Dynamical Behavior And Synchronization Of Chaotic Chemical Reactors Model

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Abstract In this paper, we discuss the dynamical properties of a chemical reactor model including Lyapunov exponents, bifurcation, stability of equilibrium and chaotic attractors as well as necessary conditions for this system to generate chaos. We study the synchronization of chemical reactors model via sliding mode control scheme. The stability of this proposed method is proved by Barbalate’s lemma. Numerical Simulation is provided for illustration and verification of the proposed method.

Keywords Chemical reactor · chaos · synchronization · sliding mode.

1. Introduction

Chaos, is an interesting phenomenon in nonlinear dynamical systems, has been studied over the last four decades [2, 16, 20, 23, 24, 31, 32]. Chaotic and hyperchaotic systems are nonlinear deterministic systems that displays complex and unpredictable behavior. Also these systems are sensitive respect to initial conditions. The chaotic and hyperchaotic systems have many important fields in applied nonlinear sciences, such as laser physics, secure communications, nonlinear circuits, control, neural networks, and active wave propagation [3, 4, 7, 13, 16, 17, 22, 25, 29].

The synchronization of chaotic systems has been investigated since its introduction in the paper by Pecora and Carrol in 1990 [24] and has been widely investigated in many fields, such as physics, chemistry, ecological science and secure communications [5, 14, 31]. Various techniques and methods have been proposed to achieve chaos synchronization and anti-synchronization such as adaptive control [9, 19, 30], adaptive sliding mode control [26], sliding mode control [33], active control [10] and nonlinear control [1]. Fortunately,
some existing methods of synchronizing can be generalized to anti-synchronization chaotic systems. Recently synchronization of chaotic complex systems studied in [21].

Dynamics of chemical reactors model has been studied in [11, 12]. The chaotic behavior of chemical reactor model has been studied in [15] by means of computer assisted proof. Synchronization of two identical chemical reactors model has been obtained via linear feedback controller in [28].

We study dynamical qualitative behavior of chemical reactor model. For this purpose, we verify the stability of fixed points and characteristic of chaos for proposed model. We apply sliding mode to synchronization of the model.

This paper is organized as follows: In section 2, the dynamical properties of chemical reactor model including Lyapunov exponents, bifurcations and stability of equilibria, will be discussed. We using sliding mode control method for chaos synchronization of two identical chemical reactors model in section 3. By using the Barbalate's lemma, proved that the error system is asymptotically stable in origin. In section 4, numerical simulations are computed to check the analytical expressions. Our concluding remarks are presented in section 5.

2. Chaotic Chemical Reactor Model

Chemical dynamics in a well-stirred reactor provides one of the most clear-cut examples of complex non-equilibrium behavior, since it can generate deterministic chaos from the intrinsic nonlinearities of the dynamics. Since this form of chaos is amenable to a small number of macro variables, one may reasonably expect that it constitutes an ideal case study for understanding the passage from microscopic to macroscopic behavior [12]. Chaotic dynamics is characterized by its sensitivity to initial conditions and is sensitive to external disturbances. Questions such as chaotic dynamics amplify internal noises and destroy the macroscopic description, and what the deterministic chemical chaos would become in the picture of a microscopic description beyond the phenomenological kinetics, are of much interest.

An interesting chemical system is established in [12], which is described by following relations:

\[
A_1 + X \xleftrightarrow{k_1} 2X, \quad X + Y \xleftrightarrow{k_2} 2Y, \quad A_5 + Y \xleftrightarrow{k_3} A_2, \quad X + Z \xleftrightarrow{k_4} A_3, \quad A_4 + Z \xleftrightarrow{k_5} 2Z, 
\]

where \(A_1, A_4\) and \(A_5\) are initiators, \(A_2\) and \(A_3\) are products. The corresponding nonlinear dynamic system is introduced, as follow:
\[
\begin{align*}
\dot{x} &= a_1 x - k_{-1} x^2 - xy - xz \\
\dot{y} &= xy - a_5 y \\
\dot{z} &= a_4 z - xz - k_{-5} z^2,
\end{align*}
\]

(2.1)

where \(x, y\) and \(z\) are positive functions, and \(a_1, a_4, a_5, k_{-1}\) and \(k_{-5}\) are positive parameters. Now we discuss some properties of (2.1).

