\ &+h\theta_{21}\left(2(b+c)(h(b+c)+1)-a\sqrt{a^2+4c}(2h(b+c)+1)\right)\\ &<\left(h\sqrt{a^2+4c}+1\right)\left(h\left(-\left(a^2+2(b+c)\right)\right)+ah\sqrt{a^2+4c}+2\theta_{11}-2\right).\end{aligned}$$

On the other hand, $\det M\left(x^*, y^*\right) > 1$ if the following inequality holds true:

$$
\begin{aligned}
& h\theta_{21}\left(a^4h + a^2(2bh + 4ch + 1) - a^3h\sqrt{a^2+4c}\right) \\
& + h\theta_{21}\left(2(b+c)(h(b+c)+1) - a\sqrt{a^2+4c}(2h(b+c)+1)\right) \\
& > \left(h\sqrt{a^2+4c}+1\right)\left(h\left(-\left(a^2+2(b+c)\right)\right) + ah\sqrt{a^2+4c} + 2\theta_{11} - 2\right).
\end{aligned}
$$

Consequently, the fixed point (x^*, y^*) of (13) is a sink if $\det M\left(x^*, y^*\right) < 1$ and source if ,$\det M\left(x^*, y^*\right) > 1$. On the other hand, at $h = 0.01$ and $c = 15.5$ the regions for sink and source are depicted in Fig. 4. Moreover, from Fig. 2 and Fig. 4, it is easy to see that dynamical behaviors of both continuous and its discrete counterpart are almost identical with an appropriate choice of step size h.

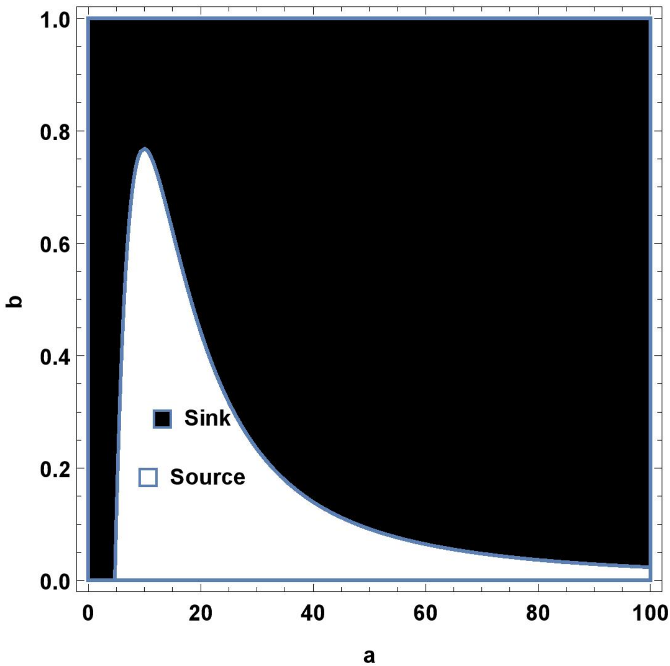


Figure 4. Dynamical classification of positive equilibrium of system (13).

Taking h as bifurcation, system (13) undergoes codimension-1 Neimark-Sacker bifurcation when h passes through small neighborhood of h_1, where h_1 is positive root of the following equation:

$$\begin{aligned}
&h\theta_{21}\left(a^4h+a^2(2bh+4ch+1)-a^3h\sqrt{a^2+4c}\right)\\
&+h\theta_{21}\left(2(b+c)(h(b+c)+1)-a\sqrt{a^2+4c}(2h(b+c)+1)\right)\\
&=\left(h\sqrt{a^2+4c}+1\right)\left(h\left(-\left(a^2+2(b+c)\right)\right)+ah\sqrt{a^2+4c}+2\theta_{11}-2\right),
\end{aligned}$$

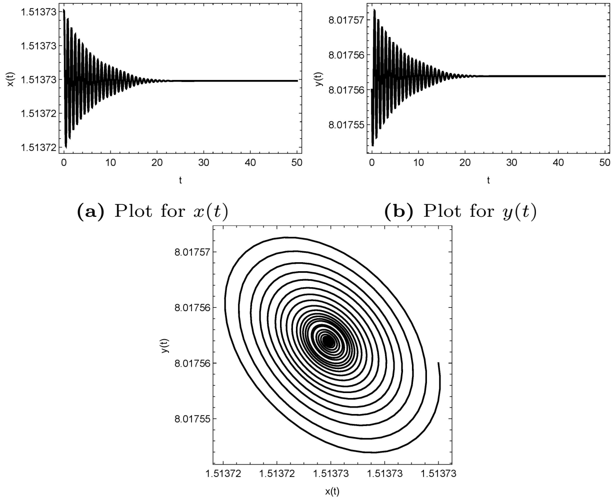
and

$$\left|\frac{1}{1+bh_1+\frac{1}{4}\left(a-\sqrt{a^2+4c}\right)^2h_1}+\theta_{11}(h_1)\right|<2.$$

6 Numerical simulations

In this section, we consider some appropriate numerical simulation for illustration and validation of theoretical investigation. For this, Mathematica packages are implemented for bifurcation diagrams and other relevant numerical simulation. Moreover, validity of bifurcation control is also checked. In the end, emergence of Neimark-Sacker bifurcation is explored in proposed discrete-time chemical reaction system.

