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Anti-Synchronization of Brusselator Chemical Reaction Systems via Adaptive Control

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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 anti-synchronization of the identical Brusselator chemical reaction systems. The main chemical anti-synchronization 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, chemical reactions, Brusselator, BZ reaction,anti-synchronization, control, etc.

Introduction

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 [1-2].

The classical chaotic systems like Lorenz system [3], Rössler system [4] were followed by the discovery of many 3-D chaotic systems such as Arneodo system [5], Sprott systems [6], Chen system [7], Lü-Chen system[8], Cai system[9], Tigan system [10], etc.

Many new chaotic systems have been also discovered in the recent years such as Sampath system [11], Sundarapandian systems [12-13], Vaidyanathan systems [14-33], Pehlivan system [34], Pham system [35], etc.

Chaos theory has very useful applications in many fields of science and engineering such as oscillators[36], lasers [37-38],biology [39-40], chemical reactions [41-43], neural networks[44-45], electrical circuits [46], etc.

In the 1970s, nonlinear oscillations and bifurcations were discovered first by modelling and then by experiments for the autocatalytic Brusselators and the Belousov-Zhabotinsky chemical reaction [47-48]. The autocatalytic chemical reaction phenomenon plays a vital role for the breakdown of the stability of the thermodynamical branch.

A simple chemical model that exhibits complex dynamics is the Brusselator model, which is an example of an autocatalytic oscillating chemical reaction [49]. 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 anti-synchronization design for the identical Brusselator chemical reaction systems using Lyapunov stability theory [50].

In control theory, active control method is used when the system parameters are available for measurement [51-66]. Adaptive control is a popular control technique used for stabilizing systems when the system parameters are unknown [67-80]. There are also other popular methods available for control and synchronization of systems such as backstepping control method [81-86], sliding mode control method [87-98], etc. In this work, we use adaptive control for asymptotically anti-synchronizingthe identical Brusselator chemical reaction systems.

Brusselator Chemical Reaction Model

The mechanism for the classical Brusselator chemical model [49] is given 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:

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

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.

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

Thus, the unique equilibrium point of (12) is easily 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

$$J_0 = J(E_0) = \begin{bmatrix} b-1 & a^2 \\ -b & -a^2 \end{bmatrix} \quad (13)$$

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

$$\lambda^2 + (a^2 - b + 1)\lambda + a^2 = 0 \quad (14)$$

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

$$a^2 - b^2 + 1 > 0 \text{ or } b < a^2 + 1 \quad (15)$$

Also, the equilibrium point E_0 is unstable if

$$a^2 - b^2 + 1 < 0 \text{ or } b > a^2 + 1 \quad (16)$$

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 $a = 1 \; mole/l$, $b = 3 \; mole/l$ where $b > a^2 + 1$.

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).

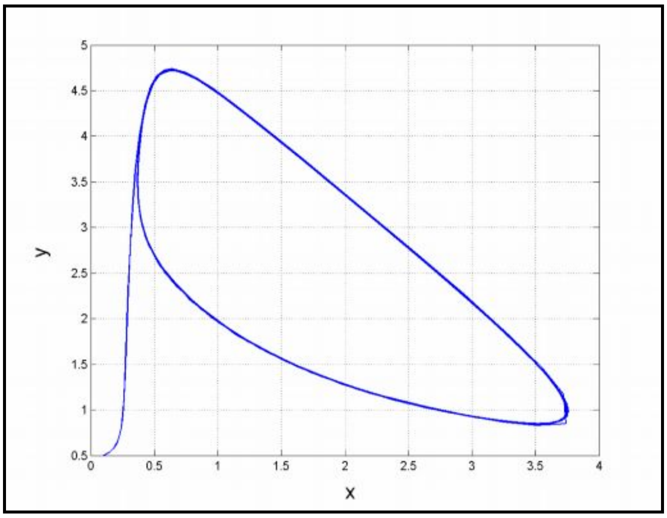

Figure 1.Limit Cycle of the Brusselator Chemical Reaction System

Adaptive Anti-Synchronization of Identical Brusselator ChemicalReaction Systems

In this section, we use adaptive control to design an adaptive control law for globally anti-synchronizing the states of identical Brusselator chemicalreaction systemswith unknown parameters.

As the master system, we consider the Brusselator chemical reaction system given by the 2-D dynamics-

$$\begin{cases} \dot{x}_1 = a + x_1^2 y_1 - (b+1)x_1 \\ \dot{y}_1 = bx_1 - x_1^2 y_1 \end{cases} \tag{17}$$

In (17), x_1, y_1 are the states and a, b are unknown system parameters.

