GLOBAL DYNAMICS OF AN AUTOCATALATOR MODEL

VALERY G. ROMANOVSKI^{1,2,3,4}, YILEI TANG^{4,5} AND STEVAN MACESIC⁶

Abstract In addition, we consider an autocatalator model for its global dynamics. Applying qualitative method to the model, we judge the number of all possible equilibria and analyze all local properties of equilibria, even though the coordinate of equilibria are difficult to be calculated. Moreover, the number of limit cycles is obtained by Hopf bifurcation in \mathbb{R}^3 . For globally asymptotic stabilities of equilibria, we provide a suitable Liapunov function and prove the global stability of the origin when this equilibrium is simple and asymptotically stable. At last, we discussed the integrability of the model and foliate the phase space on invariant surfaces.

1. INTRODUCTION

Efficient and simple chemical reaction models can represent real dynamical systems that are helpful for explaining molecular mechanisms. In the growing development of nonlinear dynamics, there are numerous simple prototype autocatalator models [9, 10, 23, 24] that are practical and useful for examination of dynamical properties of the complex nonlinear real systems.

In this paper the autocatalator [9, 10], a simple model of oscillatory chemical reaction, was analyzed. Although this model is simple it proved to be very useful as basis for modeling complex systems [6, 11, 19, 20]. For the purpose of this paper the model was modified to simulate dynamics of an open reactor, i. e. the continuously well-stirred tank reactor (CSTR), where continuous inflow and outflow of species is present.

Dynamics of this model, and therefore time evolution of concentrations of chemical species, can be described by system

(1.1)
$$\dot{r} = j_0 r_0 - (k_1 + j_0)r,$$
$$\dot{a} = k_1 r - (k_2 + j_0)a - k_3 a b^2,$$
$$\dot{b} = k_2 a - (k_4 + j_0)b + k_3 a b^2,$$

which are derived based on mass action kinetics. The system of ODEs (1.1) consists of three differential equations where r(t), a(t) and b(t) represent concentration of the chemical species and they are function of time. Parameters $k_1 - k_4$ represent reaction rate constants while j_0 represents specific flow rate (rate at which species inflow and outflow from reactor). Parameter r_0 represents concentrations of the specie r in stock solution that is the concentration of species r that inflow in the system at the rate j_0 and it is constant. The values of concentrations and all parameters in system must be nonnegative in order to describe physically meaningful solutions.

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In this paper, we analyze all properties of equilibria of system (1.1), including equilibria at infinity. The Hopf bifurcation is discussed for the existence and numbers of limit cycles in \mathbb{R}^3 . We prove the global stability of the positive equilibrium from a suitable Liapunov function. Finally, we discuss the existence of first integrals and foliate the phase space on invariant surfaces determined by these first integrals.

The organization of this paper is as follows. In section 2, we give qualitative properties for system (1.1) and research the Hopf bifurcation at equilibria. Section 3 is devoted to the research of global asymptotic stability at the origin of (1.1). And the existing region of closed orbits is studied. In section 4, we give the existence and expressions of first integrals. In the last section, we make a conclusion of above investigations and discuss phase portraits of system (1.1) in \mathbb{R}^3 or that restricted on invariant surfaces.

2. LOCAL DYNAMICS OF SYSTEM

In order to consider more general cases, we let all parameters in system (1.1) be positive in this section. We first give local properties of positive equilibria for system (1.1). To make the calculation easier, we use the changes of variables and parameters

$$x = \frac{j_0 r_0}{k_4 + j_0} x_1, \quad y = \frac{k_1 j_0 r_0}{(k_4 + j_0)^2} y_1, \quad z = \frac{k_2 k_1 j_0 r_0}{(k_4 + j_0)^3} z_1,$$

$$K_1 = \frac{k_1 + j_0}{k_4 + j_0}, \quad K_2 = \frac{k_2 + j_0}{k_4 + j_0}, \quad K_3 = \frac{k_1^2 k_2^2 k_3 j_0^2 r_0^2}{(k_4 + j_0)^7}, \quad K_4 = \frac{k_1^2 k_2 k_3 j_0^2 r_0^2}{(k_4 + j_0)^6}$$

and a time rescaling $dt = dt_1/(k_4 + j_0)$, which reduce system (1.1) into the following system,

(2.1)
$$\begin{aligned} \dot{x} &= 1 - k_1 x, \\ \dot{y} &= x - k_2 y - k_3 y z^2, \\ \dot{z} &= y - z + k_4 y z^2, \end{aligned}$$

where for simplicity we denote x_1, y_1, z_1 and K_j by x, y, z and k_j as j = 1, 2, 3, 4 respectively. Assuming that $E_*(x_*, y_*, z_*)$ is a generic positive equilibrium of system (2.1), we have

(2.2)
$$x_* = 1/k_1, \quad y_* = z_*/(k_4 z_*^2 + 1)$$

and z_* is a positive zero of the cubic polynomial in z

(2.3)
$$h(z) := c_0 + b_0 z + a_0 z^2 + z^3,$$

where $a_0 = -\frac{k_4}{k_1k_3} < 0$, $b_0 = \frac{k_2}{k_3} > 0$ and $c_0 = -\frac{1}{k_1k_3} < 0$. The derivative

