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A Novel Chemical Chaotic Reactor System and its Adaptive Control

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Abstract: Chaos theory has a manifold variety of applications in science and engineering. In this paper, new chemical chaotic reactor equations are 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 adaptive control 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 global chaos control of the novel chemical chaotic reactor system via adaptive control method.

Keywords: Chaos, chaotic systems, chemical reactor, adaptive 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 [13-40], Pehlivan system [41], Pham system [42], 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 is to device a feedback mechanism so that the trajectories of the slave system asymptotically track the trajectories of the master system. Because of the butterfly effect which causes exponential divergence of two trajectories of the system starting from nearby initial conditions, the 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 [43-62]. Adaptive control is a popular control technique used for stabilizing systems when the system parameters are unknown [63-76]. There are also other popular methods available for control and synchronization of systems such as backstepping control method [77-83], sliding mode control method [84-95], etc.

Recently, chaos theory is found to have important applications in several areas such as chemistry [96-97], biology [98-100], memristors [101-103], electrical circuits [104], etc.

This paper investigates first the qualitative properties of a chemical chaotic reactor model discovered by

Huang in 2005 [105]. 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 properites 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 adaptive control 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 [105] consist of the following five steps given below.

$$A_1 + X \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} 2X \tag{1a}$$

$$X + Y \xrightarrow{k_2} 2Y \tag{1b}$$

$$A_5 + Y \xrightarrow{k_3} A_2 \tag{1c}$$

$$X + Z \xrightarrow{k_4} A_3 \tag{1d}$$

$$A_4 + Z \underset{k_{-5}}{\overset{k_5}{\rightleftarrows}} 2Z \tag{1e}$$

Equations (1a) and (1e) indicate reversible steps, while equations (1b), (1c) and (1d) indicate non-reversible steps of the Huang chemical reactor [105]. 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

$$\begin{cases} \dot{x} = a_1 x - k_{-1}x^2 - xy - xz \\ \dot{y} = xy - a_5 y \\ \dot{z} = a_4 z - xz - k_{-5}z^2 \end{cases} \tag{2}$$

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

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

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

$$a = 30,\ \ b = 16.5,\ \ c = 10,\ \ p = 0.5,\ \ q = 0.5 \tag{4}$$

For numerical simulations, we take the initial conditions

$$x(0) = 1.8,\ \ y(0) = 2.5,\ \ z(0) = 0.6 \tag{5}$$

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

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

$$L_1 = 0.4001,\ \ L_2 \quad 0,\ \ L_3 \quad -11.8762 \tag{6}$$

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

$$D_L = 2 + \frac{L_1 + L_2}{|L_3|} = 2.0337 \tag{7}$$

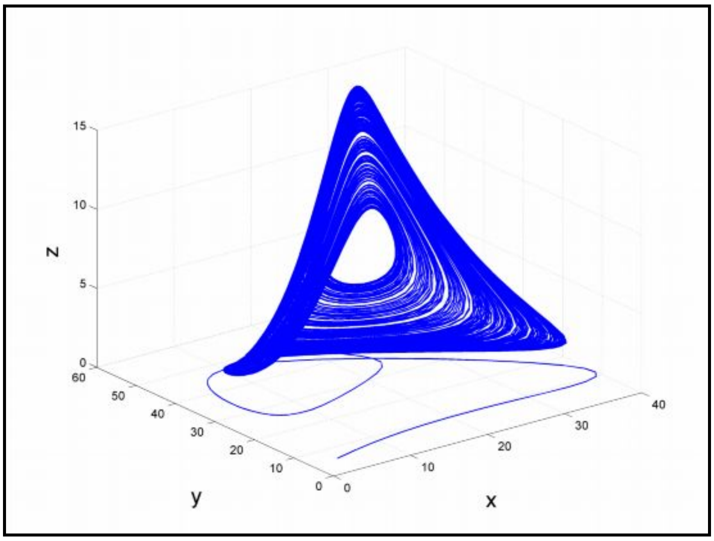

Figure 1. The 3-D phase portrait of the Huang chemical chaotic reactor

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

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

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

$$a = 30, \quad b = 16.5, \quad c = 10, \quad p = 0.5, \quad q = 0.5, \quad r = 0.01 \tag{9}$$