As the slave system, we consider the Brusselator chemical reaction system given by the 2-D dynamics

$$\begin{cases} \dot{x}_2 = a + x_2^2 y_2 - (b+1)x_2 + u_x \\ \dot{y}_2 = bx_2 - x_2^2 y_2 + u_y \end{cases} \tag{18}$$

The anti-synchronization error between the Brusselator systems (17) and (18) is defined by

$$\begin{cases} e_x = x_2 + x_1 \\ e_y = y_2 + y_1 \end{cases} \tag{19}$$

We note that the errors $e_x \to 0$ and $e_y \to 0$ if and only if $x_2 \to -x_1$ and $y_2 \to -y_1$. Thus, when the identical Brusselator chemical reaction systems (17) and (18) are anti-synchronized, their states will be equal in magnitude, but opposite in sign.

The error dynamics is obtained as

$$\begin{cases} \dot{e}_x = 2a + x_2^2 y_2 + x_1^2 y_1 - (b+1)e_x + u_x \\ \dot{e}_y = be_x - x_2^2 y_2 - x_1^2 y_1 + u_y \end{cases} \tag{20}$$

We take the adaptive control as

$$\begin{cases} u_x = -2\hat{a}(t) - x_2^2 y_2 - x_1^2 y_1 + (\hat{b}(t)+1)e_x - k_x e_x \\ u_y = -\hat{b}(t)e_x + x_2^2 y_2 + x_1^2 y_1 - k_y e_y \end{cases} \tag{21}$$

Substituting (21) into (20), we obtain the closed-loop error dynamics as

$$\begin{cases} \dot{e}_x = 2[a - \hat{a}(t)] - [b - \hat{b}(t)]e_x - k_x e_x \\ \dot{e}_y = [b - \hat{b}(t)]e_x - k_y e_y \end{cases} \tag{22}$$

We define the parameter estimation errors as

$$\begin{cases} e_a(t) = a - \hat{a}(t) \\ e_b(t) = b - \hat{b}(t) \end{cases} \tag{23}$$

In view of (23), we can simplify the closed-loop error dynamics (22) as

$$\begin{cases} \dot{e}_x = 2e_a - e_b e_x - k_x e_x \\ \dot{e}_y = e_b e_x - k_y e_y \end{cases} \tag{24}$$

Differentiating (23) with respect to time, we get

$$\begin{cases} \dot{e}_a(t) = -\dot{\hat{a}}(t) \\ \dot{e}_b(t) = -\dot{\hat{b}}(t) \end{cases} \tag{25}$$

Next, we consider the candidate Lyapunov function given by

$$V(e_x, e_y, e_a, e_b) = \frac{1}{2}\left(e_x^2 + e_y^2 + e_a^2 + e_b^2\right) \tag{26}$$

Differentiating V along the trajectories of (24) and (25), we obtain

$$\dot{V} = -k_x e_x^2 - k_y e_y^2 + e_a\left[2e_x - \dot{\hat{a}}\right] + e_b\left[e_x(e_y - e_x) - \dot{\hat{b}}\right] \tag{27}$$

In view of (27), we take the parameter estimates as follows:

$$\begin{cases} \dot{\hat{a}} = 2e_x \\ \dot{\hat{b}} = e_x(e_y - e_x) \end{cases} \tag{28}$$

Theorem 1. *The identical Brusselator chemical reaction systems (17) and (18) with unknown system parameters are globally and exponentially anti-synchronized for all initial states by the adaptive feedback control law (21) and the parameter update law (28), where* k_x, k_y *are positive gain constants.*

Proof. The quadratic Lyapunov function V defined by Eq. (26) is a positive definite function on R^4.

Substituting the parameter update law (28) into (27), the time-derivative of V is obtained as

$$\dot{V} = -k_x e_x^2 - k_y e_y^2, \tag{29}$$

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

Thus, by Lyapunov stability theory [52], we conclude that the anti-synchornization 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

We take the gain constants as $k_x = 30$ and $k_y = 30$. We take $\alpha = 1$ and $\beta = 2$.
We take the parameters as $a = 1$ and $b = 4$. Also, we take $\hat{a}(0) = 2.3$ and $\hat{b}(0) = 10.5$.
The initial state of the master system (17) is taken as $x_1(0) = 5.2$ and $y_1(0) = 4.3$.
The initial state of the slave system (18) is taken as $x_2(0) = 1.8$ and $y_2(0) = 3.2$.

Figures 2-3 show the anti-synchronization of the Brusselator chemical reactions systems (17) and (18). Figure 4 shows the time-history of the anti-synchronization errors e_1, e_2.