The equilibrium points of system (2.1) can be found by solving the following equations:

\[
\begin{align*}
a_1 x - k_{-1} x^2 - xy - xz &= 0 \\
xy - a_5 y &= 0 \\
a_4 z - xz - k_{-5} z^2 &= 0.
\end{align*}
\]

(2.2)

Applying Groebner basis and elimination theory [8], equilibrium points of (2.1) are obtained:

\[
\begin{align*}
E_1 &= (0,0,0) & E_2 &= (a_5, a_1 - a_5 k_{-1}, 0) \\
E_3 &= \left(\frac{a_1}{k_{-1}}, 0, 0\right) & E_4 &= \left(\frac{-a_4 + k_{-5} a_1 - k_{-5} a_5 k_{-1} + a_5}{k_{-5}}, \frac{a_4 - a_5}{k_{-5}}\right) \\
E_5 &= (0,0, \frac{a_4}{k_{-5}}) & E_6 &= \left(\frac{-a_4 + k_{-5} a_1}{-1 + k_{-5} k_{-1}}, 0, \frac{a_4 k_{-1} - a_1}{-1 + k_{-5} k_{-1}}\right).
\end{align*}
\]

(2.3)

The Jacobian matrix of system (2.1) is:

\[
J = \begin{bmatrix}
  a_1 - 2k_{-1} x - y - z & -x & -x \\
  y & -a_5 & 0 \\
  -z & 0 & a_4 - x - 2k_{-5} z
\end{bmatrix}.
\]

(2.4)

The eigenvalues of \(J\) at \(E_i (i = 1, 2, \ldots, 6)\) for and \(a_1 = 30, a_4 = 16.5, a_5 = 10, k_{-1} = 0.5\) and \(k_{-5} = 0.5\) are:

\[
\begin{align*}
\lambda_{E_1} &= (-10, 16.5, 30) & \lambda_{E_2} &= (-7.5 + i15.612, -7.5 - i15.612, -6.5) \\
\lambda_{E_3} &= (-30, -10, -43.5) & \lambda_{E_4} &= (1.186, -11.343 + 5.978, -11.343 - 5.978) \\
\lambda_{E_5} &= (-16.5, -3, -10) & \lambda_{E_6} &= (50.25 + i3.526, 50.25 - i3.526, -10).
\end{align*}
\]

(2.5)

So \(E_1, E_2, E_4\) and \(E_6\) are locally unstable equilibrium points, \(E_3\) and \(E_5\) are locally stable. Figure 1, 2 show that the Lyapunov exponents and bifurcations of chemical reactors system (2.1) for \(a_4 = 16.5, a_5 = 10, k_{-1} = 0.5, k_{-5} = 0.5\) and \(28 < a_1 < 42\), with initial conditions \(x(0) = 5, y(0) = 17\) and \(z(0) = 0.3\). This means that system (2.1) for
the some values of $a_1$ is a chaotic system, since one of its Lyapunov exponents, is positive. Also it is a dissipative system, because sum of its Lyapunov exponents is negative. Figure 3 shows the attractors diagrams of system (2.1). The attractors are bounded but not a fixed point or limit cycle. It is a property of chaotic systems [6].

![Lyapunov Exponents](image)

**Figure 1:** Lyapunov exponents of (2.1), for $a_4 = 16.5$, $a_5 = 10$, $k_{-1} = 0.5$, $k_{-5} = 0.5$ and $28 < a_1 < 42$, with initial conditions $x(0) = 5,y(0) = 17$ and $z(0) = 0.3$.

### 3. Synchronization Via Sliding Mode Control

For synchronization, assume the drive and response systems are defined as follow:

\[
\begin{align*}
\dot{x} &= f(x), \\
\dot{y} &= g(y) + u,
\end{align*}
\]

where $x = (x_1,x_2,\ldots,x_n)^T$, $y = (y_1,y_2,\ldots,y_n)^T \in \mathbb{R}^n$ are the state vectors of the systems (3.1) and (3.2), and $u = (u_1,u_2,\ldots,u_n)^T$ is an $n$-dimensional control signal. Let $e = y - x$, is the error of synchronization. Then, the error dynamical system between drive and response systems is:

\[
\dot{e} = \dot{y} - \dot{x} = g(y) - f(x) + u = g(e + x) - f(x) + u.
\]
The goal is to design an appropriate sliding mode controller $u$ such that for any initial condition $x_0$ and $y_0$, we have:
\[
\lim_{t\to\infty} \|e\| = \lim_{t\to\infty} \|y(t) - x(t)\| = 0,
\]
where $\|\cdot\|$ is the Euclidean norm.