For numerical simulations, we take the initial conditions

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

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

$$L_1 = 0.4354, \quad L_2 \quad 0, \quad L_3 \quad -11.9273 \tag{11}$$

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

$$D_L = 2 + \frac{L_1 + L_2}{|L_3|} = 2.0365 \tag{12}$$

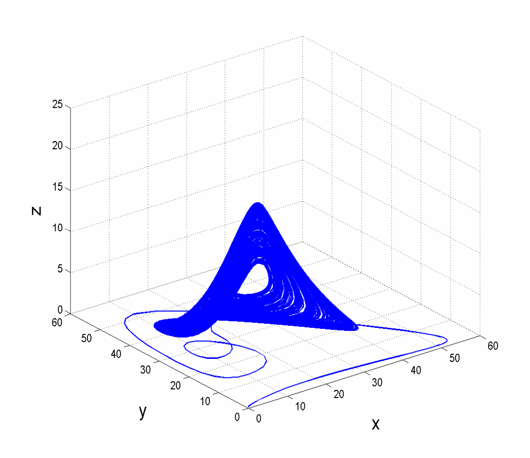

Figure 2. The 3-D phase portrait of the novel chemical chaotic reactor (8)

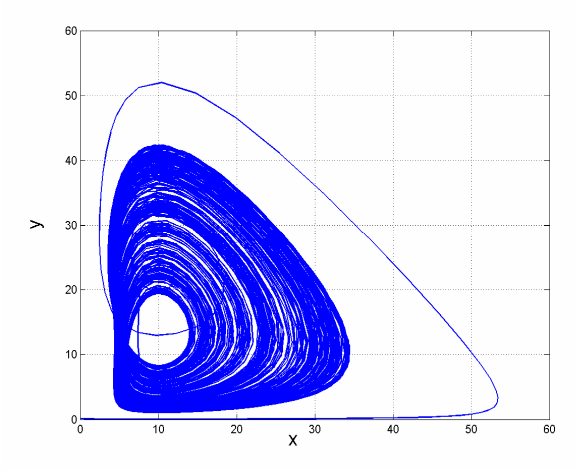

Figure 3. The 2-D projection of the novel chemical chaotic reactor (8) on the (x, y) plane

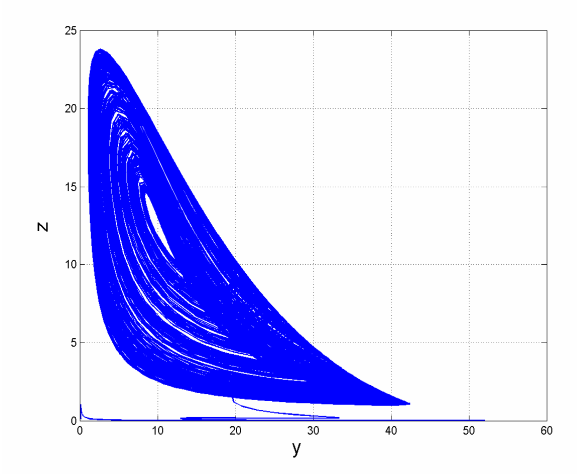

Figure 4. The 2-D projection of the novel chemical chaotic reactor (8) on the (y, z) plane

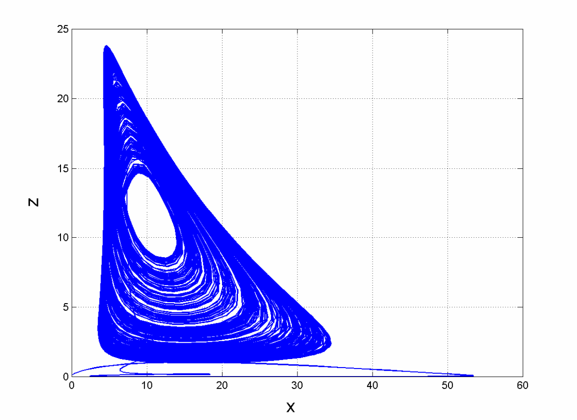

Figure 5. The 2-D projection of the novel chemical chaotic reactor (8) on the (x,z) plane

4. Adaptive Control of the Novel Chemical Chaotic Reactor

In this section, we use adaptive 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

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

In (13), x, y, z are the states of the system. We suppose that the system parameters a, b, c, p, q, r are unknown and use estimates of the parameters to derive the adaptive controls u_x, u_y, u_z. 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 α, β, γ, respectively. Thus, the regulation errors are defined by

$$\begin{cases} e_x = x - \alpha \\ e_y = y - \beta \\ e_z = z - \gamma \end{cases} \tag{14}$$

