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Dynamics and Control of Brusselator Chemical Reaction

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Abstract: In the 1970s, nonlinear oscillations and bifurcations were discovered first by modelling and then by experiments for the autocatalytic Brusselators and the Belousov-Zhabotinsky (BZ) chemical reaction. The autocatalytic chemical reaction phenomenon plays a vital role for the breakdown of the stability of the thermodynamical branch. This research work investigates the dynamics and qualitative properties of the autocatalytic Brusselator chemical reaction. Then this work discusses the adaptive control of the Brusselator chemical reaction so as to regulate its states to desired steady-state values. The main result is established using Lyapunov stability theory. MATLAB plots have been shown to illustrate all the main results discussed in this research work.
Keywords: Chemical systems, oscillations, chemical reactions, Brusselator, B-Z reaction, adaptive control, etc.

Introduction

In the 1970s, nonlinear oscillations and bifurcations were discovered first by modelling and then by experiments for the autocatalytic Brusselators and the Belousov-Zhabotinsky (BZ) chemical reaction [1-2]. The autocatalytic chemical reaction phenomenon plays a vital role for the breakdown of the stability of the thermodynamical branch.

A dynamical system is called*chaotic,* the system variables should contain some nonlinear terms and the system must satisfy three properties: boundedness, infinite recurrence and sensitive dependence on initial conditions [3-4]. The first known chaotic system was discovered by Lorenz in 1963[5]. Subsequently, Rössler discovered a 3-D chaotic chemical reaction system in 1976 [6].

The classical chaotic systems were followed by the finding of many 3-D chaotic systems such as Arneodo system [7], Sprott systems [8], Chen system [9], Lü-Chen system[10], Cai system[11], Tigan system [12], etc. Many new chaotic systems have been also discovered in the recent years such as Sampath system [13], Sundarapandian systems [14-15], Vaidyanathan systems [16-35], Pehlivan system [36], Pham system [37], etc.

Chaos theory has very useful applications in many fields of science and engineering such as oscillators[38], lasers [39-40],biology [41-42], chemical reactions [43-45], neural networks[46-47],robotics [48-49], electrical circuits [50], etc.

A simple chemical model that exhibits complex dynamics is the Brusselator model, which is an example of an autocatalytic oscillating chemical reaction [51]. This model could present the limit cycle, Hopf bifurcation and also the chaotic behaviour when a certain sinusoidal force acts on the system. This force could be created by the heat convection, microwaves etc., that its behaviour is sinusoidal with a small intensity.

This paper describes the modelling and properties of the Brusselator dynamics.This paper also derives

new results of adaptive feedback controller design for the Brusselator system using Lyapunov stability theory [52].

In control theory, active control method is used when the system parameters are available for measurement [53-68]. Adaptive control is a popular control technique used for stabilizing systems when the system parameters are unknown [69-82]. There are also other popular methods available for control and synchronization of systems such as backstepping control method [83-88], sliding mode control method [89-100], etc. In this work, we use adaptive control method for regulating the outputs of the Brusselator chemical reaction model.

Brusselator Chemical Reaction Model

The mechanism for the classical Brusselator chemical model [51] is as follows:

$$A \xrightarrow{k_1} X \tag{1}$$
$$B + X \xrightarrow{k_2} Y + D \tag{2}$$
$$2X + Y \xrightarrow{k_3} 3X \tag{3}$$
$$X \xrightarrow{k_4} E \tag{4}$$

The Brusselator chemical reaction model describes a chemical system that converts a reactant A to a final product E through four steps and four intermediate species, X, B, Y and D. The steps (2) and (3) are bimolecular, and autocatalytic trimolecular reactions respectively. Based on the mechanism of Brusselator reaction, product E is resulted from species X in step (4). In addition, species X is the result of steps (1) and (3). These relationships could show the sensitivity to initial conditions.

We denote the concentrations of $A, B, D, E, X,$ and Y by $[A], [B], [D], [E], [X],$ and $[Y]$, respectively. Then the evolutions of the concentrations of the species as a function of the time t using mass action law are given as follows:

$$\frac{d[A]}{dt} = -k_1[A] \tag{5}$$
$$\frac{d[B]}{dt} = -k_2[B][X] \tag{6}$$
$$\frac{d[D]}{dt} = k_2[B][X] \tag{7}$$
$$\frac{d[E]}{dt} = k_4[X] \tag{8}$$
$$\frac{d[X]}{dt} = k_1[A] - k_2[B][X] + k_3[X]^2[Y] - k_4[X] \tag{9}$$
$$\frac{d[Y]}{dt} = k_2[B][X] - k_3[X]^2[Y] \tag{10}$$

where $k_j, (j = 1, 2, 3, 4)$ is the reaction rate and represented in units of $(mole/l \cdot s)^{-1}$.