For studying chaos synchronization of chemical reactor model for parameter values $a_1 = 30$, $a_4 = 16.5$, $a_5 = 10$, $k_{-1} = 0.5$ and $k_{-5} = 0.5$ which generates chaotic behavior. We use the idea of sliding mode control technique for synchronization of two identical chaotic systems and stability obtained by Barbalate's lemma [18, 24, 27].

Our aim is to design a controller and make the response system follow the drive system, until they ultimately become the same. Let, the drive and response systems are defined as follow:
\[
\begin{array}{l}
\dot{x}_1 = a_1 x_1 - k_{-1} x_1^2 - x_1 y_1 - x_1 z_1 \\
\dot{y}_1 = x_1 y_1 - a_5 y_1 \\
\dot{z}_1 = a_4 z_1 - x_1 z_1 - k_{-5} z_1^2 \\
\end{array}
\] (3.4)

and

\[
\begin{array}{l}
\dot{x}_2 = a_1 x_2 - k_{-1} x_2^2 - x_2 y_2 - x_2 z_2 + u_1 \\
\dot{y}_2 = x_2 y_2 - a_5 y_2 + u_2 \\
\dot{z}_2 = a_4 z_2 - x_2 z_2 - k_{-5} z_2^2 + u_3 ,
\end{array}
\] (3.5)

where \( u_1, u_2 \) and \( u_3 \) are control functions. We discuss the synchronization via sliding mode control. Let \( e_x = x_2 - x_1 \), \( e_y = y_2 - y_1 \) and \( e_z = z_2 - z_1 \). Then the error dynamical system of (3.4) and (3.5) is:

\[
\begin{array}{l}
\dot{e}_x = e_x[a_1 - 2k_{-1} x_1 - y_1 - z_1 + k_1 e_x - e_y - e_z] + U_1 \\
\dot{e}_y = e_y[e_x + x_1 - a_5] + U_2 \\
\dot{e}_z = e_z[a_4 - x_1 - 2k_{-5} z_1 - e_x - k_{-5} e_z] + U_3 ,
\end{array}
\] (3.6)

**Figure 3.** Attractor of (2.1), for \( a_1 = 30, a_4 = 16.5, a_5 = 10, k_{-1} = 0.5 \) and \( k_{-5} = 0.5 \) with initial conditions \( x(0) = 5, y(0) = 17 \) and \( z(0) = 0.3 \).
where

\[
\begin{align*}
U_1 &= -e_y x_1 - x_2 x_1 + u_1 \\
U_2 &= -e_x y_1 + u_2 \\
U_3 &= -e_x z_1 + u_3.
\end{align*}
\] (3.7)

Sliding mode control [18, 27] is a robust control method. The first step is to select an appropriate sliding surface. The sliding surface can be designed as:

\[
\begin{align*}
s_1(t) &= \lambda_1 e_x(t) \\
s_2(t) &= \lambda_2 e_y(t) \\
s_3(t) &= \lambda_3 e_z(t),
\end{align*}
\] (3.8)

where surface parameters \( \lambda_i \) are positive constants. The next step is to determine an input signal \( U(t) \) to guarantee that the error system trajectories reach to the sliding surface \( s(t) = 0 \). The sliding mode control law is proposed as:

\[
\begin{align*}
U_1 &= -\eta_1 \text{sign}(s_1) \\
U_2 &= -\eta_2 \text{sign}(s_2) \\
U_3 &= -\eta_3 \text{sign}(s_3),
\end{align*}
\] (3.9)

where \( \eta_i, (i = 1, 2, 3) \) are the switching gain and positive. By note that the chaotic properties all states of (3.4) and (3.5) are bounded, then there exist \( L_1, L_2 \) and \( L_3 \) such that:

\[
\begin{align*}
a_1 - 2k_{-1} x_1 - y_1 - z_1 + k_1 e_x - e_y - e_z &< L_1 \\
e_x + x_1 - a_5 &< L_2 \\
a_4 - x_1 - 2k_{-5} z_1 - e_x - k_{-5} e_z &< L_3
\end{align*}
\] (3.11)

We note that \( x_1, y_1 \) and \( z_1 \) are positive and bounded mole functions.