(2.4)
$$h'(z) := b_0 + 2a_0 z + 3z^2$$

has two real zeros

(2.5)
$$\xi_{\pm} = \frac{-a_0 \pm \sqrt{a_0^2 - 3b_0}}{3},$$

when $a_0^2 - 3b_0 \ge 0$. We find that real $\xi_{\pm} > 0$ if they exist since $a_0 < 0$ and $b_0 > 0$. From Lemma 3.1, the characteristic polynomial of (2.3) is calculated as

$$\Delta_3 = \frac{4k_1^4k_2^3k_3 - k_1^2k_2^2k_4^2 - 18k_1^2k_2k_3k_4 + 27k_1^2k_3^2 + 4k_4^3}{(108k_1^4k_3^4)}$$

Although parameter conditions can be directly presented for the cases that system (2.1) exists 3, 2, 1 or 0 positive equilibria respectively by Lemma 3.1 (see Appendix), we will not show them because of tedious subcases and expressions for these conditions. However, applying properties of cubic polynomial h(z) together with Lemma 3.1, we not only completely determine the numbers of positive equilibria of system (2.1) but also give concrete and relatively simple conditions of parameters as follows.

Theorem 2.1. System (2.1) has at least one positive equilibrium and at most three positive equilibria. Moreover, system (2.1) has (i) three positive equilibria if and only if $\Delta_3 < 0$, (ii) two positive equilibria if and only if $\Delta_3 = 0$, $a_0b_0 < c_0$ and $a_0^2 - 3b_0 > 0$ or (iii) a unique positive equilibrium in remaining cases. Moreover, if system (2.1) has two positive equilibria, then the z-coordinate of one positive equilibria must be a zero of multiplicity 2 of h(z).

Proof. From the analysis above (2.3), it is easy to see that the number of positive equilibria of system (2.1) is equivalent to the number of different positive zeros of cubic polynomial h(z). Thus, system (2.1) has at most three positive equilibria since the degree of h(z) is there with respect to z. Moreover, we have that

(2.6)
$$h(0) = -\frac{1}{k_1 k_3} < 0, \qquad h'(0) = \frac{k_2}{k_3} > 0, \qquad h(\pm \infty) = \pm \infty$$

by (2.3) and (2.4), yielding that h(z) has at least one positive zero by well-known Intermediate Value Theorem [27] and then system (2.1) has at least one positive equilibrium.

Using the case (III4) of Table 1 in Lemma 3.1, we obtain that h(z) has exactly three different positive zeros if and only if $\Delta_3 < 0$ since $a_0 < 0$, $b_0 > 0$ and $c_0 < 0$ in (2.3). Besides, these three different positive zeros of h(z) are simple, as shown in Figure 1. Hence, statement (i) of this theorem is proved.



FIGURE 1. h(z) has three different zeros in \mathbb{R}_+ , all of which are simple.

When h(z) has two different positive zeros, one of them is of multiplicity 2 by (2.6), indicating that $h(\xi_+) = 0$ or $h(\xi_-) = 0$, as shown in Figure 2. Applying the case (II4) of Table 1 in Lemma 3.1, we obtain that h(z) has two positive zeros including a zero of multiplicity 2 if and only if $\Delta_3 = 0$ and $a_0b_0 < c_0$ for (2.3). In order to guarantee that h(z)has exactly two different positive zeros, we need add the condition $a_0^2 - 3b_0 > 0$ by (2.5) in case that h(z) has a zero of multiplicity 3. Thus, statement (ii) of this theorem is proved. Because h(z) has at least one positive zero, the remaining cases except (i) and (ii) in this theorem correspond to the situation that h(z) has exactly one positive zero. The proof of this theorem is completed.



FIGURE 2. h(z) has two different zeros in \mathbb{R}_+ , one of which is of multiplicity 2.

Notice that Δ_3 can be negative under some parameter conditions and the number of 3 different positive for h(z) is reachable. For example, when k_3 is small and $k_1^2 k_2^2 - 4k_4 > 0$ we get $\Delta_3 < 0$, since the numerator of Δ_3 equals $-k_4^2 (k_1^2 k_2^2 - 4k_4)$ as $k_3 = 0$.

Using Lemma 3.1 and Theorem 2.1, we can exhibit the coordinates of all equilibria of system (2.1). However, these expressions of coordinates are complicated, which can cause big difficulty in analysing the properties of equilibria. So, we consider the generic positive equilibrium $E_*(x_*, y_*, z_*)$ of system (2.1). For its qualitative properties, we are interested in the complicated cases, i.e., the equilibrium is degenerate or the matrix of linear part of system (2.1) at the equilibrium has a pair of pure imaginary eigenvalues. These two cases mean that the matrix of linear part of system (2.1) has a zero eigenvalue or may cause Hopf bifurcation.

Theorem 2.2. The generic positive equilibrium $E_*(x_*, y_*, z_*)$ of system (2.1) is degenerate if and only if $z_* = \sqrt{\alpha_{\pm}}$, $h(\sqrt{\alpha_{\pm}}) = 0$ and $k_2k_4 \ge 9k_3$, where α is given in (2.10). The Hopf bifurcation happens at E_* if and only if $z_* = \sqrt{\beta_{\pm}}$, $h(\sqrt{\beta_{\pm}}) = 0$, $k_2 < 1$, $k_3 \le k_2k_4 + 3k_4 - 2\sqrt{2k_2k_4^2 + 2k_4^2}$ and $D_* < 0$, where β and D_* are given in (2.11) and (2.8) respectively.

