Control of Chaos in Nonlinear Chemical Reactor

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ABSTRACT
In this paper, it is shown that chaotic nonlinear chemical process can be controlled based on the Poincare map based control algorithm. An isothermal autocatalytic CSTR, which has chaotic dynamics, is successfully controlled and period 2 orbit is generated in a normal chaotic region with small perturbation of the control parameter.

INTRODUCTION

Nonlinear oscillation and chaos, peculiar characteristics of nonlinear systems, can be found in many chemical processes because of their inherently nonlinear and structurally unstable dynamics. Recently, numbers of papers have been showing that typical chemical processes have chaotic feature[1, 2, 3, 4, 5]. Because of omnipresence of chaos among chemical processes, control of chaotic system recently becomes a focal point of great interest.

In order to suppress chaos, if the dynamics of the processes shows undesirable chaotic behavior and eliminating chaos by changing design parameters is not allowed, a method of controlling chaos is necessary. Some methods which regulate chaos have been appeared lately, in the literatures [6, 7, 10, 14, 15]. For example, Fowler [6] devised an algorithm using a state estimator based on the Kalman filter which can regulate chaotic Lorenz equation. Hartley and Mossayebi[14] showed that proportional - integral controller can regulate chaotic Lorenz system in normally chaotic region. Ott et al. [7] developed an algorithm, based upon Poincare section and return map of given nonlinear dynamical system and successfully applied to Henon's map. The power of the method has been demonstrated in a few physical and chemical systems [8, 9, 11, 12, 13].

In this paper, we demonstrated the Poincare map based approach to control a chaotic reaction system consisted of parallel cubic autocatalators.

AUTOCATALYTIC CONTINUOUSLY STIRRED TANK REACTOR

We consider a system consisting of two parallel, isothermal autocatalytic reactions taking place in a CSTR (Continuously Stirred Tank Reactor). The kinetics of the system proceeds according to the following steps

$$A + 2B \rightarrow 3B \qquad \text{(i)}$$
$$B \rightarrow C \qquad \text{(ii)}$$
$$D + 2B \rightarrow 3B \qquad \text{(iii)}$$

which are governed by the following rate equations

$$-\gamma_A = k_1 C_A C_B^2 \qquad (1)$$
$$\gamma_C = k_2 C_B \qquad (2)$$
$$-\gamma_D = k_3 C_D C_B^2 \qquad (3)$$

When the reaction is carried out in a CSTR, the system can be described by three ordinary differential equations. If we define the dimesionless concentration for C_A, C_B, and C_D,

$$x_1 = \frac{C_A}{C_{A0}},\quad x_2 = \frac{C_B}{C_{B0}},\quad x_3 = \frac{C_D}{C_{D0}} \qquad (4)$$

Damkohler numbers for species A, D and B,

$$D_{a1}=\frac{k_1 C_{B0}^2 V}{Q},\quad D_{a2}=\frac{k_3 C_{B0}^2 V}{Q},\quad D_{a3}=\frac{k_2 V}{Q} \qquad (5)$$

ratios of species in the feed and dimensionless time,

$$\gamma_1=\frac{C_{A0}}{C_{B0}},\quad \gamma_2=\frac{C_{D0}}{C_{B0}},\quad \tau=\frac{t\cdot Q}{V} \qquad (6)$$

then the equations governing the system are given by

$$\frac{dx_1}{d\tau}=1-x_1-Da_1\cdot x_1\cdot x_3^2 \qquad (7)$$

$$\frac{dx_2}{d\tau}=1-x_2-Da_2\cdot x_2\cdot x_3^2 \qquad (8)$$

$$\frac{dx_3}{d\tau}=1-(1+Da_3)x_2+\gamma_1 Da_1\cdot x_1\cdot x_3^2 + \gamma_2 Da_2\cdot x_2\cdot x_3^2 \qquad (9)$$

At $Da_1 = 18000$, $Da_2 = 80$, $Da_3 = 80$, $\gamma_1 = 1.5$ and $\gamma_2=4.2$, the continuous autonomous system of eqs (7)-(9), shows chaos [5]. The trajectories of eqs (7) - (9) eventually approaches to chaotic attractor independent of initial condition after sufficient period of time. Two dimensional phase plane of the system, x_1 versus x_2 and x_1 versus x_3 are shown in **Fig. 1** and **Fig. 2,** respectively. The calculations were carried out on a IBM RS/6000 350 using the LSODE subroutine. The relative error tolerance and the absolute error tolerance was held at 10^{-6}. We obtain a first return map, which is a plot of n+1 th versus n th piercing values of a state variable, on the following surface section

$$x_1 = 0.25 \text{ and } \dot{x}_1 > 0 \qquad (10)$$

as indicated in **Fig. 1** by the horizontal line. First return map of given system are localized in a thin band as shown in **Fig. 3.** The map does not have any fixed point, i.e. the first return map does not intersect bisectrix. Henon's algorithm [16] was applied to obtain numerical piercing values during the integration.