The error dynamics is obtained as

$$\begin{cases} \dot{e}_x = a(e_x + \alpha) - p(e_x + \alpha)^2 - (e_x + \alpha)(e_y + \beta) - (e_x + \alpha)(e_z + \gamma) + u_x \\ \dot{e}_y = (e_x + \alpha)(e_y + \beta) + r(e_x + \alpha) - c(e_y + \beta) + u_y \\ \dot{e}_z = b(e_z + \gamma) - (e_x + \alpha)(e_z + \gamma) - q(e_z + \gamma)^2 + u_z \end{cases} \tag{15}$$

We consider the adaptive controller defined by

$$\begin{cases} u_x = -\hat{a}(t)(e_x + \alpha) + \hat{p}(t)(e_x + \alpha)^2 + (e_x + \alpha)(e_y + \beta) + (e_x + \alpha)(e_z + \gamma) - k_x e_x \\ u_y = -(e_x + \alpha)(e_y + \beta) - \hat{r}(t)(e_x + \alpha) + \hat{c}(t)(e_y + \beta) - k_y e_y \\ u_z = -\hat{b}(t)(e_z + \gamma) + (e_x + \alpha)(e_z + \gamma) + \hat{q}(t)(e_z + \gamma)^2 - k_z e_z \end{cases} \tag{16}$$

where k_x, k_y, k_z are positive gain constants.

Substituting (16) into (15), we get the closed-loop error dynamics as

$$\begin{cases} \dot{e}_x = [a-\hat{a}(t)](e_x+\alpha)-[p-\hat{p}(t)](e_x+\alpha)^2-k_xe_x \\ \dot{e}_y = [r-\hat{r}(t)](e_x+\alpha)-[c-\hat{c}(t)](e_y+\beta)-k_ye_y \\ \dot{e}_z = [b-\hat{b}(t)](e_z+\gamma)-[q-\hat{q}(t)](e_z+\gamma)^2-k_ze_z \end{cases} \tag{17}$$

We define the parameter estimation errors as

$$\begin{cases} e_a(t)=a-\hat{a}(t) \\ e_b(t)=b-\hat{b}(t) \\ e_c(t)=c-\hat{c}(t) \\ e_p(t)=p-\hat{p}(t) \\ e_q(t)=q-\hat{q}(t) \\ e_r(t)=r-\hat{r}(t) \end{cases} \tag{18}$$

Using (18), the closed-loop system (17) can be simplified as

$$\begin{cases} \dot{e}_x = e_a(e_x+\alpha)-e_p(e_x+\alpha)^2-k_xe_x \\ \dot{e}_y = e_r(e_x+\alpha)-e_c(e_y+\beta)-k_ye_y \\ \dot{e}_z = e_b(e_z+\gamma)-e_q(e_z+\gamma)^2-k_ze_z \end{cases} \tag{19}$$

Differentiating (18) with respect to time, we get

$$\begin{cases} \dot{e}_a(t)=-\dot{\hat{a}}(t) \\ \dot{e}_b(t)=-\dot{\hat{b}}(t) \\ \dot{e}_c(t)=-\dot{\hat{c}}(t) \\ \dot{e}_p(t)=-\dot{\hat{p}}(t) \\ \dot{e}_q(t)=-\dot{\hat{q}}(t) \\ \dot{e}_r(t)=-\dot{\hat{r}}(t) \end{cases} \tag{20}$$

Next, we consider the candidate Lyapunov function defined by

$$V(e_x,e_y,e_z,e_a,e_b,e_c,e_p,e_q,e_r)=\frac{1}{2}\left(e_x^2+e_y^2+e_z^2+e_a^2+e_b^2+e_c^2+e_p^2+e_q^2+e_r^2\right) \tag{21}$$

Differentiating (21) along the trajectories of (19) and (20), we get the following dynamics

$$\begin{aligned} \dot{V} = {} & -k_xe_x^2-k_ye_y^2-k_ze_z^2+e_a\left[e_x(e_x+\alpha)-\dot{\hat{a}}\right]+e_b\left[e_z(e_z+\gamma)-\dot{\hat{b}}\right]+e_c\left[-e_y(e_y+\beta)-\dot{\hat{c}}\right] \\ & +e_p\left[-e_x(e_x+\alpha)^2-\dot{\hat{p}}\right]+e_q\left[-e_z(e_z+\gamma)^2-\dot{\hat{q}}\right]+e_r\left[e_y(e_x+\alpha)-\dot{\hat{r}}\right] \end{aligned} \tag{22}$$

