Chaos Synchronization of Chemical Models

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Abstract

Chaos synchronization of identical chemical reactors with different initial conditions is investigated by two approaches: linear coupling and a novel coupling which is proposed for the first time. Both approaches are studied under bidirectional and unidirectional schemes. The conditions to achieve stability of synchronization are determined by the Lyapunov theorem for linear coupling method. Also, stability condition is obtained when novel coupling is applied. In each section, numerical simulations are presented to verify the theoretical results.

Keywords: Chemical reactor, chaos synchronization, stability.

1. Introduction

Synchronization of coupled dynamical systems is an important field of nonlinear dynamics. Its effects in oscillators are widely used in chemical reactors (Cruz et al., 2009; Chen, 2008; Kurkina & Kuretuva, 2004). The idea of synchronizing two identical chaotic systems that start with different initial conditions was introduced by Pecora and Carrols (1990). It consists of linking the trajectories of one system to the corresponding trajectories of the other so that they remain in step with each other through the transmission of a signal. A variety of approaches have been proposed for the synchronization of chaotic systems [Lian et al; 2002; Tan et al., 2003; Jiang & Zheng, 2005); However they can be classified into two cases: bidirectional and unidirectional scenarios (Chen et al., 1998). Bidirectional coupling involves the situation wherein the two chaotic systems influence each other mutually. Since this bidirectional coupling is believed to be generic in a majority of natural processes, it has generated utmost interest in the scientific community. However, it is easy to motivate studying the synchronization phenomena under unidirectional coupling as there may exist numerous nonlinear processes that function within the premises of master-slave configuration (Cruz et al., 2009). This will be discussed in the next section.

There are many control techniques to determine coupling terms such that error dynamics converges to zero. A general one is based on negative linear feedback of error dynamics. Moreover there are many nonlinear feedback based synchronization techniques where the coupling terms are nonlinear functions of error dynamics In this paper we use two schemes for coupling: first we start by linear coupling scheme in both bidirectional and unidirectional ways. We prove the stability of error dynamics by the Lyapunov theorem (Slotine & Li, 1991). Then we propose a novel method to couple both unidirectional and bidirectional for synchronization of two identical chaotic chemical reactors. We show that our coupling scheme can synchronize the considered system effectively and in a short time. Also, we study asymptotic stability of error dynamics theoretically. The rest of the paper is organized as follows: Next section is devoted to a brief introduction on synchronization problem. In section 3 the model of a well known chemical reactor is brought in. The chaotic behavior of this model has been studied in (Haung, 2005). Section 4 presents the synchronization problem with linear coupling in unidirectional and bidirectional schemes. In section 5, first the stability of synchronization by a new coupling scheme is shown by simulation. Then validity of the proposed method is revealed by the stability theory. The final section is dedicated to compare the linear coupling and the novel coupling schemes and weakness and advantages of these methods are studied.

2. Synchronization Problem

Consider the following chaotic systems described by

$$\dot{X} = F(X,U), \quad \dot{Y} = F(Y,V)$$

where $X, Y \in R^n$, are the state variables, $U, V \in R^m$, are the control inputs and $F : R^n \times R^m \to R^n$ determines the dynamic of systems. The synchronization is to design U, V such that the states of both systems follow each other asymptotically (Chen et al., 1998). Dynamic of the error of synchronization can be expressed as

$$\dot{E} = F(X,U) - F(Y,V)$$

where $E = X - Y$. The aim of synchronization is to make $\lim_{t\to\infty} \| E \| = 0$ by choosing a suitable U and V .

The bidirectional coupling scheme uses $U = G_1(X,Y)$ and $V = G_2(X,Y)$ where both systems influence each other. If $G_2(X,Y) = -G_1(X,Y) = KE$ where $K = \mathrm{diag}\{\kappa\}$, then the coupling terms are linear. In the unidirectional scheme we utilize $U = 0$ and the second system does not affect the first one. This scheme is often called master-slave configuration.

3. Chemical Reactor Dynamic

The well-stirred chemical reactor dynamic has been studied in (Haung, 2005) which consists of the following five reversible steps

$$A_1 + X \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} 2X, \quad X + Y \underset{k_{-2}}{\overset{k_2}{\rightleftarrows}} 2Y, \quad A_5 + Y \underset{k_{-3}}{\overset{k_3}{\rightleftarrows}} A_2, \quad X + Z \underset{k_{-4}}{\overset{k_4}{\rightleftarrows}} A_3, \quad A_4 + Z \underset{k_{-5}}{\overset{k_5}{\rightleftarrows}} 2Z.$$

Here, A_1, A_4 and A_5 are initiators, A_2 and A_3 are products. The intermediates whose dynamics are followed are X, Y and Z. The corresponding non-dimensionalized dynamical evolution equations read

$$\begin{cases} \dot{x} = (a_1 - k_{-1}x - y - z)x \\ \dot{y} = (x - a_5)y \\ \dot{z} = (a_4 - x - k_{-5}z)z \end{cases} \tag{1}$$

Where x, y and z are positive mole functions, and a_1, a_4, a_5, k_{-1} and k_{-5} are positive parameters.
For the following value of parameters, system (1) is chaotic.

$$a_1 = 30,\ a_4 = 16.5,\ a_5 = 10,\ k_{-1} = 0.5,\ k_{-5} = 0.5 \tag{2}$$

Fig. 1 shows the chaotic trajectory of system (1) with initial conditions $[x(0), y(0), z(0)] = [5,17,0.3]$. Note that the state variables of the system are always nonnegative because of the inherent properties.

