

A Novel Chemical Chaotic Reactor System and its Output Regulation via Integral Sliding Mode Control

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Abstract: Chaos theory has a manifold variety of applications in science and engineering. In this paper, a new chemical chaotic reactor is derived by modifying the chemical chaotic reactor system obtained by the Huang (2005). This paper gives a summary description of the chemical reactor dynamics and the chaos dynamic analysis. Next, new results are obtained for the output regulation of the novel chemical chaotic reactor system. MATLAB plots have been shown to illustrate the phase portraits of the novel chemical chaotic attractor and the output regulation of the novel chemical chaotic reactor system via integral sliding mode control.

Keywords: Chaos, chaotic systems, chemical reactor, chemical engineering, sliding mode control, output regulation, chaos control, stability.

1. Introduction

A dynamical system is called *chaotic* if it satisfies the three properties: boundedness, infinite recurrence and sensitive dependence on initial conditions [1-2]. Chaos theory investigates the qualitative and numerical study of unstable aperiodic behaviour in deterministic nonlinear dynamical systems.

In 1963, Lorenz [3] discovered a 3-D chaotic system when he was studying a 3-D weather model for atmospheric convection. After a decade, Rössler [4] discovered a 3-D chaotic system, which was constructed during the study of a chemical reaction. These classical chaotic systems paved the way to 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 like Sundarapandian systems [11, 12], Vaidyanathan systems [13-43], Pehlivan system [44], Pham system [45], etc.

Recently, there is significant result in the chaos literature in the synchronization of physical and chemical systems. A pair of systems called master and slave systems are considered for the synchronization process and the design goal of anti-synchronization is to devise a feedback mechanism so that the state trajectories of the master and slave systems are equal in magnitude and opposite in sign asymptotically. Because of the butterfly effect which causes exponential divergence of two trajectories of the system starting from nearby initial conditions, the anti-synchronization of chaotic systems is seemingly a challenging research problem.

In control theory, active control method is used when the parameters are available for measurement [46-65]. Adaptive control is a popular control technique used for stabilizing systems when the system parameters are unknown [66-80]. There are also other popular methods available for control and synchronization of systems such as backstepping control method [81-87], sliding mode control method [88-

100], intelligent control [101-110], etc.

Recently, chaos theory is found to have important applications in several areas such as chemistry [111-128], biology [129-160], memristors [161-163], electrical circuits [164], etc.

This paper investigates first the qualitative properties of a chemical chaotic reactor model discovered by Huang in 2005 [165]. Huang derived the chemical reactor model by considering reactor dynamics with five steps (2 reversible and 3 non-reversible). Then a novel chemical chaotic reactor model is derived. The qualitative properties of the novel chemical chaotic reactor model are described. This paper also derives new results for the global chaos control of the novel chemical chaotic reactor model via integral sliding mode method. MATLAB plots are shown to illustrate the phase portraits and global chaos control of the novel chemical chaotic reactor.

2. Huang's Chemical Chaotic Reactor

The well-stirred chemical reactor dynamics of Huang and Yang [165] consist of the following five steps given below.



Equations (1a) and (1e) indicate reversible steps, while equations (1b), (1c) and (1d) indicate non-reversible steps of the Huang chemical reactor [165]. In (1), A_1, A_4, A_5 are initiators and A_2, A_3 are products. The intermediates whose dynamics are followed are X, Y and Z .

Assuming an ideal mixture and a well-stirred reactor, the macroscopic rate equations for the Huang's chemical reactor can be written in non-dimensionalized form as

$$\begin{cases} \dot{x} = a_1x - k_{-1}x^2 - xy - xz \\ \dot{y} = xy - a_5y \\ \dot{z} = a_4z - xz - k_{-5}z^2 \end{cases} \quad (2)$$

In (2), x, y, z are the mole fractions of X, Y and Z . Also, the rate constants k_1, k_3 and k_5 are incorporated in the parameters a_1, a_4 and a_5 .

To simplify the notations, we rename the constants and express the chemical reactor system (2) as

$$\begin{cases} \dot{x} = ax - px^2 - xy - xz \\ \dot{y} = xy - cy \\ \dot{z} = bz - xz - qz^2 \end{cases} \quad (3)$$

The system (3) is *chaotic* when the system parameters are chosen as

$$a = 30, \quad b = 16.5, \quad c = 10, \quad p = 0.5, \quad q = 0.5 \quad (4)$$

For numerical simulations, we take the initial conditions

$$x(0) = 1.8, \quad y(0) = 2.5, \quad z(0) = 0.6 \quad (5)$$

The 3-D phase portrait of the chemical chaotic reactor (2) is depicted in Figure 1.