In order to show emergence of Hopf bifurcation, first we choose $a= 15.2$, $c= 25.3$ and $b\in[0.5,1.5]$. Then, we will verify that system (3) is unstable for $0.5\le b<b_0= 1.098109805678854$, asymptotically for $b_0<b\le 1.5$, and it will undergo Hopf bifurcation at $b\equiv b_0= 1.098109805678854$. Furthermore, if one choose $a= 15.2$, $c= 25.3$ and $b= 1.15$, then $(1.514, 8.02)$ is unique positive equilibrium point for system (3). On the other hand, the complex conjugate multipliers for the variational matrix of system (3) about $(x^*,y^*)=(1.51373, 8.01756)$ are given by $\lambda_{1,2}=-0.211744\pm 7.91723i$ with $\Re(\lambda_{1,2})=-0.211744<0$ showing that equilibrium is asymptotically stable. Moreover, the plots for state-variables and associated phase portrait are shown in Fig. 5.



(a) Plot for $x(t)$ **(b)** Plot for $y(t)$

(c) Phase portrait

Figure 5. Plots and phase portrait for the system (3) with $a = 15.2$, $c = 25.3$ and $b = 1.15$, and $(x_0, y_0) = (1.51373, 8.01756)$.

Secondly, we take $a = 15.2$, $c = 25.3$ and $b = b_0 = 1.098109805678854$, then system (3) has unique equilibrium $(1.51373, 8.1403)$ with multipliers $\lambda_{1,2} = \pm\, 7.86012i$. On the other hand, we have $\alpha(b)$ is given as follows:

$$\alpha(b) = -\,b + \frac{83.5315}{b + 2.29137} - 23.5463.$$

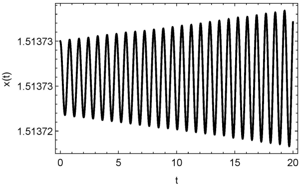
Taking into account transversality condition, one has

$$\rho = \frac{d}{db}\alpha(b)|_{b=b_0} = -\,4.13543 < 0.$$

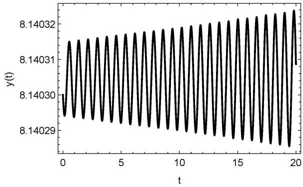
Therefore, necessary and sufficient conditions for appearance of Hopf bifurcation are satisfied at $b = b_0 = 1.098109805678854$. On the other hand, due to some tedious computation, the first Lyapunov exponent is calculated as follows:

$$L_1 = -\,8.79151121928982 < 0.$$

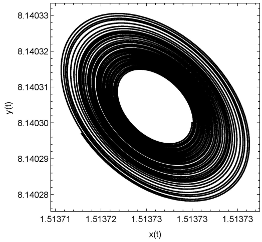
Furthermore, considering $a = 15.2$, $c = 25.3$ and $b = b_0 = 1.098109805678854$ (bifurcation point), the plots for state-variables and associated phase portrait are shown in Fig. 6.



(a) Plot for $x(t)$



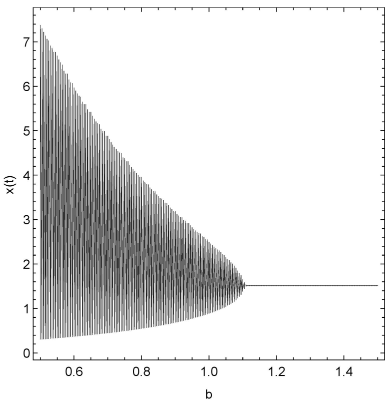
(b) Plot for $y(t)$



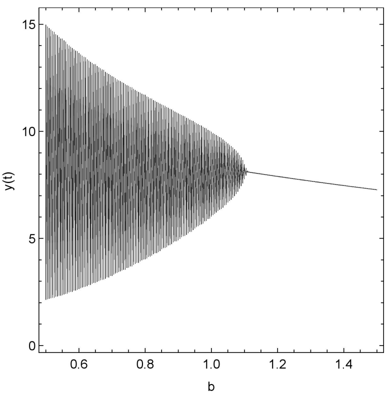
(c) Phase portrait

Figure 6. Plots and phase portrait for the system (3) with a= 15.2, c= 25.3, b= 1.098109805678854, and $(x_0, y_0) = (1.51373, 8.1403)$.