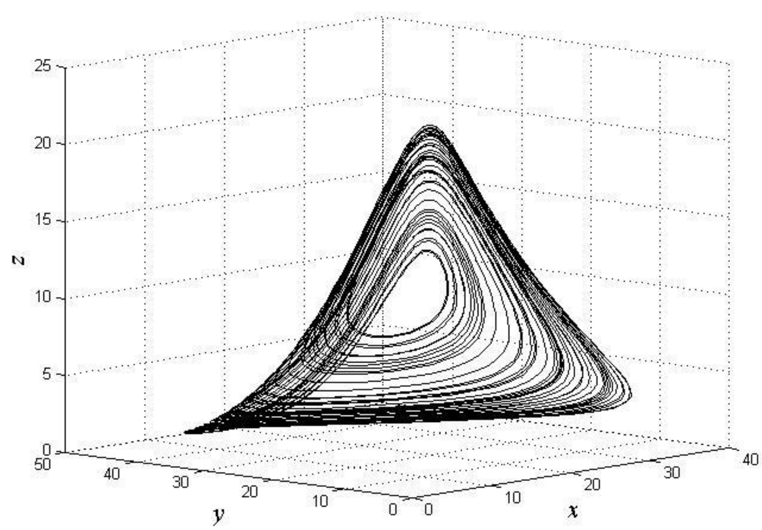

Fig. 1. Chaotic trajectory of system (1) after transition time.

4. Synchronization by Linear Coupling

A. Bidirectional Synchronization

Let us consider two well-Stirred reactors with bidirectional linear coupling as

$$\begin{cases} \dot{x}_1 = (a_1 - k_{-1}x_1 - y_1 - z_1)x_1 + \kappa(x_2 - x_1) \\ \dot{y}_1 = (x_1 - a_5)y_1 + \kappa(y_2 - y_1) \\ \dot{z}_1 = (a_4 - x_1 - k_{-5}z_1)z_1 + \kappa(z_2 - z_1) \end{cases}, \qquad \text{reactor 1} \tag{3}$$

$$\begin{cases} \dot{x}_2 = (a_1 - k_{-1}x_2 - y_2 - z_2)x_2 + \kappa(x_1 - x_2) \\ \dot{y}_2 = (x_2 - a_5)y_2 + \kappa(y_1 - y_2) \\ \dot{z}_2 = (a_4 - x_2 - k_{-5}z_2)z_2 + \kappa(z_1 - z_2) \end{cases}. \qquad \text{reactor 2} \tag{4}$$

Define the components of error vector as

$$e_x = x_1 - x_2, \quad e_y = y_1 - y_2, \quad e_z = z_1 - z_2, \tag{5}$$

The following error dynamic for e_x is

$$\dot{e}_x = (a_1 - k_{-1}x_1 - y_1 - z_1)x_1 - (a_1 - k_{-1}x_2 - y_2 - z_2)x_2 - 2\kappa e_x, \tag{6}$$

this can be simplified as

$$\begin{aligned} \dot{e}_x &= a_1(x_1 - x_2) - k_{-1}(x_1 - x_2)(x_1 + x_2) - 2\kappa e_x \\ &\quad - y_1x_1 + y_1x_2 - y_1x_2 + y_2x_2 - z_1x_1 + z_1x_2 - z_1x_2 + z_2x_2 \\ &= a_1e_x - k_{-1}(x_1 + x_2)e_x - y_1e_x - x_2e_y - z_1e_x - x_2e_z - 2\kappa e_x \\ &= [a_1 - k_{-1}(x_1 + x_2) - (y_1 + z_1) - 2\kappa \quad -x_2 \quad -x_2][e_x \quad e_y \quad e_z]^T \end{aligned}, \tag{7}$$

By similar manipulation we have

$$\dot{e}_y = y_2 e_x - (a_5 + 2\kappa - x_1)e_y, \tag{8}$$

and

$$\dot{e}_z = -z_2e_x - (k_{-5}(z_1 + z_2) - a_4 + 2\kappa + x_1)e_z, \tag{9}$$

Equations (7)-(9) can be summarized in the following system

$$\begin{bmatrix} \dot{e}_x \\ \dot{e}_y \\ \dot{e}_z \end{bmatrix} = \begin{bmatrix} -2\kappa + a_1 - k_{-1}(x_1 + x_2) - (y_1 + z_1) & -x_2 & -x_2 \\ y_2 & -2\kappa - a_5 + x_1 & 0 \\ -z_2 & 0 & -2\kappa + a_4 - k_{-5}(z_1 + z_2) - (x_2 + x_1) \end{bmatrix} \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix}, \tag{10}$$

We have the following theorem.