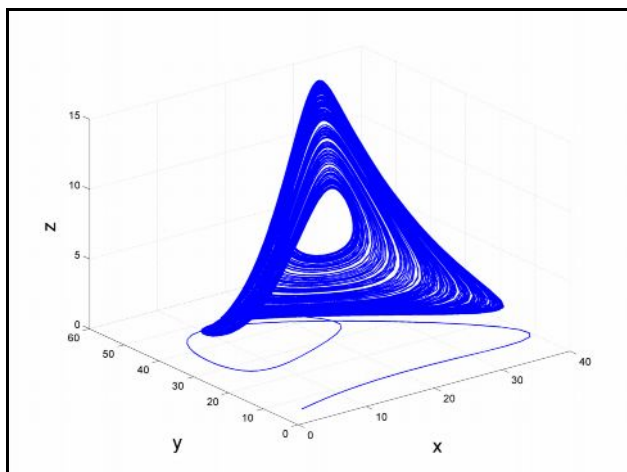


Figure 1. The 3-D phase portrait of the Huang chemical chaotic reactor

The Lyapunov exponents of the Huang's chemical chaotic attractor (3) are derived in MATLAB as

$$L_1 = 0.4001, \quad L_2 = 0, \quad L_3 = -11.8762 \quad (6)$$

Thus, the Lyapunov dimension of the chemical chaotic attractor (3) is deduced as

$$D_L = 2 + \frac{L_1 + L_2}{|L_3|} = 2.0337 \quad (7)$$

3. A Novel Chemical Chaotic Reactor System

In this section, we propose a novel chemical chaotic reactor system by modifying Huang's system (3) as

$$\begin{cases} \dot{x} = ax - px^2 - xy - xz \\ \dot{y} = xy + rx - cy \\ \dot{z} = bz - xz - qz^2 \end{cases} \quad (8)$$

The novel 3-D system (8) is *chaotic* when the parameter values are taken as

$$a = 30, \quad b = 16.5, \quad c = 10, \quad p = 0.5, \quad q = 0.5, \quad r = 0.01 \quad (9)$$

For numerical simulations, we take the initial conditions

$$x(0) = 0.1, \quad y(0) = 0.2, \quad z(0) = 0.1 \quad (10)$$

The 3-D phase portrait of the novel chemical chaotic reactor (8) is depicted in Figure 2. The 2-D projections of the strange attractor of the novel chemical reactor (8) on the (x, y) , (y, z) and (x, z) coordinate planes are depicted in Figures 3-5, respectively.

The Lyapunov exponents of the novel chemical chaotic reactor (8) are obtained as

$$L_1 = 0.4354, \quad L_2 = 0, \quad L_3 = -11.9273 \quad (11)$$

Also, the Lyapunov dimension of the novel chemical chaotic reactor (8) is obtained as

$$D_L = 2 + \frac{L_1 + L_2}{|L_3|} = 2.0365 \quad (12)$$

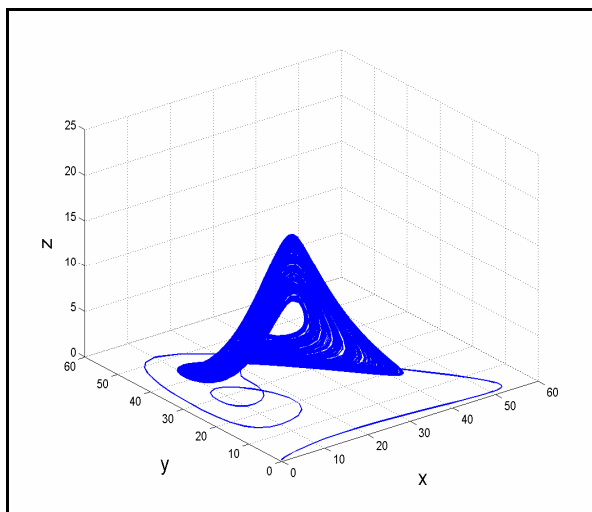


Figure 2. The 3-D phase portrait of the novel chemical chaotic reactor (8)