Proof. By (2.2) and (2.3), the Jacobian matrix of system (2.1) at E_* is

$$J(E_*) := \begin{pmatrix} -k_1 & 0 & 0\\ 1 & -k_3 z_*^2 - k_2 & -2k_3 z_*^2 / (k_4 z_*^2 + 1)\\ 0 & k_4 z_*^2 + 1 & -1 + 2k_4 z_*^2 / (k_4 z_*^2 + 1) \end{pmatrix}.$$

Expanding the characteristic polynomial of the matrix $J(E_*)$, we compute eigenvalues of matrix $J(E_*)$ as

(2.7)
$$-k_1, \qquad \frac{1}{2(k_4 z_*^2 + 1)} \Big(T_* \pm \sqrt{\Delta_*} \Big),$$

where

$$T_* = -k_3k_4z_*^4 + (-k_2k_4 - k_3 + k_4)z_*^2 - k_2 - 1, \qquad \Delta_* = T_*^2 + \frac{4(k_4z_*^2 + 1)^2D_*}{k_1},$$

and

(2.8)
$$D_* = \frac{k_1(-k_3k_4z_*^4 + k_2k_4z_*^2 - 3k_3z_*^2 - k_2)}{k_4z_*^2 + 1}$$

being the determinant of matrix $J(E_*)$.

Clearly, equilibrium $E_*(x_*, y_*, z_*)$ of system (2.1) is degenerate if and only if at least one of its eigenvalues equals zero, i.e., $D_* = 0$, indicating $\Delta_* = 0$. Moreover, the Jacobian matrix $J(E_*)$ has three eigenvalues

(2.9)
$$-k_1, \qquad \frac{T_*}{k_4 z_*^2 + 1}, \qquad 0,$$

when $D_* = 0$. Solving the equation $D_* = 0$, we obtain that

(2.10)
$$z_*^2 = \alpha_{\pm} := \frac{k_2 k_4 - 3k_3 \pm \sqrt{(k_2 k_4 - 3k_3)^2 - 4k_2 k_3 k_4}}{2k_3 k_4},$$

indicating $k_2k_4 \ge 9k_3$ since $(k_2k_4-3k_3)^2-4k_2k_3k_4 = (k_2k_4-9k_3)(k_2k_4-k_3)$ and z*>0. Thus, the determinant D_* has positive zeros with respect to z_* if and only if $k_2k_4 \ge 9k_3$. In this case, from $D_* = 0$ we actually have two positive zeros $\sqrt{\alpha_{\pm}}$, which can coalesce into one positive zeros $\sqrt{(k_2k_4-3k_3)/(2k_3k_4)}$ of multiplicity 2 if $k_2k_4 = 9k_3$. Substituting the positive zeros of D_* into (2.3), we get $h(\sqrt{\alpha_{\pm}}) = 0$ and $k_2k_4 \ge 9k_3$. Therefore, equilibrium $E_*(x_*, y_*, z_*)$ of system (2.1) is degenerate if and only if $z_* = \sqrt{\alpha_{\pm}}$, $h(\sqrt{\alpha_{\pm}}) = 0$ and $k_2k_4 \ge 9k_3$.

The matrix $J(E_*)$ has a pair of pure imaginary eigenvalues if and only if $T_* = 0$ and $D_* < 0$ by (2.7) and (2.8). Solving from $T_* = 0$, we get

(2.11)
$$z_*^2 = \beta_{\pm} := \frac{-k_2k_4 - k_3 + k_4 \pm \sqrt{(-k_2k_4 - k_3 + k_4)^2 - 4k_3k_4(k_2 + 1)}}{2k_3k_4}$$

yielding $-k_2k_4 - k_3 + k_4 \ge 2\sqrt{k_3k_4(k_2+1)} > 0$ to guarantee that $z^* > 0$. Thus, the equation $T_* = 0$ has positive zeros with respect to z_* if and only if

(2.12)
$$k_2 < 1, \quad k_3 \le k_2 k_4 + 3k_4 - 2\sqrt{2k_2 k_4^2 + 2k_4^2}.$$

In particular, T_* has two positive zeros $z_* = \sqrt{\beta_{\pm}}$, which can coalesce into one positive zero $\sqrt{(-k_2k_4 - k_3 + k_4)/(2k_3k_4)}$ of multiplicity 2 if $k_3 = k_2k_4 + 3k_4 - 2\sqrt{2k_2k_4^2 + 2k_4^2}$. Substituting the positive zeros of T_* into (2.3), we get that $h(\sqrt{\beta_{\pm}}) = 0$ under conditions (2.12). Therefore, the Hopf bifurcation happens at equilibrium $E_*(x_*, y_*, z_*)$ of system (2.1) if and only if $z_* = \sqrt{\beta_{\pm}}$, $h(\sqrt{\beta_{\pm}}) = 0$, $k_2 < 1$, $k_3 \le k_2k_4 + 3k_4 - 2\sqrt{2k_2k_4^2 + 2k_4^2}$ and $D_* < 0$ by (2.11), (2.12) and (2.7).