Theorem 1: The origin of (10) is asymptotically stable if κ is chosen sufficiently large.

Proof: The origin is an equilibrium point for (10) and a suitable Lyapunov function is of the form (Slotine & Li, 1991)

$$V = \tfrac{1}{2}(e_x^2 + e_y^2 + e_y^2), \tag{11}$$

Computing time derivative of V along the trajectories of (10), we find

$$\begin{aligned} \dot{V} &= e_x\dot{e}_x + e_y\dot{e}_y + e_y\dot{e}_z \\ &= -(k_{-1}(x_1 + x_2) + y_1 + z_1 + 2\kappa - a_1)e_x^2 - x_2e_ye_x - x_2e_ze_x + \\ &\quad y_2 e_xe_y - (a_5 + 2\kappa - x_1)e_y^2 - z_2e_xe_z - (k_{-5}(z_1 + z_2) - a_4 + 2\kappa + x_1)e_z^2 \end{aligned} \tag{12}$$

or equivalently

$$\dot{V} = -[e_x \quad e_y \quad e_z]^T Q [e_x \quad e_y \quad e_z], \tag{13}$$

where $Q = [q_{ij}],\ i, j = 1,2,3$ is the following matrix

$$Q = \begin{bmatrix} 2\kappa - a_1 + k_{-1}(x_1 + x_2) + y_1 + z_1 & \frac{x_2 - y_2}{2} & \frac{x_2 + z_2}{2} \\ \frac{x_2 - y_2}{2} & (2\kappa + a_5 - x_1) & 0 \\ \frac{x_2 + z_2}{2} & 0 & 2\kappa - a_4 + k_{-5}(z_1 + z_2) + x_1 \end{bmatrix} \tag{14}$$

To ensure that the origin is asymptotically stable, the matrix Q would be positive definite. This is the case if the following three inequalities hold:

$$q_{11} > 0, \qquad q_{11}q_{22} - q_{12}q_{21} > 0, \qquad \det(Q) > 0, \tag{15}$$

Hence by the first condition on the left of (15) we have $2\kappa - a_1 + k_{-1}(x_1 + x_2) + (y_1 + z_1) > 0$. Since we always have $k_{-1}(x_1 + x_2) + (y_1 + z_1) \geq 0$, a choice for κ independent of states is

$$2\kappa > a_1. \tag{16}$$

Also since a chaotic system has bounded trajectories, there exists a positive constant ℓ, such that

$$0 \leq x_i, y_i, z_i \leq \ell, \qquad i = 1,2,$$

Thus the second inequality in (15) becomes

$$(2\kappa - a_1)(2\kappa + a_5 - \ell) > \ell^2, \tag{17}$$

Similarly the third condition is held if

$$(2\kappa - a_1)(2\kappa + a_5 - \ell)(2\kappa - a_4 - \ell(1 + 2k_{-5})) > \ell^2[(2\kappa + a_5 + \ell) + (2\kappa - a_4 + \ell(1 + 2k_{-5}))], \tag{18}$$

Considering (16)-(18) we may choose sufficiently large κ so that $\dot{V} < 0$ for the error vector $e \neq 0$ and the origin of (10) is asymptotically stable. This completes the proof.■

As a notable feature we know that negativeness of the time derivative of Lyapunov function is a sufficient condition for the stability, i.e. $\dot{V} < 0$ is a conservative condition. So although theorem 1 implies a large coupling strength κ for stability of the origin of error dynamics, systems (3) and (4) are synchronized by the smaller coupling strength κ. Fig. 2 shows the time history of error with $\kappa = 0.5$ where theorem 1 entails $\kappa > 7.5$. There it is demonstrated that error components e_x, e_y and e_z go to zero after a short time.

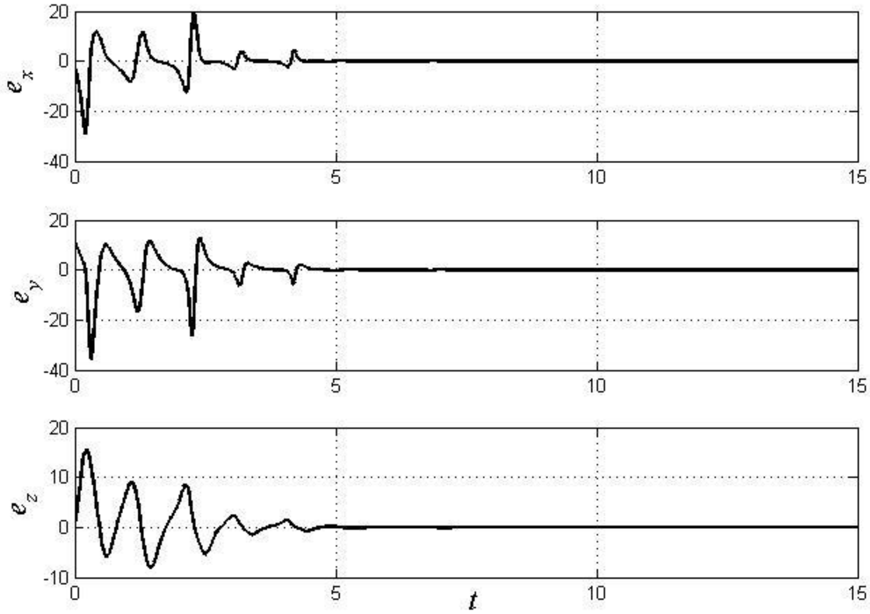

Fig. 2. Time history of error dynamics for linear bidirectional coupling method with $\kappa = 0.5$.