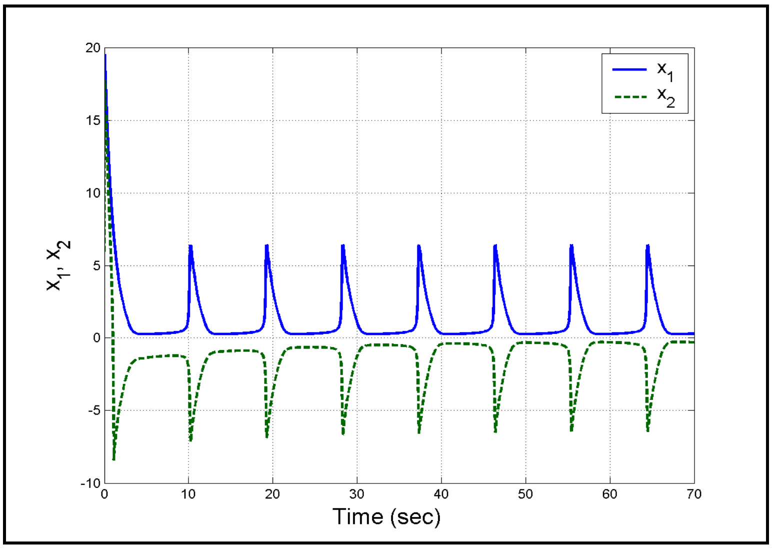

Figure2. Anti-synchronization of the states x_1 and x_2 of Brusselator chemical reaction systems

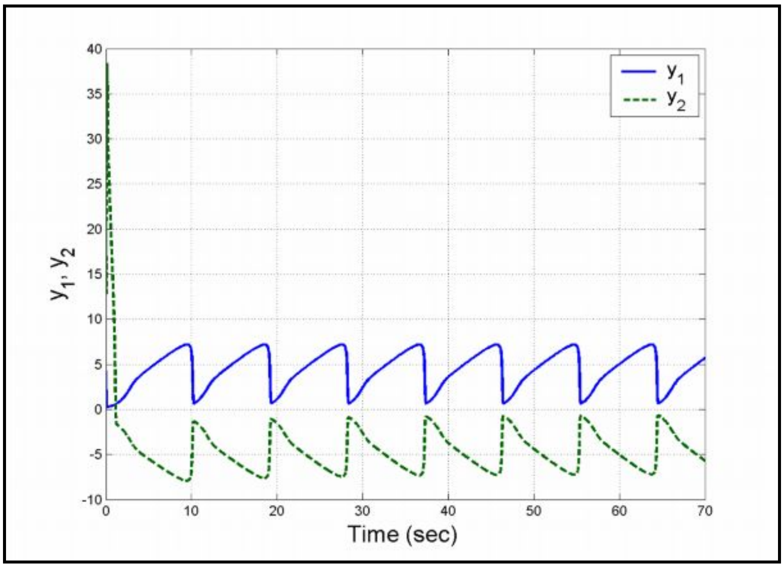

Figure3.Anti-synchronization of the states y_1 and y_2 of Brusselator chemical reaction systems

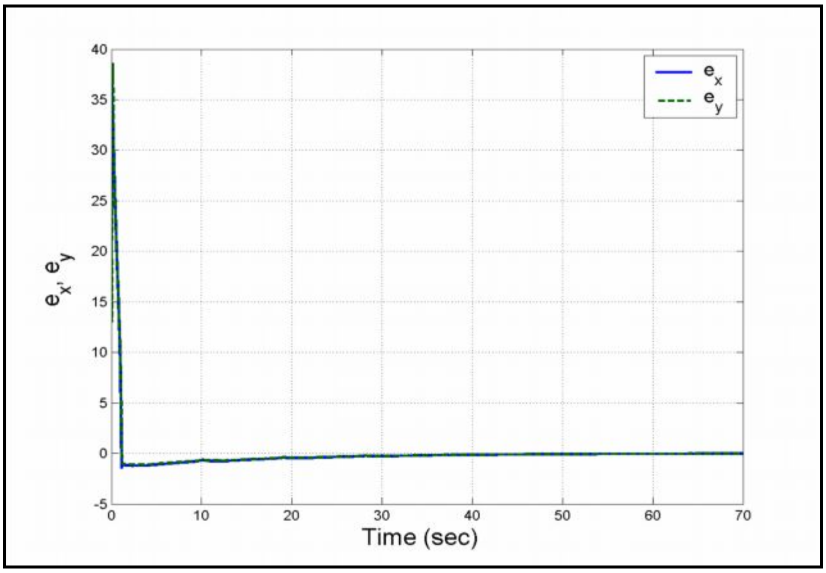

Figure4.Time-history of the anti-synchronization errors e_1, e_2

Conclusions

In this paper, new results have been derived for the analysis and adaptive anti-synchronization 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 anti-synchronization of identical Brusselator chemical reaction systems. The main results have been proved using Lyapunov stability theory and numerical simulations have been illustrated using MATLAB.

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