In view of (22), we take the following parameter update law:

$$\begin{cases} \dot{\hat{a}}(t)=e_x\left(e_x+\alpha\right) \\ \dot{\hat{b}}(t)=e_z\left(e_z+\gamma\right) \\ \dot{\hat{c}}(t)=-e_y\left(e_y+\beta\right) \\ \dot{\hat{p}}(t)=-e_x\left(e_y+\beta\right) \\ \dot{\hat{q}}(t)=-e_z\left(e_z+\gamma\right)^2 \\ \dot{e}_r(t)=e_y\left(e_x+\alpha\right) \end{cases} \tag{23}$$

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

Theorem 1. The adaptive control law (16) and the parameter update law (23) achieve global output regulation of the novel chemical chaotic reactor defined by (13), where k_x, k_y, k_z are positive gain constants.

Proof. The result is proved using Lyapunov stability theory [106].

The quadratic Lyapunov function V defined by (21) is positive definite on R^9.

Substituting the parameter update law (23) into (22), we get the time derivative of V as

$$\dot{V} = -k_x e_x^2 - k_y e_y^2 - k_z e_z^2, \tag{24}$$

which is negative semi-definite on R^9.

Thus, by Barbalat's lemma in Lyapunov stability theory [106], it follows that the closed-loop error dynamics (19) is globally exponentially stable.

This completes the proof. ■

5. Numerical Simulations

We use the classical fourth-order Runge-Kutta method with step-size $h = 10^{-8}$ to solve the system of differential equations (13) and (23), when the adaptive control law (16) is implemented.

We take the parameter values of the novel chemical chaotic reactor (13) as in the chaotic case, viz.

$$a = 30, \quad b = 16.5, \quad c = 10, \quad p = 0.5, \quad q = 0.5, \quad r = 0.01 \tag{25}$$

We take the gain constants as $k_x = 6$, $k_y = 6$ and $k_z = 6$.

We take the constant reference signals (set-point values) as $\alpha = 1$, $\beta = 2$ and $\gamma = 3$.

We take the initial values of the chemical chaotic reactor (13) as $x(0) = 5.2$, $y(0) = 11.4$, and $z(0) = 16.7$.

We take the initial values of the parameter estimates as $\hat{a}(0) = 2$, $\hat{b}(0) = 7$, $\hat{c}(0) = 2$, $\hat{p}(0) = 2$, $\hat{q}(0) = 4$ and $\hat{r}(0) = 6$.

Figures 6-8 show the output regulation of the novel chemical chaotic reactor system (13).

Figure 9 shows the time-history of the regulation errors e_x, e_y, e_z.

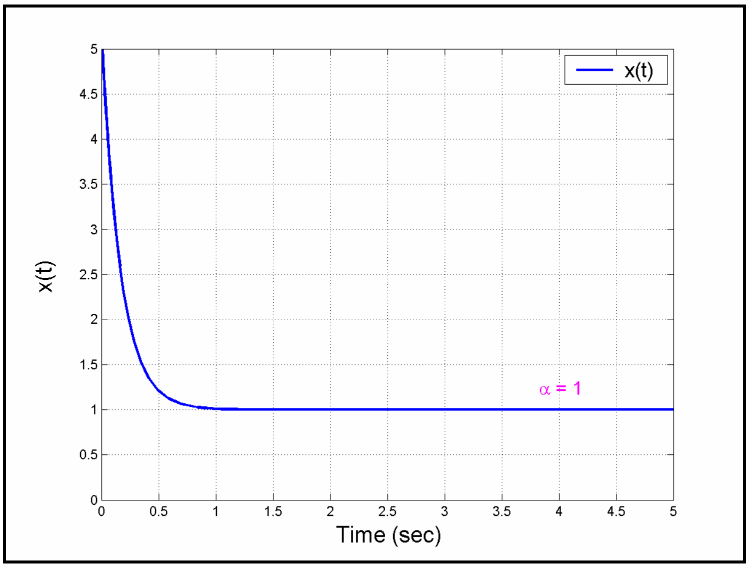

Figure 6. The state $x(t)$ of the novel chemical reactor system tracking $\alpha = 1$