A. Unidirectional Synchronization

Now consider the master-slave configuration of coupled chemical reactors where control signal just apply to slave system which yields

$$\begin{cases} \dot{x}_1 = (a_1 - k_{-1}x_1 - y_1 - z_1)x_1 \\ \dot{y}_1 = (x_1 - a_5)y_1 \\ \dot{z}_1 = (a_4 - x_1 - k_{-5}z_1)z_1 \end{cases}, \quad \text{master reactor}$$

$$\begin{cases} \dot{x}_2 = (a_1 - k_{-1}x_2 - y_2 - z_2)x_2 + \kappa(x_1 - x_2) \\ \dot{y}_2 = (x_2 - a_5)y_2 + \kappa(y_1 - y_2) \\ \dot{z}_2 = (a_4 - x_2 - k_{-5}z_2)z_2 + \kappa(z_1 - z_2) \end{cases}, \quad \text{slave reactor} \tag{19}$$

By the errors defined in (5), we have the same error dynamics as (10) where 2κ is changed into κ. So the stability results are the same as (16)-(18) and theorem 1 remains valid. Fig. 3 shows the trajectories of the error dynamics in phase plane for $\kappa = 0.8$. It reveals stability of the origin of error dynamics.

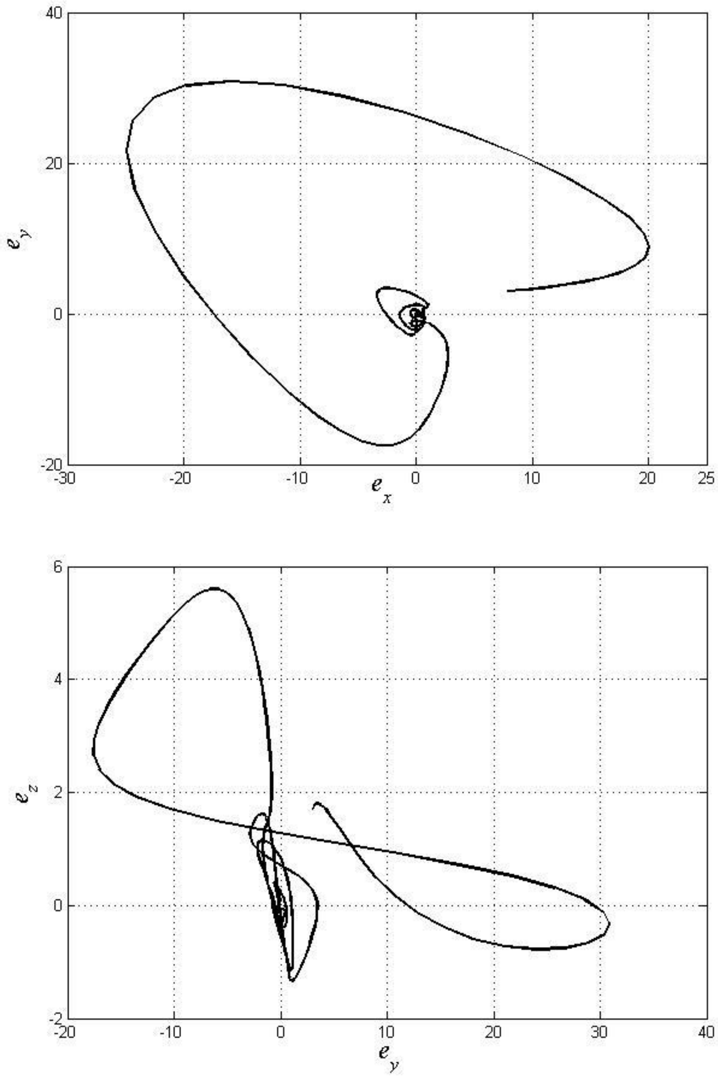

Fig. 3. Phase planes of error dynamics for linear unidirectional coupling method with $\kappa = 0.8$.

5. *Synchronization by Novel Coupling*

A. Bidirectional Synchronization

Again consider the corresponding dynamics of reactors. If we replace $x_2 \leftrightarrow x_1$ in the third equations of reactors then a new coupling systems are obtained as

$$\begin{cases} \dot{x}_1 = (a_1 - k_{-1}x_1 - y_1 - z_1)x_1 \\ \dot{y}_1 = (x_1 - a_5)y_1 \\ \dot{z}_1 = (a_4 - x_2 - k_{-5}z_1)z_1 \end{cases}, \quad \text{new reactor 1} \qquad (20)$$

$$\begin{cases} \dot{x}_2 = (a_1 - k_{-1}x_2 - y_2 - z_2)x_2 \\ \dot{y}_2 = (x_2 - a_5)y_2 \\ \dot{z}_2 = (a_4 - x_1 - k_{-5}z_2)z_2 \end{cases}, \quad \text{new reactor 2} \qquad (21)$$

Both systems (20) and (21) remain chaotic and become synchronized. Fig. 4 shows the state variables of both systems which follow each other after a short transient time.