Remark that by (2.7) and (2.8) the generic positive equilibrium $E_*(x_*, y_*, z_*)$ of system (2.1) is asymptotically stable if $D_* < 0$ and $T_* < 0$, or E_* is unstable with a two-dimensional unstable manifold (resp. stable manifold) and a one-dimensional stable manifold (resp. unstable manifold) if $D_* < 0$ and $T_* > 0$ (resp. $D_* > 0$). When $D_* = 0$ and $T_* > 0$ (resp. $T_* < 0$), from (2.9) equilibrium E_* has a one-dimensional unstable manifold, a one-dimensional stable manifold and a one-dimensional center manifold (resp. a two-dimensional stable manifold and a one-dimensional center manifold). When $D_* = 0$ and $T_* = 0$, from (2.9) equilibrium E_* has a one-dimensional stable manifold and an two-dimensional center manifold. When $T_* = 0$ and $D_* < 0$, from (2.7) equilibrium E_* has a one-dimensional stable manifold and an two-dimensional center manifold.

In order to simplify the calculation, we fix one positive equilibrium on the plane $z = z_0$. Without loss of generality, we let $z_0 = 1$. Thus, there exists a positive equilibrium

 $E_1(1/k_1, 1/(k_1(k_2 + k_3)), 1)$ of system (2.1) if

(2.13)
$$k_4 = \tilde{k}_4 := k_1 k_2 + k_1 k_3 - 1,$$

where $k_1k_2 + k_1k_3 - 1 > 0$. Actually, we can solve three positive zeros of h(z) in (2.3) as 1 and

$$z_{\pm} = \frac{k_1 k_2 - 1 + \sqrt{(k_1 k_2 - 1)^2 - 4k_1 k_3}}{2k_1 k_3}$$

if $k_4 = \tilde{k}_4$ and $k_1k_2 - 1 - 2\sqrt{k_1k_3} \ge 0$. Hence, we have the following lemma by above zeros and (2.2) directly.

Lemma 2.3. Supposing that $k_4 = \tilde{k}_4$, system (2.1) has three positive equilibria $E_1(1/k_1, 1/(k_1(k_2+k_3)), 1)$ and $E_{\pm}(1/k_1, z_{\pm}/(k_4 z_{\pm}^2 + 1), z_{\pm})$ if and only if $k_1 k_2 - 1 - 2\sqrt{k_1 k_3} > 0$ and $z_{\pm} \neq 1$, two positive equilibria E_1 and $E_2(1/k_1, z_2/(k_4 z_2^2 + 1), z_2)$ if and only if $k_1 k_2 - 1 - 2\sqrt{k_1 k_3} = 0$, where $z_2 = (k_1 k_2 - 1)/(2k_1 k_3) \neq 1$, or a unique positive equilibrium E_1 in remaining cases.

Theorem 2.4. Assuming that $k_4 = k_4$. Equilibrium $E_1(1/k_1, 1/(k_1(k_2+k_3)), 1) E_1$ is asymptotically stable if $-k_1(k_2+k_3)(k_2+k_3-1) - 2 < 0$ and $k_1k_2 - k_1k_3 - 2 < 0$. When $k_1k_2 - k_1k_3 - 2 > 0$ (or $-k_1(k_2+k_3)(k_2+k_3-1) - 2 > 0$ and $k_1k_2 - k_1k_3 - 2 < 0$), equilibrium E_1 is unstable. When $k_1k_2 - k_1k_3 - 2 = 0$, equilibrium E_1 is degenerate. When $-k_1(k_2+k_3)(k_2+k_3-1) - 2 = 0$ and $k_1k_2 - k_1k_3 - 2 < 0$, equilibrium E_1 has a center manifold of dimension two and a stable manifold of dimension one. Moreover, at most two limit cycles of system (2.1) can appear from the Hopf bifurcation.

Proof. A routine computation shows that the Jacobian matrix of system (2.1) at E_1 is

$$J(E_1) := \begin{pmatrix} -k_1 & 0 & 0\\ 1 & -k_2 - k_3 & -2k_3/(k_1(k_2 + k_3))\\ 0 & k_1k_2 + k_1k_3 & (2k_1k_2 + 2k_1k_3 - 2)/(k_1(k_2 + k_3)) - 1 \end{pmatrix}.$$

By (2.7), eigenvalues of matrix $J(E_1)$ as $-k_1$ and

$$\frac{1}{2(k_1(k_2+k_3)}\Big(-k_1(k_2+k_3)(k_2+k_3-1)-2\\\pm\Big((-k_1(k_2+k_3)(k_2+k_3-1)-2)^2+4k_1(k_2+k_3)^2(k_1k_2-k_1k_3-2)\Big)^{\frac{1}{2}}\Big).$$

From (2.8), the determinant of matrix $J(E_1)$ is equal to $D_1 = k_1k_2 - k_1k_3 - 2$.

Obviously, E_1 is asymptotically stable if $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 < 0$ and $k_1k_2 - k_1k_3 - 2 < 0$. When $k_1k_2 - k_1k_3 - 2 > 0$ (resp. $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 > 0$ and $k_1k_2 - k_1k_3 - 2 < 0$), equilibrium E_1 is unstable. When $k_1k_2 - k_1k_3 - 2 = 0$, equilibrium E_1 is degenerate, and its Jacobian matrix $J(E_1)$ has at least one zero eigenvalue. When $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 = 0$ and $k_1k_2 - k_1k_3 - 2 < 0$, equilibrium E_1 has a center manifold of dimension two and a stable manifold of dimension one.