Since the species D and E do not influence others, we ignore (7) and (8). Moreover, for simplicity, we suppose that $[A]$ and $[B]$ are maintained constant, *i.e.* $[A] = a$ and $[B] = b$, where $a, b > 0$, and all reaction rates k_j, $(j = 1, 2, 3, 4)$ are set equal to unity.

Thus, the ordinary differential equations that describe the Brusselator chemical reaction are as follows:

$$\begin{cases} \dfrac{d[X]}{dt} = a + [X]^2[Y] - (b+1)[X] \\ \dfrac{d[Y]}{dt} = b[X] - [X]^2[Y] \end{cases} \tag{11}$$

To simplify the notation, we define $x = [X]$ and $y = [Y]$.

Then we can represent the Brusselator chemical reaction given in (11) in a compact form as follows.

$$\begin{cases} \dot{x} = a + x^2 y - (b+1)x \\ \dot{y} = bx - x^2 y \end{cases} \tag{12}$$

The equilibrium points of (12) are obtained by solving the nonlinear equations

$$a + x^2 y - (b+1)x = 0 \tag{13a}$$

$$x(b - xy) = 0 \tag{13b}$$

From (13b), either $x = 0$ or $b - xy = 0$.

If we take $x = 0$, then (13a) reduces to $a = 0$, which is inadmissible.

Thus, we must have $b - xy = 0$ or $xy = b$.

Using this, we can simplify (13a) as

$$a + bx - (b+1)x = 0 \text{ or } x = a. \tag{14}$$

Then we obtain y as $y = \dfrac{b}{x} = \dfrac{b}{a}$.

Thus, the unique equilibrium point of (12) is obtained as $E_0 : (x, y) = \left(a, \dfrac{b}{a} \right)$.

The Jacobian matrix of (12) at the equilibrium point E_0 is obtained as

$$J_0 = J(E_0) = \begin{bmatrix} b-1 & a^2 \\ -b & -a^2 \end{bmatrix} \tag{15}$$

The characteristic equation of the Jacobian matrix J_0 is easily obtained as

$$\lambda^2 + (a^2 - b + 1)\lambda + a^2 = 0 \tag{16}$$

By Routh's theorem, the equilibrium point E_0 is stable if and only if

$$a^2 - b^2 + 1 > 0 \text{ or } b < a^2 + 1 \tag{17}$$

Also, the equilibrium point E_0 is unstable if

$$a^2 - b^2 + 1 < 0 \text{ or } b > a^2 + 1 \tag{18}$$

Therefore, for $b > a^2 + 1$, the Brusselator chemical model (12) has a limit cycle.

Assuming $b = a^2 + 1$, the Brusselator chemical model (12) exhibits Hopf bifurcation.

For numerical simulations, we take

$a = 1\ mole/l,\ b = 3\ mole/l$

We note that

$b > a^2 + 1.$

We take the initial values of the concentrations x and y as

$x(0) = 0.1\ mole/l,\ y(0) = 0.5\ mole/l$

Figure 1 shows the limit cycle of the Brusselator chemical reaction system (12).

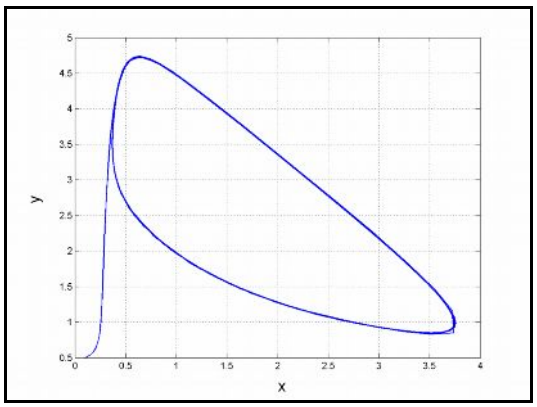

Figure1.Limit Cycle of the Brusselator Chemical Reaction System

Adaptive Control of the Brusselator ChemicalReaction System

In this section, we use adaptive control method to design an adaptive feedback control law for regulating the outputs of the Brusselator chemicalreaction system with unknown parameters.