Moreover, for a= 15.2, c= 25.3 and $b \in [0.5, 1.5]$ bifurcation diagrams for system (3) are depicted in Fig. 7.



(a) Bifurcation diagram for $x(t)$

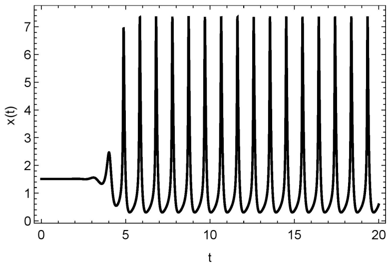


(b) Bifurcation diagram for $x(t)$

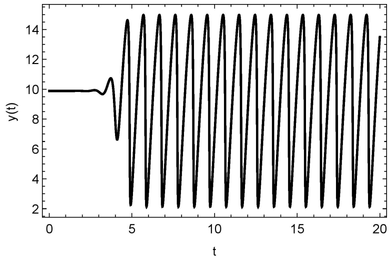
Figure 7. Bifurcation diagrams for the system (3) with a= 15.2, c= 25.3, $b \in [0.5, 1.5]$, and $(x_0, y_0) = (1.51373, 8.1403)$.

Next, in order see the behavior of the system in bifurcation region, that is, $0.5 \leq b < b_0 = 1.098109805678854$, we choose a= 15.2, c= 25.3 and

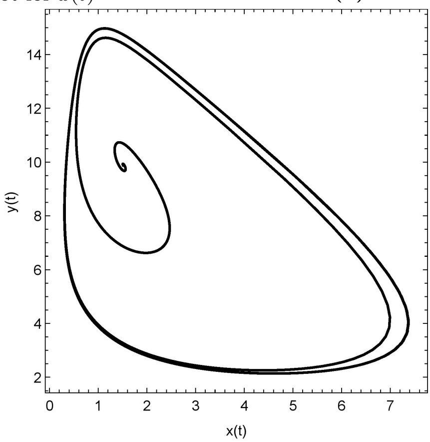
b= 0.5. Then, system (3) has unique positive equilibrium $(1.51373, 9.88454)$ with multipliers of Jacobian matrix about $(x^*, y^*) = (1.51373, 9.88454)$ are given by $\lambda_{1,2}$= $2.93935 \pm 6.49921i$ having $\Re(\lambda_{1,2}) = 2.93935 > 0$. Consequently, equilibrium is a source and plots of system are depicted in Fig. 8. In Fig. 8c, a limit cycle is depicted for the system (3) at b= 0.5.



(a) Plot for $x(t)$



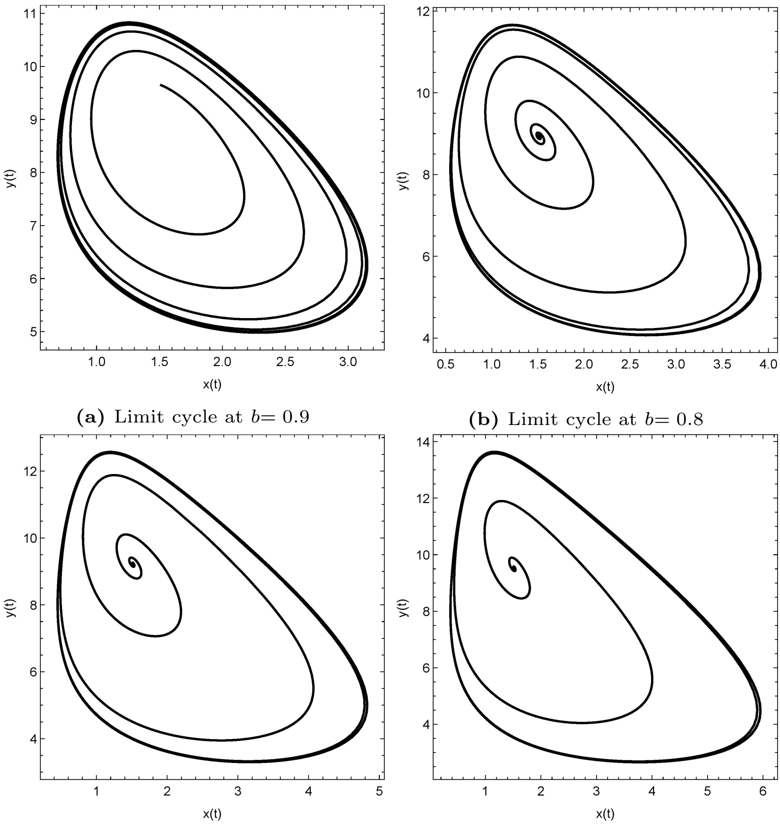
(b) Plot for $y(t)$



(c) Phase portrait

Figure 8. Plots and phase portrait for the system (3) with a= 15.2, c= 25.3, b= 0.5, and $(x_0, y_0) = (1.51373, 9.88454)$.