When $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 = 0$, i.e.,

$$k_1 = \tilde{k}_1 := -\frac{2}{(k_2 + k_3)(k_2 + k_3 - 1)},$$

matrix $J(E_1)$ has a negative eigenvalue $\lambda_3 = -k_1$ and a pair of pure imaginary eigenvalues

$$\lambda_{\pm} = \pm i\sqrt{2k_3 - (k_2 + k_3)^2},$$

where i is the imaginary unit. By tedious calculation, the associated eigenvectors with respect to λ_+ , λ_- and λ_3 are

$$\begin{split} \phi_1 &:= (0, k_3(k_2 + k_3 - 1)/(\sqrt{(k_2 + k_3)^2 - 2k_3} + k_2 + k_3), 1)^T, \\ \phi_2 &:= (0, k_3(k_2 + k_3 - 1)/(-\sqrt{(k_2 + k_3)^2 - 2k_3} + k_2 + k_3), 1)^T, \\ \phi_3 &:= ((k_2^6 + 6k_2^5k_3 + 15k_2^4k_3^2 + 20k_2^3k_3^3 + 15k_2^2k_3^4 + 6k_2k_3^5 + k_3^6 - 2k_2^5 - 12k_2^4k_3 \\ &- 28k_2^3k_3^2 - 32k_2^2k_3^3 - 18k_2k_3^4 - 4k_3^5 + k_2^4 + 8k_2^3k_3 + 16k_2k_3^3 + 5k_3^4 - 2k_2^2k_3 \\ &+ 18k_2^2k_3^2 - 4k_2k_3^2 - 2k_3^3 - 4)/(2(k_2^2 + 2k_2k_3 + k_3^2 - k_2 - k_3)(k_2 + k_3)), \\ &(k_2^3 + 3k_2^2k_3 + 3k_2k_3^2 + k_3^3 - k_2^2 - 2k_2k_3 - k_3^2 - 2)/(2(k_2 + k_3)), 1)^T, \end{split}$$

respectively.

Let $X = (x, y, z)^T$, $U = (u, v, w)^T$, $\Phi_0 = (\phi_1, \phi_2, \phi_3)$ and

$$\Phi_1 = \begin{pmatrix} 1 & i & 0 \\ 1 & -i & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Following the method of standard form in [3], moving E_1 to the origin and making a change $X = \Phi_0 \Phi_1 U$, we rewrite system (2.1) as

(2.14)
$$\dot{U} = \begin{pmatrix} 0 & -\sqrt{2k_3 - (k_2 + k_3)^2} & 0\\ \sqrt{2k_3 - (k_2 + k_3)^2} & 0 & 0\\ 0 & 0 & -k_1 \end{pmatrix} U + \begin{pmatrix} F_1(u, v, w)\\ F_2(u, v, w)\\ F_3(u, v, w) \end{pmatrix},$$

where

$$\begin{split} F_1(u,v,w) = &(k_2+k_3+1)\Big(-(2k_2+2k_3-1)u^2-2\sqrt{2k_3-(k_2+k_3)^2}uv-(2k_3^2+6k_2^2k_3\\ &-(2k_2^3+6k_2^2k_3+6k_2k_3^2+2k_3^3-3k_2^2-6k_2k_3-3k_3^2+k_2+k_3-2)uw/((k_2+k_3)(k_2+k_3-1))-(2k_2^3+6k_2^2k_3+6k_2k_3^2+2k_3^3-3k_2^2-6k_2k_3-3k_3^2+k_2+k_3-4)w^2/(4(k_2+k_3)(k_2+k_3-1))-\sqrt{2k_3-(k_2+k_3)^2}vw-2(k_2+k_3)u^3\\ &-2\sqrt{2k_3-(k_2+k_3)^2}u^2v-(k_2^3+3k_2^2k_3+3k_2k_3^2+k_3^3-k_2^2-2k_2k_3-k_3^2\\ &-2)w^3/(4(k_2+k_3)(k_2+k_3-1))-(3k_2^3+9k_2^2k_3+9k_2k_3^2+3k_3^3-3k_2^2-3k_3^2\\ &-6k_2k_3-2)u^2w/((k_2+k_3)(k_2+k_3-1))-(3k_2^3+9k_2^2k_3+9k_2k_3^2+3k_3^3-3k_2^2-3k_3^2\\ &-6k_2k_3-3k_3^2-4)uw^2/(2(k_2+k_3)(k_2+k_3-1))-\sqrt{2k_3-(k_2+k_3)^2}vw^2/2)\Big), \\ F_2(u,v,w) =&((k_2+k_3)^2+k_2-k_3)\Big((2k_2+2k_3-1)u^2/\sqrt{2k_3-(k_2+k_3)^2}+(2k_2^3+6k_2^2k_3+6k_2k_3^2+2k_3^3-3k_2^2-6k_2k_3-3k_3^2+k_2+k_3-4)w^2/(4\sqrt{2k_3-(k_2+k_3)^2})(k_2+k_3-1))+vw\\ &+2(k_2+k_3)(k_2+k_3-1))+2uv+(2k_2^3+6k_2^2k_3+6k_2k_3^2+2k_3^3-3k_2^2-6k_2k_3-3k_3^2+k_2+k_3-4)w^2/(4\sqrt{2k_3-(k_2+k_3)^2})(k_2+k_3-1))+vw\\ &+2(k_2+k_3)u^3/\sqrt{2k_3-(k_2+k_3)^2}+(k_2^3+3k_2^2k_3+3k_2k_3^2+k_3^3-k_2^2-2k_2k_3-k_3^2-2k_2k_3+k_3^2-2k_2k_3-k_3^2-2k_2k_3-k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3+3k_2k_3^2+k_3-4)w^2/((k_2+k_3-1))+vw\\ &+2(k_2+k_3)u^3/\sqrt{2k_3-(k_2+k_3)^2}+(k_2^3+3k_2^2k_3+3k_2k_3^2+k_3^3-3k_2^2-2k_2k_3-k_3^2-2k_2k_3-k_3^2-2k_2k_3-k_3^2-2k_2k_3-4k_3^2-2k_2k_3-3k_3^2-2k_2k_3-3k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-3k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-3k_3^2-2k_2k_3-3k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_3^2-2k_2k_3-4k_2k_3^2+2k_3+2k_3^2-3k_3^2\\ &-2k_2k_3-4k_3^2-2(k_2+k_3)^2(k_2+k_3)^2(k_2+k_3)(k_2+k_3-1))+vw^2/2\Big),\\ F_3(u,v,w) = 2w/((k_2+k_3)(k_2+k_3-1)). \end{split}$$