In this section, we consider the controlled Brusselator chemical reaction system given by the 2-D dynamics

$$\begin{cases} \dot{x} = a + x^2 y - (b+1)x + u_x \\ \dot{y} = bx - x^2 y + u_y \end{cases} \tag{19}$$

In (19), x, y are the states and u_x, u_y are the adaptive feedback controls to be found using estimates of the unknown parameters a, b of the system (19).

Our control goal is to drive the states of the Brusselator chemical reaction system (19) to desired values of the states, say, α, β, respectively.

Thus, we define the tracking errors as

$$\begin{cases} e_x(t) = x(t) - \alpha \\ e_y(t) = y(t) - \beta \end{cases} \tag{20}$$

The tracking error dynamics is obtained as

$$\begin{cases} \dot{e}_x = a + (e_x + \alpha)^2 (e_y + \beta) - (b+1)(e_x + \alpha) + u_x \\ \dot{e}_y = b(e_x + \alpha) - (e_x + \alpha)^2 (e_y + \beta) + u_y \end{cases} \tag{21}$$

We consider the adaptive controller defined by

$$\begin{cases} u_x = -\hat{a}(t) - (e_x + \alpha)^2 (e_y + \beta) + [\hat{b}(t) + 1](e_x + \alpha) - k_x e_x \\ u_y = -\hat{b}(t)(e_x + \alpha) + (e_x + \alpha)^2 (e_y + \beta) - k_y e_y \end{cases} \tag{22}$$

where k_x, k_y are positive gain constants.

Substituting (22) into (21), we get the closed-loop control system given by

$$\begin{cases} \dot{e}_x = [a - \hat{a}(t)] - [b - \hat{b}(t)](e_x + \alpha) - k_x e_x \\ \dot{e}_y = [b - \hat{b}(t)](e_x + \alpha) - k_y e_y \end{cases} \tag{23}$$

We define parameter estimation errors as follows:

$$\begin{cases} e_a = a - \hat{a}(t) \\ e_b = b - \hat{b}(t) \end{cases} \tag{24}$$

Using (24), we can simplify the error dynamics (23) as follows.

$$\begin{cases} \dot{e}_x = e_a - e_b(e_x + \alpha) - k_x e_x \\ \dot{e}_y = e_b(e_x + \alpha) - k_y e_y \end{cases} \tag{25}$$

Differentiating the parameter estimation errors (8) with respect to time, we get

$$\begin{cases} \dot{e}_a = -\dot{\hat{a}}(t) \\ \dot{e}_b = -\dot{\hat{b}}(t) \end{cases} \tag{26}$$

Next, we consider the candidate Lyapunov function given by

$$V(e_x, e_y, e_a, e_b) = \frac{1}{2}\left(e_x^2 + e_y^2 + e_a^2 + e_b^2\right) \tag{27}$$

Differentiating V along the trajectories of (25) and (26), we obtain

$$\dot{V} = -k_x e_x^2 - k_y e_y^2 + e_a\left[e_x - \dot{\hat{a}}\right] + e_b\left[(e_y - e_x)(e_x + \alpha) - \dot{\hat{b}}\right] \tag{28}$$

In view of (28), we take the parameter estimates as follows:

$$\begin{cases} \dot{\hat{a}} = e_x \\ \dot{\hat{b}} = (e_y - e_x)(e_x + \alpha) \end{cases} \tag{29}$$

Theorem 1. *The Brusselator chemical reaction system (19) is exponentially regulated to the steady-state values α, β by the adaptive feedback control law (22) and the parameter update law (29), where k_x, k_y are positive gain constants.*

Proof. The quadratic Lyapunov function V defined by Eq. (27) is a positive definite function on R^4.

Substituting the parameter update law (29) into (28), the time-derivative of V is obtained as

$$\dot{V} = -k_x e_x^2 - k_y e_y^2, \tag{30}$$

which is a negative semi-definite function on R^4.