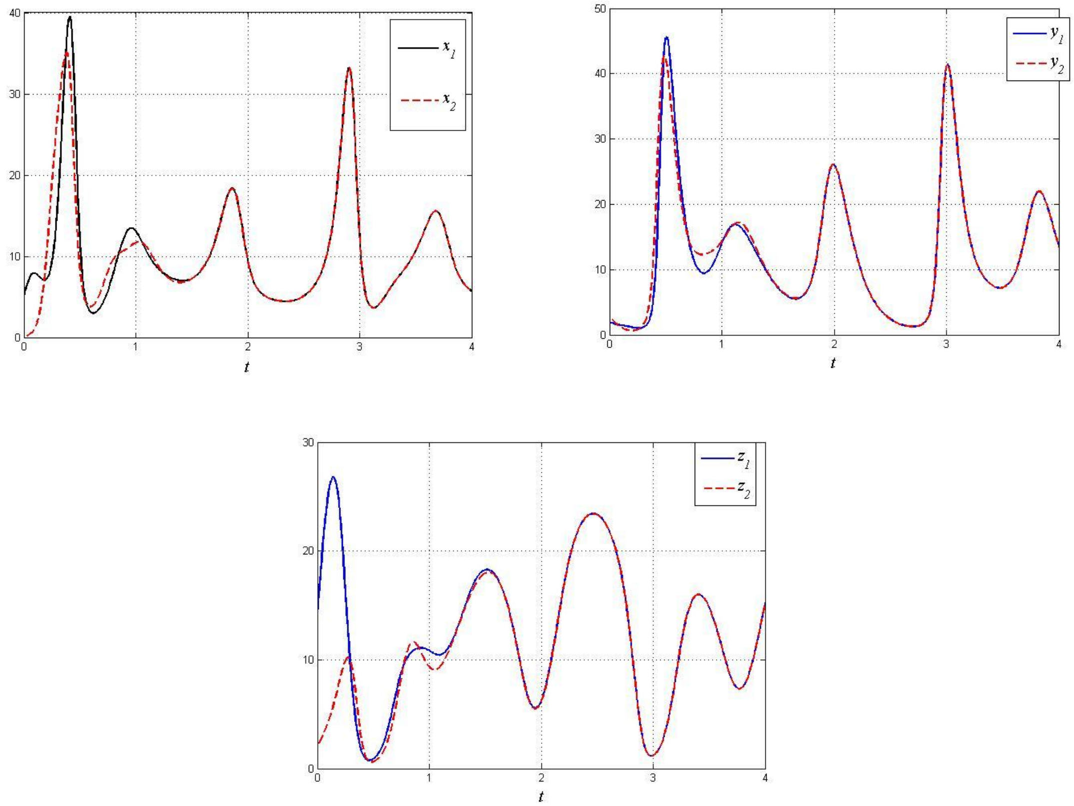

Fig. 4. Comparisons of systems trajectories by using bidirectional coupling $x_2 \leftrightarrow x_1$.

This is because of the dynamics of error signals: By definition (5) of error signals we have

$$\dot{e}_x = [a_1 - k_{-1}(x_1 + x_2) - (y_1 + z_1) \quad -x_2 \quad -x_2][e_x \quad e_y \quad e_z]^T . \tag{22}$$

By similar manipulations we have

$$\dot{e}_y = [y_2 \quad -a_5 + x_1 \quad 0][e_x \quad e_y \quad e_z]^T ,$$

and

$$\dot{e}_z = [0 \quad 0 \quad a_4 - k_{-5}(z_1 + z_2) - (x_2 + x_1)][e_x \quad e_y \quad e_z]^T ,$$

So the error dynamics are obtained as the following system

$$\begin{bmatrix} \dot{e}_x \\ \dot{e}_y \\ \dot{e}_z \end{bmatrix} = \begin{bmatrix} a_1 - k_{-1}(x_1 + x_2) - (y_1 + z_1) & -x_2 & -x_2 \\ y_2 & -a_5 + x_1 & 0 \\ 0 & 0 & a_4 - k_{-5}(z_1 + z_2) - (x_2 + x_1) \end{bmatrix} \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix}, \tag{23}$$

or

$$\begin{bmatrix} \dot{e}_x \\ \dot{e}_y \\ \dot{e}_z \end{bmatrix} = \begin{bmatrix} \lambda_1 & -x_2 & -x_2 \\ y_2 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix} = A \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix}. \tag{24}$$

At last (24) is stable if the matrix $A + A^T$ is negative definite (Slotine & Li, 1991). This is occurred if

$$S_1 = 2\lambda_1 < 0, \quad S_2 = 4\lambda_1\lambda_2 - (x_2 - y_2)^2 > 0, \quad S_3 = -2\lambda_2 x_2^2 + 2\lambda_3 S_2 < 0 , \tag{25}$$

The above parameters are time dependent. In Fig. 5, $(-S_1, S_2/100, -S_3/10^4)$ are plotted. It can be seen that these are positive almost all the times. Thus the error dynamics may be stable, and so the states in both systems become identical which are seen in Fig. 4.