The center manifold \mathcal{M}^c of E_1 is a plane which tangents to the invariant eigenspace w = 0 at E_1 . Hence, we can reduce system (2.14) on the center manifold as

$$\dot{u} = -\sqrt{2k_3 - (k_2 + k_3)^2}v - (k_2 + k_3 + 1)(2k_2 + 2k_3 - 1)u^2 - 2\sqrt{2k_3 - (k_2 + k_3)^2}(k_2 + k_3 + 1)uv - 2(k_2 + k_3 + 1)(k_2 + k_3)u^3 - 2\sqrt{2k_3 - (k_2 + k_3)^2}(k_2 + k_3 + 1)u^2v,$$

$$(2.15) \qquad \dot{v} = \sqrt{2k_3 - (k_2 + k_3)^2}u + \frac{(2k_2 + 2k_3 - 1)((k_2 + k_3)^2 + k_2 - k_3)}{\sqrt{2k_3 - (k_2 + k_3)^2}}u^2 + 2((k_2 + k_3)^2 + k_2 - k_3)uv + \frac{2(k_2 + k_3)((k_2 + k_3)^2 + k_2 - k_3)}{\sqrt{2k_3 - (k_2 + k_3)^2}}u^3 + 2((k_2 + k_3)^2 + k_2 - k_3)u^2v.$$

From the classical Hopf bifurcation theory in [18, 36], restricted on the center manifold \mathcal{M}^c , equilibrium E_1 is a weak focus or a center since system (2.1) is analytical. If the order of the first non-zero Liapunov coefficient at E_1 is n, then it is a weak focus of order n. With the

help of Maple V.13 software, the first-order Liapunov coefficient L_1 is calculated as

$$L_1 := -\frac{4k_3(k_2+k_3)^3 - (k_2+k_3)(k_2^2 - 6k_2k_3 + 2k_3 + k_3^2 - 1) - 4k_3}{4(k_2^2 + 2k_2k_3 + k_3^2 - 2k_3)}$$

Notice that the sign of L_1 cannot be fixed. For instance, if we let $k_3 = 0.3$ and $k_2 = 0.4$, then $L_1 = -0.4077272728$; if we let $k_3 = 0.3$ and $k_2 = 0.47$, then $L_1 = 2.389669014$. Therefore, at least one limit cycle appears from the Hopf bifurcation when $|-k_1(k_2+k_3)(k_2+k_3-1)-2|$ is small enough. Moreover, the limit cycle is stable if $L_1 < 0$, and is unstable if $L_1 > 0$. When $L_1 \equiv 0$, we compute the second-order Liapunov coefficient

$$\begin{split} L_2 :=& 23k_2 - 70k_2^2k_3 - 100k_2^3 + 162k_2^4 + 187k_2^5 - 211k_2^6 - 182k_2^7 + 92k_2^8 - 23k_3 - 52k_2k_3 \\ &- 43k_2^2 + 662k_2^3k_3 + 471k_2^4k_3 - 1522k_2^5k_3 - 962k_2^6k_3 + 976k_2^7k_3 + 648k_2^8k_3 + 187k_3^2 \\ &- 272k_2k_3^2 + 586k_2^2k_3^2 + 918k_2^3k_3^2 - 4061k_2^4k_3^2 - 2270k_2^5k_3^2 + 4256k_2^6k_3^2 + 2592k_2^7k_3^2 \\ &- 478k_3^3 + 314k_2k_3^3 + 2022k_2^2k_3^3 - 6204k_2^3k_3^3 - 3290k_2^4k_3^3 + 10192k_2^5k_3^3 + 6048k_2^6k_3^3 \\ &+ 2367k_2k_3^4 - 6301k_2^2k_3^4 - 3330k_2^3k_3^4 + 14840k_2^4k_3^4 + 9072k_2^5k_3^4 + 979k_3^5 - 3890k_2k_3^5 \\ &- 2342k_2^2k_3^5 + 13552k_2^3k_3^5 + 9072k_2^4k_3^5 - 1043k_3^6 - 1002k_2k_3^6 + 7616k_2^2k_3^6 + 6048k_2^3k_3^6 \\ &+ 72k_2^9 + 164k_3^4 - 190k_3^7 + 2416k_2k_3^7 + 2592k_2^2k_3^7 + 332k_3^8 + 648k_2k_3^8 + 72k_3^9 \\ &+ \lambda_0^2 \Big(- 23 - 2k_2 + 140k_2^2 + 26k_2^3 - 301k_2^4 - 136k_2^5 + 184k_2^6 + 112k_2^7 + 388k_2k_3 \\ &- 44k_3 + 100k_2^2k_3 - 1436k_2^3k_3 - 544k_2^4k_3 + 1344k_2^5k_3 + 784k_2^6k_3 + 384k_3^2 + 114k_2k_3^2 \\ &- 2886k_2^2k_3^2 - 1008k_2^3k_3^2 + 3960k_2^4k_3^2 + 2352k_2^5k_3^2 + 72k_3^3 - 2668k_2k_3^3 - 1120k_2^2k_3^3 \\ &+ 6080k_2^3k_3^3 + 424k_3^6 + 3920k_2^4k_3^3 - 917k_3^4 - 712k_2k_3^4 + 5160k_2^2k_3^4 + 3920k_2^3k_3^4 - 192k_3^5 \\ &+ 2304k_2k_3^5 + 2352k_2^2k_3^5 + 784k_2k_3^6 + 112k_3^7 + \lambda_0^2(-18 - 70k_2 - 74k_2^2 - 220k_2k_3 \\ &+ 30k_2^3 + 92k_2^4 + 40k_2^5 - 94k_3 + 42k_2^2k_3 + 368k_2^3k_3 + 200k_2^4k_3 + 400k_2^2k_3^3 - 146k_3^2 - 6k_2k_3^2 + 552k_2^2k_3^2 + 400k_2^2k_3^2 + 368k_2k_3^3 + 92k_4^4 + 40k_3^5)\Big), \end{split}$$