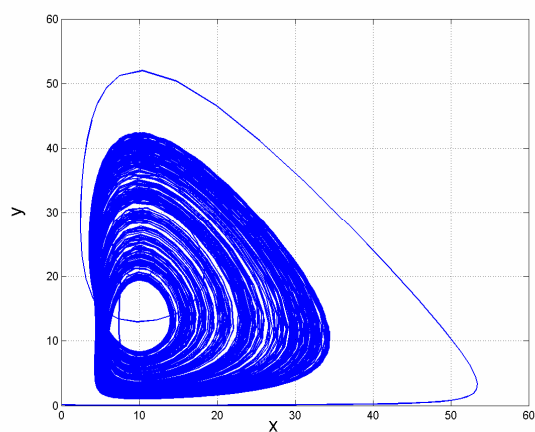


Figure 3. The 2-D projection of the novel chemical chaotic reactor (8) on the (x, y) plane

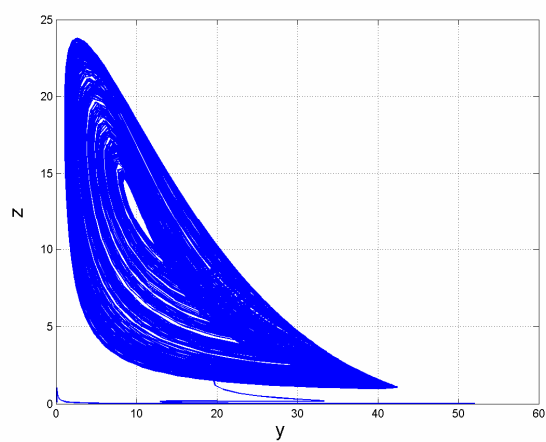


Figure 4. The 2-D projection of the novel chemical chaotic reactor (8) on the (y, z) plane

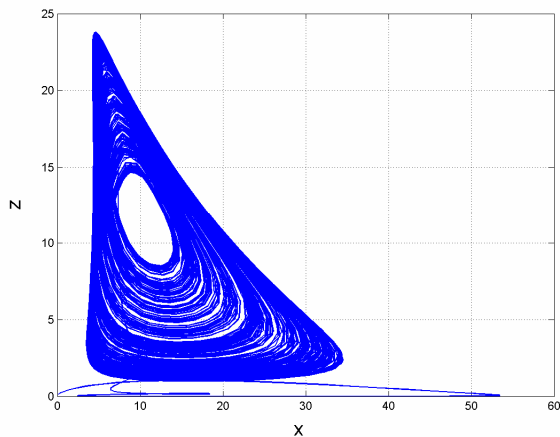


Figure 5. The 2-D projection of the novel chemical chaotic reactor (8) on the (x, z) plane

4. Output Regulation of the Novel Chemical Chaotic Reactor

In this section, we use integral sliding mode control method to regulate the states of the novel chemical chaotic reactor with unknown system parameters. We use Lyapunov stability theory to prove the main result derived in this section.

Thus, we consider the novel chemical reactor dynamics given by

$$\begin{cases} \dot{x} = ax - px^2 - xy - xz + u_x \\ \dot{y} = xy + rx - cy + u_y \\ \dot{z} = bz - xz - qz^2 + u_z \end{cases} \quad (13)$$

In (13), x, y, z are the states of the system. The design goal is to find feedback controls u_x, u_y, u_z so that the system states x, y, z are regulated to the reference values $\alpha_x, \alpha_y, \alpha_z$, respectively.

Thus, the regulation errors are defined by

$$\begin{cases} e_x(t) = x(t) - \alpha_x \\ e_y(t) = y(t) - \alpha_y \\ e_z(t) = z(t) - \alpha_z \end{cases} \quad (14)$$

The error dynamics is obtained as

$$\begin{cases} \dot{e}_x = ax - px^2 - xy - xz + u_x \\ \dot{e}_y = xy + rx - cy + u_y \\ \dot{e}_z = bz - xz - qz^2 + u_z \end{cases} \quad (15)$$