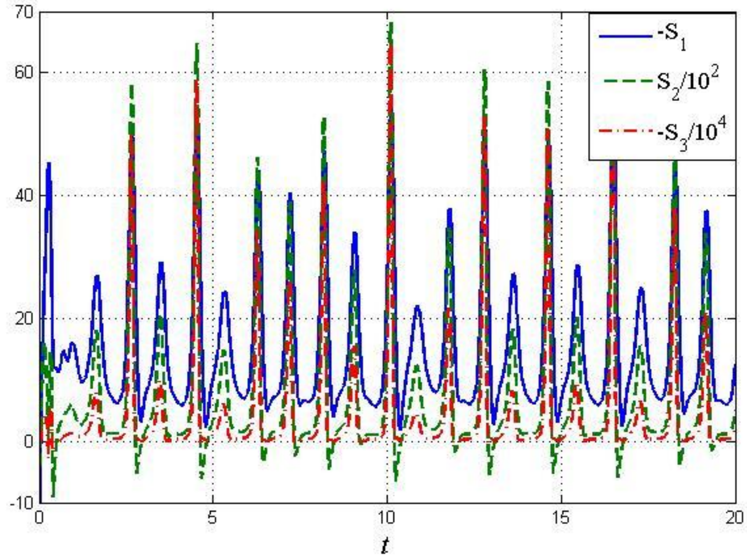

Fig. 5. The establishment of (25) for the stability of (24).

Now we couple two systems by substituting $z_2 \leftrightarrow z_1$ in the first equations of the reactors of model (1), which yields

$$\begin{cases} \dot{x}_1 = (a_1 - k_{-1}x_1 - y_1 - z_2)x_1 \\ \dot{y}_1 = (x_1 - a_5)y_1 \\ \dot{z}_1 = (a_4 - x_1 - k_{-5}z_1)z_1 \end{cases} , \quad \text{new reactor 1} \tag{26}$$

$$\begin{cases} \dot{x}_2 = (a_1 - k_{-1}x_2 - y_2 - z_1)x_2 \\ \dot{y}_2 = (x_2 - a_5)y_2 \\ \dot{z}_2 = (a_4 - x_2 - k_{-5}z_2)z_2 \end{cases} , \quad \text{new reactor 2} \tag{27}$$

Then these systems are synchronized with each other. Stability results are obtained as the previous case. Fig. 6 shows that the error dynamics go to zero after a short time and faster than the previous synchronizations.

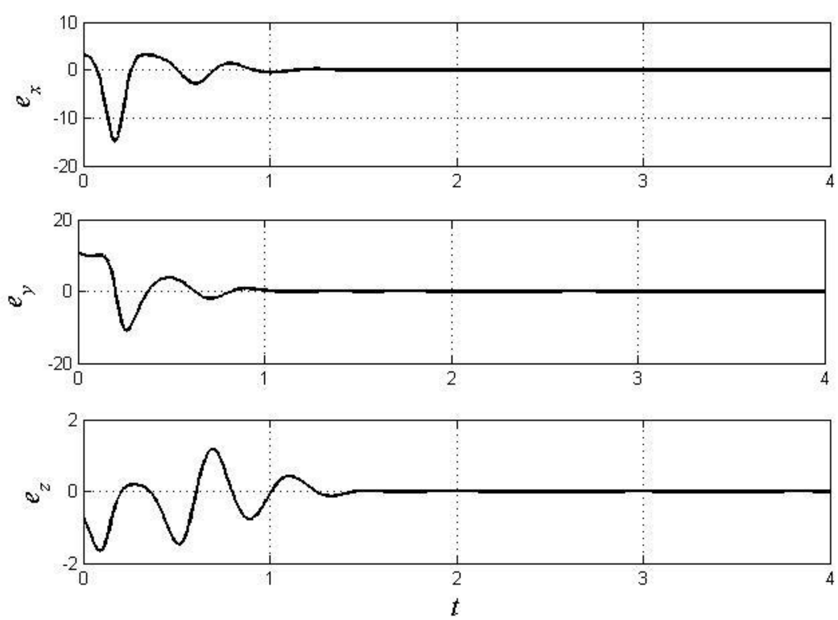

Fig. 6. Time history of error dynamics using bidirectional coupling $z_2 \leftrightarrow z_1$.