On the other hand, for b= 0.9, b= 0.8, b= 0.7 and b= 0.6 limit cycles are depicted in Fig. 9.



(a) Limit cycle at b= 0.9

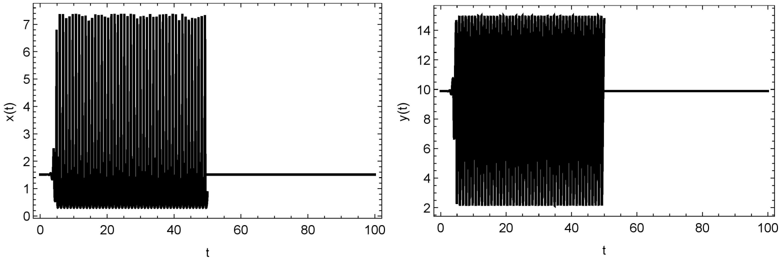
(b) Limit cycle at b= 0.8

(c) Limit cycle at b= 0.7

(d) Limit cycle at b= 0.6

Figure 9. Limit cycles for the system (3) with a= 15.2, c= 25.3 and various values of b.

Finally, effectiveness of bifurcation control is checked in the bifurcation region. For this, assume that a= 15.2, c= 25.3 and b= 0.5 for controlled system (10), then this system is controllable if $k_1 \leq 0.877134$, $k_2 < k_1 - 0.594736$, or $k_1 > 0.877134$, $k_2 < 0.28239$. For k_1= 1.5 and k_2= 0.1, bifurcation control procedure is activated for system (3) for $50 \leq t \leq 100$ and corresponding plots are depicted in Fig. 10.

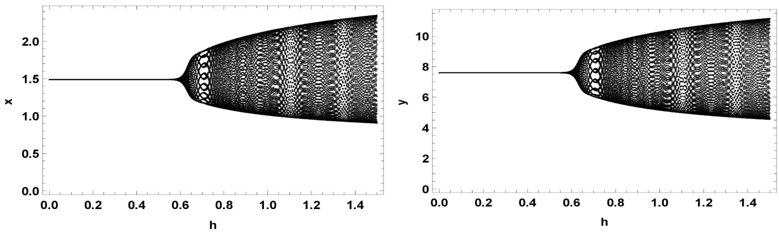


(a) Plot for $x(t)$

(b) Plot for $y(t)$

Figure 10. Activated control procedure for the system (3) with a= 15.2, c= 25.3, b= 0.5, and $50 \leq t \leq 100$.

Finally, appearance of Neimark-Sacker bifurcation in map (13) about is positve fixed is discussed. For this, we take $a = 15.5$, $b = 1.4$, $c = 25.3$, and $h \in [0, 1.5]$. Then, positive fixed point (1.489, 7.61) becomes nonhyperbolic at $h = 0.55822$ yielding Neimark-Sacker bifurcation. On the other hand, bifurcation diagrams for the map (13) are depicted in Fig. 11.



(a) Bifurcation diagram for x_n

(b) Bifurcation diagram for y_n

Figure 11. Bifurcation diagrams for the system (13) with a= 15.5, c= 25.3, $b = 1.4$, $h \in [0, 1.5]$, and $(x_0, y_0) = (1.489, 7.6)$.

7 Concluding remarks

A chemical reaction model for two interacting species is studied. Stability analysis is carried out around unique positive equilibrium. It is investigated that model experiences Hopf bifurcation about its interior (positive) equilibrium point. Direction of Hopf bifurcation through implementation of standard bifurcation theory of normal forms and the computation of the first Lyapunov exponent. Bifurcation control is studied via implementation of state feedback control method which has been frequently used for chaos control in discrete-time dynamical systems. Arguing as in [23–28], OGY (Ott–Grebogi–Yorke) method [22] has sometimes drawbacks for application of discrete-time models, that is, it may be ineffective for controlling chaotic or bifurcating behavior of iterative maps. But our investigation reveals that bifurcation control method is effective for wide range of control parameters. Consequently, OGY control method can be more effective for controlling bifurcation for chemical reaction systems governed by ordinary differential systems. In the end, a consistency preserving non-standard finite difference scheme is implemented to obtain a discrete-time chemical reaction model. The qualitative behavior is explored for proposed model and our investigation proves the consistency preserving properties. Taking into account the fact that the fractional-order chemical reaction systems have the potential to improve our understanding of a wide range of chemical processes and to provide new insights into the behavior and control of these systems [29–34], we will consider a fractional-order counterpart of the system (3) for our future investigation.

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