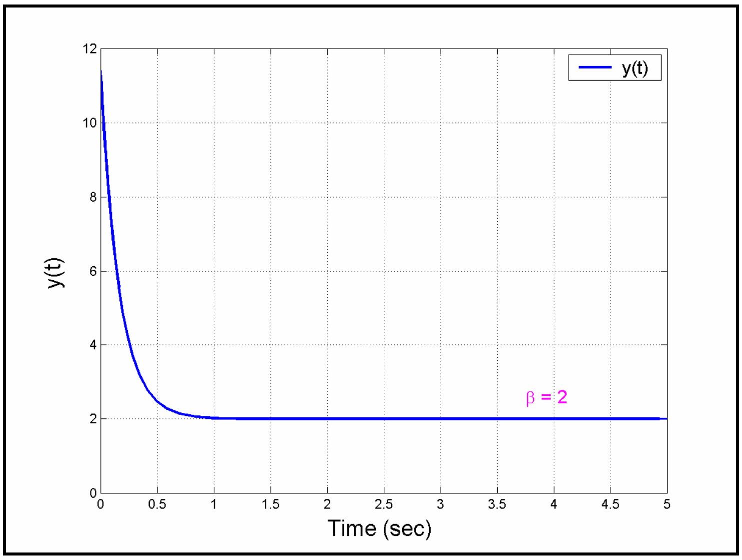

Figure 7. The state $y(t)$ of the novel chemical reactor system tracking $\beta = 2$

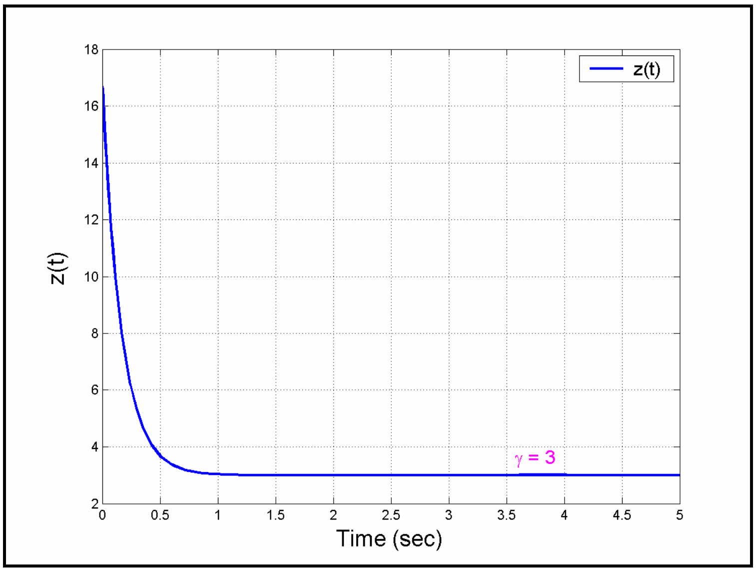

Figure 8. The state $z(t)$ of the novel chemical reactor system tracking $\gamma = 3$

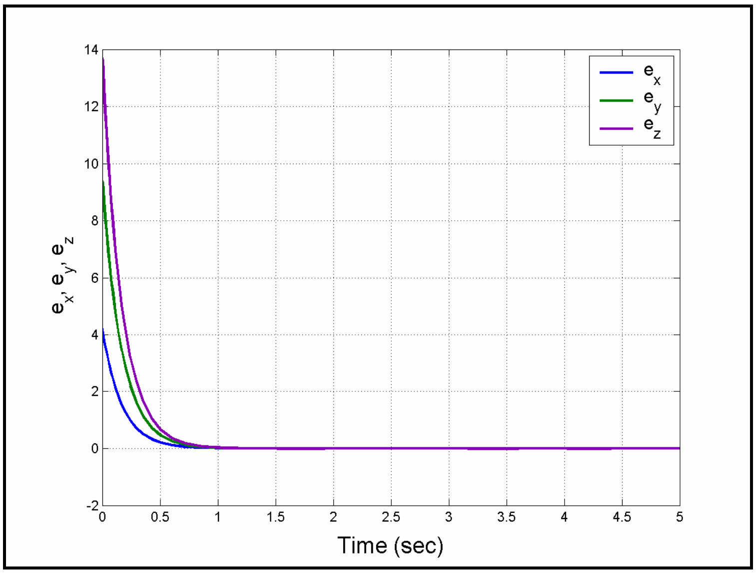

Figure 9. Time-history of the regulation errors $e_x(t), e_y(t), e_z(t)$

6. Conclusions

In this paper, a new chemical chaotic reactor equations are 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 adaptive control of the novel chemical chaotic reactor system. MATLAB plots were shown to illustrate the phase portraits of the novel chemical chaotic attractor and the global chaos control of the novel chemical chaotic reactor system via adaptive control method.

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