Based on the sliding mode control theory [166], the integral sliding surface of each error variable is defined as follows:

$$\begin{cases} s_x = \left[\frac{d}{dt} + \lambda_x \right] \left[\int_0^t e_x(\tau) d\tau \right] & e_x + \lambda_x \int_0^t e_x(\tau) d\tau \\ s_y = \left[\frac{d}{dt} + \lambda_y \right] \left[\int_0^t e_y(\tau) d\tau \right] & e_y + \lambda_y \int_0^t e_y(\tau) d\tau \\ s_z = \left[\frac{d}{dt} + \lambda_z \right] \left[\int_0^t e_z(\tau) d\tau \right] & e_z + \lambda_z \int_0^t e_z(\tau) d\tau \end{cases} \quad (16)$$

The derivative of each equation in (16) yields

$$\begin{cases} \dot{s}_x = \dot{e}_x + \lambda_x e_x \\ \dot{s}_y = \dot{e}_y + \lambda_y e_y \\ \dot{s}_z = \dot{e}_z + \lambda_z e_z \end{cases} \quad (17)$$

The Hurwitz condition is satisfied if $\lambda_x, \lambda_y, \lambda_z$ are positive constants.

Based on the exponential reaching law [166], we set

$$\begin{cases} \dot{s}_x = -\eta_x \operatorname{sgn}(s_x) - k_x s_x \\ \dot{s}_y = -\eta_y \operatorname{sgn}(s_y) - k_y s_y \\ \dot{s}_z = -\eta_z \operatorname{sgn}(s_z) - k_z s_z \end{cases} \quad (18)$$

Comparing equations (17) and (18), we get

$$\begin{cases} \dot{e}_x + \lambda_x e_x & -\eta_x \operatorname{sgn}(s_x) - k_x s_x \\ \dot{e}_y + \lambda_y e_y & -\eta_y \operatorname{sgn}(s_y) - k_y s_y \\ \dot{e}_z + \lambda_z e_z & -\eta_z \operatorname{sgn}(s_z) - k_z s_z \end{cases} \quad (19)$$

Using Eq. (15), we can rewrite Eq. (19) as follows:

$$\begin{cases} ax - px^2 - xy - xz + u_x + \lambda_x e_x & -\eta_x \operatorname{sgn}(s_x) - k_x s_x \\ xy + rx - cy + u_y + \lambda_y e_y & -\eta_y \operatorname{sgn}(s_y) - k_y s_y \\ bz - xz - qz^2 + u_z + \lambda_z e_z & -\eta_z \operatorname{sgn}(s_z) - k_z s_z \end{cases} \quad (20)$$

From Eq. (20), the control laws are obtained as follows:

$$\begin{cases} u_x = -ax + px^2 + xy + xz - \lambda_x e_x - \eta_x \operatorname{sgn}(s_x) - k_x s_x \\ u_y = -xy - rx + cy - \lambda_y e_y - \eta_y \operatorname{sgn}(s_y) - k_y s_y \\ u_z = -bz + xz + qz^2 - \lambda_z e_z - \eta_z \operatorname{sgn}(s_z) - k_z s_z \end{cases} \quad (21)$$

Next, we state and prove the main result of this section.

Theorem 1. The states x, y, z of the novel chemical chaotic reactor (13) are regulated to track the constant reference signals $\alpha_x, \alpha_y, \alpha_z$, respectively as $t \rightarrow \infty$ for all initial conditions $(x(0), y(0), z(0)) \in R^3$ by the integral sliding mode control law (21), where the constants $\lambda_x, \lambda_y, \lambda_z, \eta_x, \eta_y, \eta_z, k_x, k_y, k_z$ are all positive.

Proof. This result is proved using Lyapunov stability theory [167].

We consider the following quadratic Lyapunov function

$$V(s_x, s_y, s_z) = \frac{1}{2} (s_x^2 + s_y^2 + s_z^2) \quad (22)$$

where s_x, s_y, s_z are as defined in (16).

The time-derivative of V is obtained as

$$\dot{V} = s_x \dot{s}_x + s_y \dot{s}_y + s_z \dot{s}_z \quad (23)$$

Substituting from Eq. (18) into (23), we get

$$\dot{V} = s_x[-\eta_x \operatorname{sgn}(s_x) - k_x s_x] + s_y[-\eta_y \operatorname{sgn}(s_y) - k_y s_y] + s_z[-\eta_z \operatorname{sgn}(s_z) - k_z s_z] \quad (24)$$

Simplifying Eq. (24), we obtain

$$\dot{V} = -\eta_x |s_x| - k_x s_x^2 - \eta_y |s_y| - k_y s_y^2 - \eta_z |s_z| - k_z s_z^2 \quad (25)$$

Since $k_x, k_y, k_z > 0$ and $\eta_x, \eta_y, \eta_z > 0$, it follows from (25) that \dot{V} is a negative definite function.