B. Unidirectional Synchronization

For unidirectional synchronization first we replace x_1 by x_2 in the third equation of reactor 2 as the slave system which gives up system (21) where the master system is

$$\begin{cases} \dot{x}_1 = (a_1 - k_{-1}x_1 - y_1 - z_1)x_1 \\ \dot{y}_1 = (x_1 - a_5)y_1 \\ \dot{z}_1 = (a_4 - x_1 - k_{-5}z_1)z_1 \end{cases}, \quad \text{master reactor} \tag{28}$$

To study behavior of the coupled systems we calculate the error dynamics

$$\begin{bmatrix} \dot{e}_x \\ \dot{e}_y \\ \dot{e}_z \end{bmatrix} = \begin{bmatrix} a_1 - k_{-1}(x_1 + x_2) - (y_1 + z_1) & -x_2 & -x_2 \\ y_2 & -a_5 + x_1 & 0 \\ 0 & 0 & a_4 - k_{-5}(z_1 + z_2) - x_1 \end{bmatrix} \begin{bmatrix} e_x \\ e_y \\ e_z \end{bmatrix}, \tag{29}$$

This is comparable with (23), so the stability conditions are the same as (25) with

$$\lambda_3 = a_4 - k_{-5}(z_1 + z_2) - x_1 < 0, \tag{30}$$

Fig. 7 shows the phase planes of error dynamics.

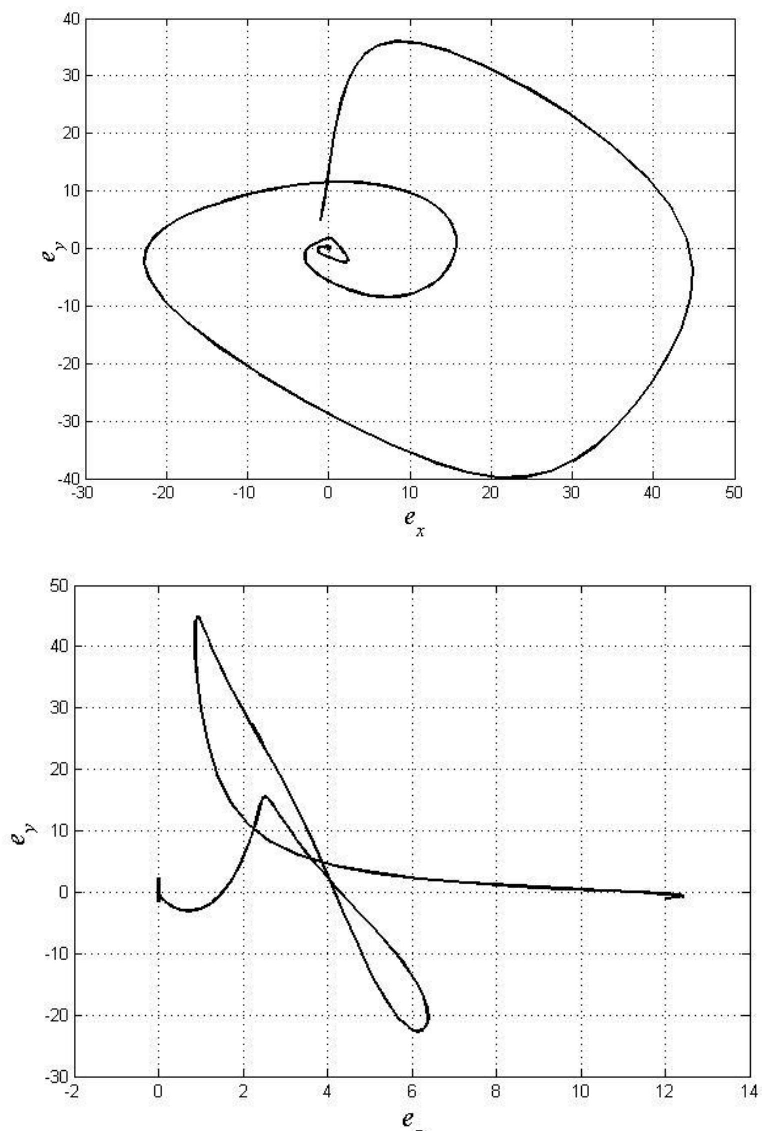

Fig. 7. Phase plane of error dynamics by using novel unidirectional coupling $x_1 \to x_2$.

Now by replacing $z_2 \to z_1$ in the first equation of the slave reactor we have (27) where the master reactor stays unchanged as (28). In Fig. 8 the time history of error dynamics are given which indicates the errors go to zero.

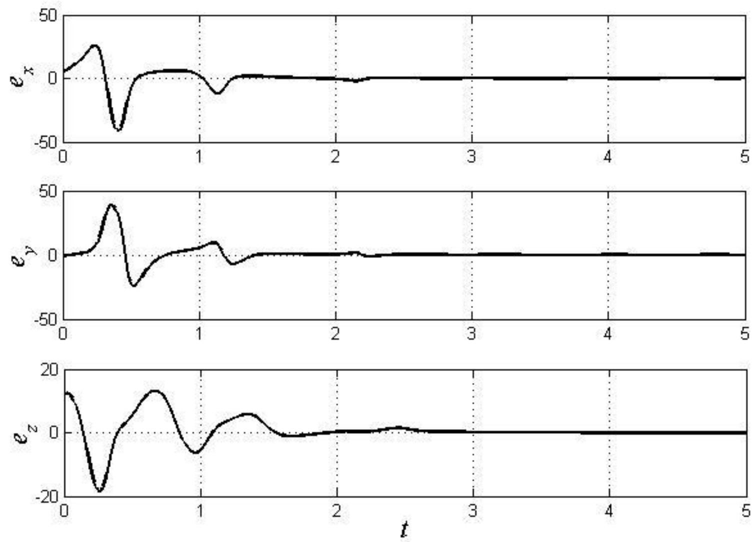

Fig. 8. Time history of error dynamics using unidirectional coupling $z_1 \to z_2$.