Thus, by Lyapunov stability theory [52], we conclude that the tracking error $e(t) \to 0$ exponentially as $t \to \infty$ for all initial conditions $e(0) \in R^2$. This completes the proof. ■

Numerical Simulations

Weuse classical fourth-order Runge-Kutta method in MATLAB with step-size $h = 10^{-8}$ for solving the systems of differential equations given by (19) and (29).

We take the gain constants as $k_x = 50$ and $k_y = 50$. We take $\alpha = 1$ and $\beta = 2$.
We take the initial conditions of the system (19) as $x(0) = 5.1$ and $y(0) = 3.7$.
We take the parameters as $a = 1$ and $b = 4$. Also, we take $\hat{a}(0) = 2.3$ and $\hat{b}(0) = 1.5$.

Figures 2-3 show the time-history of the exponential convergence of the states x, y to desired target values α, β respectively.

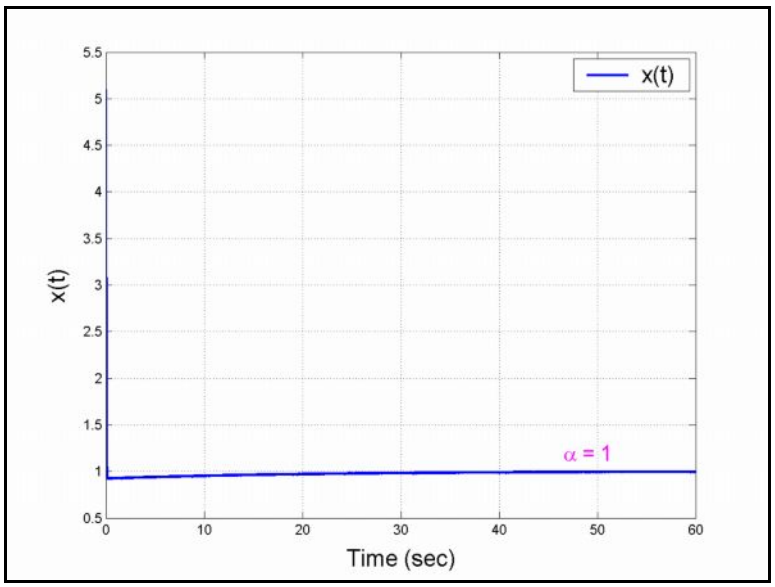

Figure 2.Regulation of the state x of the Brusselator chemical reaction system to $\alpha = 1$

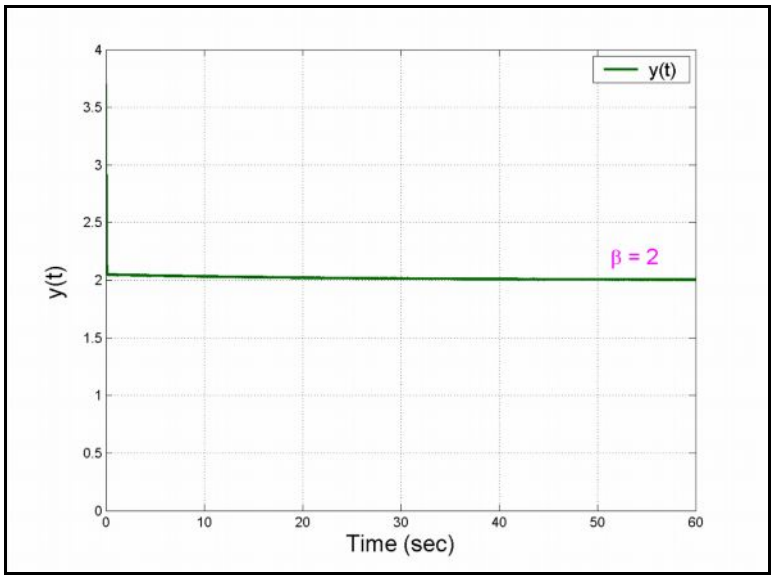

Figure 3. Regulation of the state y of the Brusselator chemical reaction system to $\beta = 2$

Conclusions

In this paper, new results have been derived for the analysis and adaptive control of the autocatalytic Brusselator chemical reaction system. After analyzing the dynamic and qualitative properties of theBrusselator chemical reaction system, we have designed an adaptive controller for the global exponential regulation of the states of the Brusselator chemical reaction system to desired steady-state values. The main results have been proved using Lyapunov stability theory and numerical simulations have been illustrated using MATLAB.

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