Thus, by Lyapunov stability theory [167], it follows that $(s_x, s_y, s_z) \rightarrow (0, 0, 0)$ as $t \rightarrow \infty$.

Hence, it is immediate that $(e_x, e_y, e_z) \rightarrow (0, 0, 0)$ as $t \rightarrow \infty$.

This completes the proof. ■

5. Numerical Simulations

We use classical fourth-order Runge-Kutta method in MATLAB with step-size $h = 10^{-8}$ for solving the system of differential equations (13) when the integral sliding mode controller (21) is implemented.

The parameter values of the novel chemical reactor (13) are taken as in the chaotic case, viz.

$$a = 30, \quad b = 16.5, \quad c = 10, \quad p = 0.5, \quad q = 0.5, \quad r = 0.01 \quad (26)$$

We take the sliding constants as

$$\lambda_x = \lambda_y = \lambda_z = 0.1, \quad \eta_x = \eta_y = \eta_z = 0.1, \quad k_x = k_y = k_z = 25 \quad (27)$$

We take the initial conditions of the novel chemical reactor (13) as

$$x(0) = 2.6, \quad y(0) = 5.9, \quad z(0) = 0.8 \quad (28)$$

We take the constant reference signals as

$$\alpha_x = 1, \quad \alpha_y = 2, \quad \alpha_z = 3 \quad (29)$$

Figure 6 shows the output regulation of the novel chemical reactor (13).

Figure 7 shows the time-history of the output regulation errors e_x, e_y, e_z .

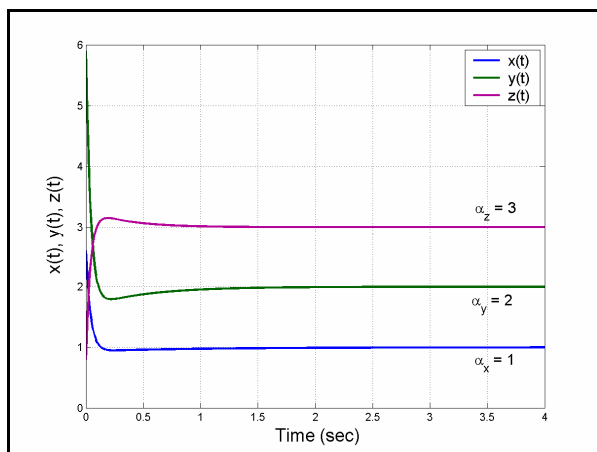


Figure 6. Output regulation of the novel chemical chaotic reactor

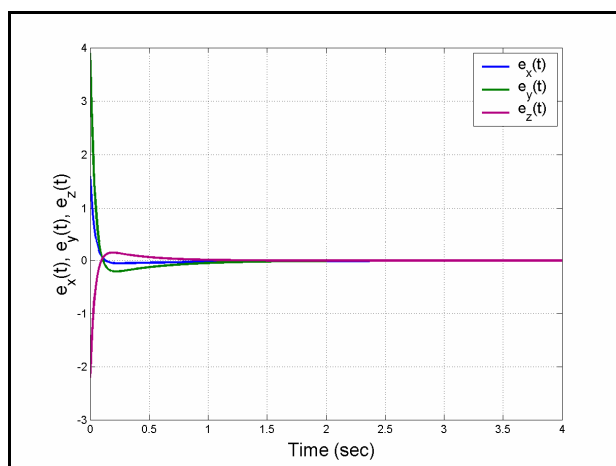


Figure 7. Time-history of the regulation errors $e_x(t), e_y(t), e_z(t)$

6. Conclusions

In this paper, a new chemical chaotic reactor is derived by modifying the chemical chaotic reactor system obtained by the Huang (2005). We gave a summary description of the chemical reactor dynamics and the chaos dynamic analysis. Next, new results were obtained for the output regulation of the novel chemical chaotic reactor system. MATLAB plots were shown to illustrate the phase portraits of the novel chemical chaotic attractor and the output regulation of the novel chemical chaotic reactor system via integral sliding mode control method.

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