where $\lambda_0 = \sqrt{2k_3 - (k_2 + k_3)^2}$. Performing the computations by the routine minAssGTZ [8] of SINGULAR [7] over the field of characteristic 32003 we obtain that there exist no common zeros of L_1 and L_2 in the parameter region $\{(k_2, k_3) \in \mathbb{R}^2_+ | 0 < k_2 + k_3 < 1, 2k_3 - (k_2 + k_3)^2 > 0\}$, which guarantees that $\lambda_0 > 0$, $k_1 > 0$ and $k_4 > 0$. Therefore, at most two limit cycles of system (2.1) can appear from the Hopf bifurcation. The proof is completed.

Remark that E_1 is asymptotically stable if $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 < 0$ and $k_1k_2 - k_1k_3 - 2 < 0$. When $k_1k_2 - k_1k_3 - 2 > 0$ (resp. $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 > 0$ and $k_1k_2 - k_1k_3 - 2 < 0$), equilibrium E_1 is unstable, having a one-dimensional (resp. a two-dimensional) unstable manifold and a two-dimensional (resp. a one-dimensional) stable manifold. When $k_1k_2 - k_1k_3 - 2 = 0$ and $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 > 0$ (resp. < 0), equilibrium E_1 is degenerate, having a center manifold of dimension one, a stable manifold of dimension two). When $k_1k_2 - k_1k_3 - 2 = 0$ and $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 > 0$ (resp. < 0), equilibrium E_1 is degenerate, having a center manifold of dimension one, a stable manifold of dimension two. When $k_1k_2 - k_1k_3 - 2 = 0$ and $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 = 0$, equilibrium E_1 is degenerate, having a center manifold of dimension one (resp. and a stable manifold of dimension two). When $k_1k_2 - k_1k_3 - 2 = 0$ and $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 = 0$, equilibrium E_1 is degenerate, having a center manifold of dimension two and a stable manifold of dimension one. When $-k_1(k_2 + k_3)(k_2 + k_3 - 1) - 2 = 0$ and $k_1k_2 - k_1k_3 - 2 < 0$, equilibrium E_1 has a center manifold of dimension two and a stable manifold of dimension one.

We give numerical examples to illustrate our results of Hopf bifurcation by computer algebra system MATLAB. When $k_4 = \tilde{k}_4$, $k_2 = 0.3295$, $k_3 = 0.6$ and $k_1 = 30.52048879$, we

obtain that $L_2 < 0, L_1 > 0$ and matrix $J(E_1)$ has a pair of pure imaginary eigenvalues λ_{\pm} . Then we find the existence of one stable limit cycle from Hopf bifurcation at weak focus $E_1(0.032764875, 0.03525, 1)$ of system (2.1), as shown in Figure 3.



FIGURE 3. One limit cycles of system (2.1) bifurcates from weak focus E_1 , where the initial value is (0.03, 0.04, 1).

When $k_4 = k_4$, $k_2 = 0.3295$, $k_3 = 0.6$ and $k_1 = 29$, we have that $L_2 < 0$, $L_1 > 0$ and the real part of a pair of conjugate complex eigenvalues of matrix $J(E_1)$ is negative. Two limit cycles of system (2.1) can bifurcate from Hopf bifurcation at weak focus $E_1(0.03448275862, 0.03709818033, 1)$. Seeing Figure 4, the orbit starting from the initial value (0.03, 0.04, 1) trends to a stable limit cycle and the orbit starting from the initial value (0.034, 0.037, 1) goes to equilibrium E_1 . Thus, after restricting system (2.1) on the center manifold and applying Poincaré-Bendixson Annular Theorem [36], we have an unstable limit cycle between the stable limit cycle and equilibrium E_1 . Actually, restricting system (2.1) on the center manifold, we find two limit cycles of system (2.15) by Hopf bifurcation, as shown in Figure 5. Specially, the outer limit cycle is stable and the inner limit cycle is unstable.

3. DISCUSSION

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FIGURE 4. Two limit cycles of system (2.1) bifurcate from weak focus E_1 .