**Theorem 3.1.** Consider the error dynamics (3.6), this system is controlled by \( U(t) \) in (3.9), such that \( \eta_1 = 2L_1 |e_x|, \eta_2 = 2L_2 |e_y| \) and \( \eta_3 = 2L_3 |e_z| \). Then the error system trajectories will converge to the sliding surface \( s(t) = 0 \).

**Proof.** We define the Lyapunov function as follow

\[
V(t) = \sum_1^3 \frac{s_i^2}{2\lambda_i^2}
\] (3.11)

there for
\[ \dot{V} = \sum_{i=1}^{3} \frac{\dot{x}_i^2}{\lambda_i^2} = e_x \dot{e}_x + e_y \dot{e}_y + e_z \dot{e}_z \]
\[ \dot{V} = e_x^2 [a_1 - 2k_x x_1 - y_1 - z_1 + k_1 e_x - e_y - e_z] + e_y^2 [e_x + x_1 - a_5] \]
\[ + e_z^2 [a_4 - x_1 - 2k_z z_1 - e_x - k_z e_z] + e_x \dot{U}_1 + e_y \dot{U}_2 + e_z \dot{U}_3, \]

then
\[ \dot{V} < e_x^2 L_1 + e_y^2 L_2 + e_z^2 L_3 + e_x \dot{U}_1 + e_y \dot{U}_2 + e_z \dot{U}_3 \]
\[ = e_x^2 L_1 + e_y^2 L_2 + e_z^2 L_3 - \eta_1 |e_x| - \eta_2 |e_y| - \eta_3 |e_z|. \]

If we let \( \eta_1 = 2L_1 |e_x|, \) \( \eta_2 = 2L_2 |e_y| \) and \( \eta_3 = 2L_3 |e_z| \) then we have
\[ \dot{V} < -[L_1 e_x^2 + L_2 e_y^2 + L_3 e_z^2] = -L |s| = -\omega(t) \leq 0 \]

where \( L |s| = \omega(t) \geq 0 \). Integrating equation (3.14) from zero to \( t \) yields:
\[ \begin{cases} V(0) - V(t) \geq 0 \Rightarrow V(0) \geq V(t) \\ V(0) - V(t) > \int_0^t \omega(\tau) d\tau. \end{cases} \]  

Then \( \lim_{t \to \infty} \int_0^t \omega(\tau) d\tau \) exists and is positive. Thus, according to the Barbalate's lemma [18], we have:
\[ \lim_{t \to \infty} \omega(t) = \lim_{t \to \infty} L |s| = 0. \]  

Since \( L \) is greater than zero, (3.16) implies \( s = 0 \). This completes the proof.

\[ \square \]

4. **Numerical Simulation**

To demonstrate and verify the validity of the proposed scheme, we discuss and illustrate the numerical simulations results for synchronization of two identical chaotic chemical reactor model.

For synchronization, systems (3.4) and (3.5) with controllers (3.7) are solved numerically by Maple 16 with Runge-Kutta method of order four.

By assuming \( a_1 = 30, a_4 = 16.5, a_5 = 10, k_x = 0.5, k_z = 0.5 \) and with initial conditions \( x_1(0) = 15, y_1(0) = 17, z_1(0) = 3, x_2(0) = 1, y_2(0) = 5, z_2(0) = 5 \), the proposed system in section 2 is chaotic. Also, we assume the constant parameters in controllers rule are \( L_1 = 0.1, L_2 = 0.5, L_3 = 1 \) and \( \lambda_i (i = 1, 2, 3) \) which are arbitrary positive constant.

The results of chaotic synchronization of two identical chaotic chemical reactor model via sliding mode control are shown in Figure 4. This shows the synchronization of (3.4) and (3.5) is achieved after small time interval. The errors due of synchronization are
plotted in Figure 5. As expected from the above analytical considerations the synchronization errors $e_x$, $e_y$ and $e_z$ converge to zero as $t \to 0$.

**Figure 4.** Synchronization of (3.4) and (3.5) with different initial conditions.

**Figure 5.** Error due synchronization of (3.4) and (3.5) with different initial conditions.
5. **CONCLUSION**

In this paper, we studied the dynamics of a chaotic chemical reactor system. The basic properties of chemical reactor model such as Lyapunov exponents, chaotic attractors, equilibria and their stability was discussed. For synchronization, we used sliding mode controller scheme. Obtained controllers laws were satisfied in Barbalate’s lemma. Numerical simulations were given to show the effectiveness of study method.

**REFERENCES**