6. Closing Remarks

To closing this paper we compare linear and nonlinear coupling schemes. First we consider bidirectional coupling in linear form presented by (3) and (4); and bidirectional nonlinear coupling given by (20) and (21). In Fig. 9 the convergence rates of error dynamics are compared for two different values of κ and also for nonlinear coupling. It is observed that transient time is comparable in both schemes for $\kappa \approx 1$. Moreover convergence rates can be increased by increasing coupling gain κ.

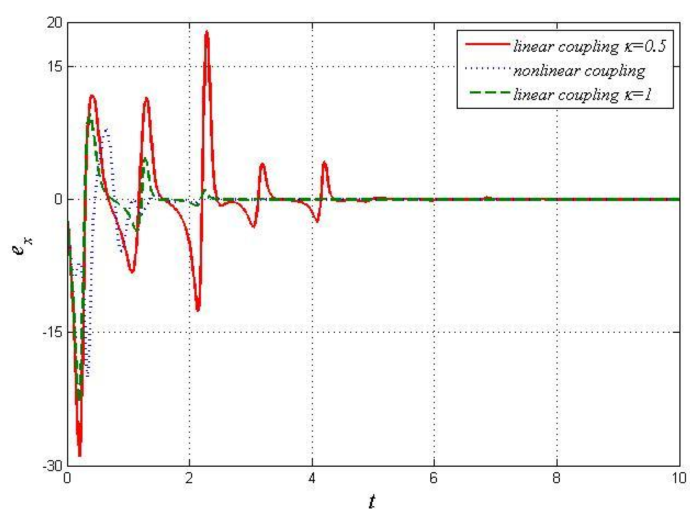

Fig. 9. Comparison of convergence rates of nonlinear and linear coupling schemes with different coupling strengths κ.

There are two significant differences between the above two methods:

i. In linear coupling the amplitude of control signal $\kappa |x_1 - x_2|$ goes to zero after transient time but in nonlinear coupling the control signals $x_i (i = 1,2)$ never go to zero. Note that it is true for unidirectional coupling.

ii. In linear coupling three signals must be transferred between systems but in the new coupling scheme it is enough to synchronize two systems only by one signal.

In section 4 we used x_i as control signal in the third equations of reactors and z_i as control signal in the first equation of reactors. But we cannot use these nonlinear coupling in the second equation. This is because the structure of the second equation of reactor is unstable:

$$\dot{y}_i = (x_i - a_5)y_i$$

In other word $x_i - a_5$ may be positive in many times, and changing this equation may increase the instability. But we can apply $y_2 \to y_1$ as nonlinear coupling in the first equation of slave reactor instead of $z_2 \to z_1$. This coupling term may stabilize the equilibrium point of chaotic slave system which is shown in Fig. 10.

Briefly, the problem of synchronization with different schemes in chaotic chemical reactors is solved in this paper. The effects of linear and nonlinear coupling terms as well as bidirectional and unidirectional coupling methods have been studied. Finally the advantages and weakness of each method are investigated.

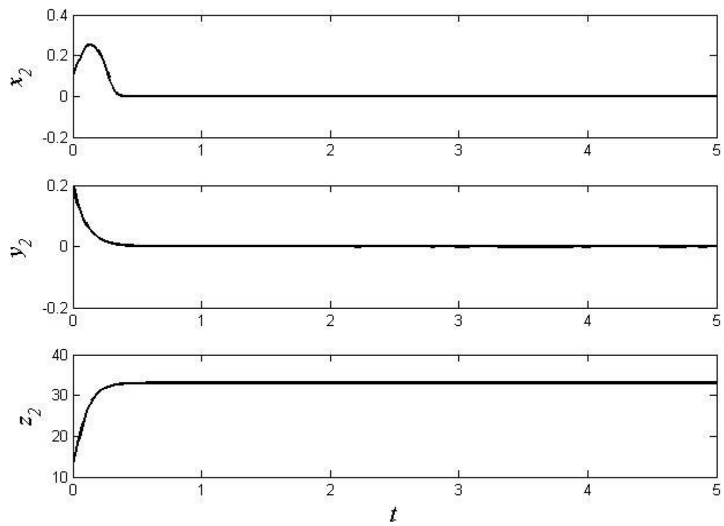

Fig. 10. Stabilizing equilibrium point of slave system by nonlinear coupling term $y_2 \to y_1$ in the first equation of slave reactor.

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