FIGURE 5. Two limit cycles of system (2.15) bifurcate from stable weak focus (0,0).

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Appendix 1: Roots of Cubic Polynomials

Consider a general cubic polynomial equation

(3.1)
$$x^3 + ax^2 + bx + c = 0$$

with real coefficients a, b, c. It is known that equation (3.1) has three roots

(3.2)

$$x_{1} = \sqrt[3]{-\frac{Q}{2} + \sqrt{\Delta_{3}}} + \sqrt[3]{-\frac{Q}{2} - \sqrt{\Delta_{3}}} - \frac{a}{3},$$

$$x_{2} = \sqrt[3]{-\frac{Q}{2} + \sqrt{\Delta_{3}}}\omega^{2} + \sqrt[3]{-\frac{Q}{2} - \sqrt{\Delta_{3}}}\omega - \frac{a}{3},$$

$$x_{3} = \sqrt[3]{-\frac{Q}{2} + \sqrt{\Delta_{3}}}\omega + \sqrt[3]{-\frac{Q}{2} - \sqrt{\Delta_{3}}}\omega^{2} - \frac{a}{3},$$

in \mathbb{C} , where $\omega := (-1 + \sqrt{3}i)/2$, $Q := 2a^3/27 + c - ab/3$ and $\Delta_3 = (4a^3c - a^2b^2 + 4b^3 - 18abc + 27c^2)/108$. One can check easily that equation (3.1) has exactly one real root x_1 and a pair of complex conjugate roots x_2 and x_3 when $\Delta_3 > 0$, three real roots x_1, x_2, x_3 when $\Delta_3 \leq 0$. In particular, $x_2 = x_3$ when $\Delta_3 = 0$ but x_1, x_2, x_3 are distinct when $\Delta_3 < 0$. Let $\Re x_j$ and $\Im x_j$ denote the real part and the imaginary part of x_j .

The following lemma is elementary but useful in discussion on the cubic polynomials for equilibria from the idea of Cardano's method.

Lemma 3.1. The cubic polynomial equation (3.1) has the following distribution of roots:

Case	Possibilities of a, b, c	Distribution of roots
I1	$a^2 < 4b, a < (>)c = 0$	$x_1 = 0, \Re x_{2,3} > (<)0, \Im x_{2,3} \neq 0$
I2	b > 0, ab = c > (resp. =, <)0	$x_1 < (\text{resp.} =, >)0, \Re x_{2,3} = 0, \Im x_{2,3} \neq 0$
I3	$\Delta_3 > 0, ab > (<)c > (<)0$	$x_1 < (>)0, \Re x_{2,3} < (>)0, \Im x_{2,3} \neq 0$
I4	$\Delta_3 > 0, c > \max(<\min)\{ab, 0\}$	$x_1 < (>)0, \Re x_{2,3} > (<)0, \Im x_{2,3} \neq 0$
II1	$a^2 = 4b, ab < (>)c = 0$	$x_1 = 0, x_2 = x_3 > (<)0$
II2	$a^2 = -b, ab = c > (<)0$	$x_1 < (>)0, x_2 = x_3 > (<)0$
II3	a > (resp. =, <)b = c = 0	$x_1 < (\text{resp.} =, >) x_2 = x_3 = 0$
II4	$\Delta_3 = 0, ab < (>)c < (>)0$	$x_1 > (<)0, x_2 = x_3 > (<)0$
II5	$\Delta_3 = 0, c > \max(<\min)\{ab, 0\}$	$x_1 < (>)0, x_2 = x_3 > (<)0$
III1	$a^2 > 4b, a < (>)0, b > 0, c = 0$	$x_1 > (=)0, x_2 > (<)0, x_3 = (<)0$
III2	b < 0, c = 0	$x_1 > 0, x_2 = 0, x_3 < 0$
III3	$\Delta_3 < 0, \ a \ge (\le)0, \ c < (>)0$	$x_1 > 0, x_2 < (>)0, x_3 < 0$
III4	$\Delta_3 < 0, \ a < (>)0, \ b > (<)0, \ c < (>)0$	$x_1 > 0, x_2 > 0, x_3 > (<)0$
III5	$\Delta_3 < 0, a < (>)0, b < (>)0, c < (>)0$	$x_1 > (<)0, x_2 < 0, x_3 < 0$

Table 1: Distribution of zeros of cubic polynomials.

 1 Department of Mathematics, Shanghai Normal University, Shanghai, 200234, P.R. China $E\text{-}mail\ address:\ Valery.Romanovski@uni-mb.si\ (V.G. Romanovski)$

 2 Faculty of Electrical Engineering and Computer Science, University of Maribor, Smetanova 17, Maribor, SI-2000 Maribor, Slovenia

 3 Faculty of Natural Science and Mathematics, University of Maribor, Koroška c.160, Maribor, SI-2000 Maribor, Slovenia

 4 Center for Applied Mathematics and Theoretical Physics, University of Maribor, Krekova 2, Maribor, SI-2000 Maribor, Slovenia

 5 School of Mathematical Science, Shanghai Jiao Tong University, Dongchuan Road 800, Shanghai, 200240, P.R. China

E-mail address: mathtyl@sjtu.edu.cn (Y. Tang)

⁶ FACULTY OF PHYSICAL CHEMISTRY, UNIVERSITY OF BELGRADE, STUDENTSKI TRG 12, BELGRADE, SERBIA

E-mail address: <macesic.stevan@gmail.com (S. Macesic)