POINCARE MAP BASED CONTROL

The main idea of the method is based on the fact that chaotic attractor is very sensitive to small perturbations because chaotic attractor has densely embedded within it an infinite number of unstable periodic orbits. The method can be applied to infinite dimensional systems,

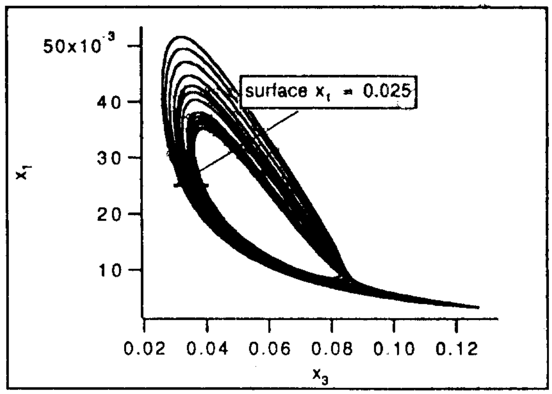

Fig. 1 Phase plane of x_1 vs. x_3.

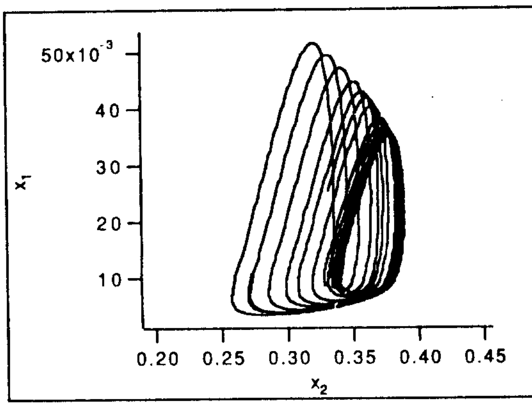

Fig. 2 Phase plane of x_1 vs. x_2.

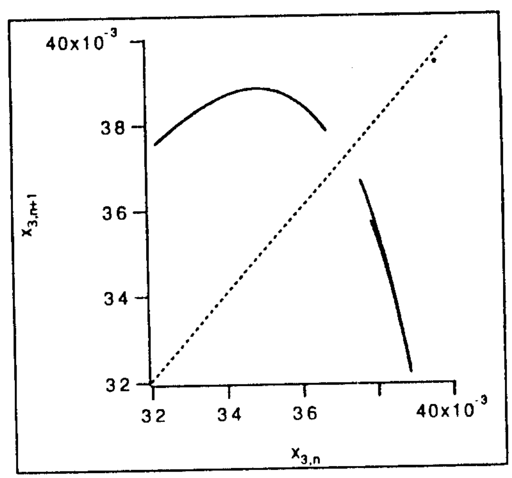

Fig. 3. Period 1 return map of x_3 at surface section $x_1 = 0.025$.

but here we restrict our attention to two dimensional map. We consider two dimensional map on the Poincare section with a scalar control variable

$$\mathbf{x}_{n+1}= \mathbf{F}(\mathbf{x}_n, u) \tag{11}$$

where $\mathbf{x} \in \mathbf{R}^2$ are the state variable, $\mathbf{F}: \mathbf{R}^2 \rightarrow \mathbf{R}^2$ and $n = 0, 1, 2, \ldots$. The control input u is manipulatable in a small range around a nominal value u_0. If the control u is varied slightly from the nominal input $u_0 = 0$ to some nearby point $u = \bar{u}$, the fixed point $\mathbf{x}_F(u)$ may changes from $\mathbf{x}_F(u)|_{u=0}=\mathbf{x}_F(0)$ to $\mathbf{x}_F(u)|_{u=\bar{u}}=\mathbf{x}_F(\bar{u})$. We define here the vector $\mathbf{g}$ as

$$\mathbf{g}=\frac{\partial \mathbf{x}_F(u)}{\partial u} \approx \frac{\mathbf{x}_F(u) - \mathbf{x}_F(0)}{u} \tag{12}$$

in the near neighborhood of the nominal value u_0 . Near the fixed point $\mathbf{x}_F(0)$, linearly approximation of map (1) can be expressed as

$$\mathbf{x}_{n+1} - \mathbf{x}_F(u) \approx \mathbf{A}[\mathbf{x}_n - \mathbf{x}_F(u)] \tag{13}$$

where $\mathbf{A}$ is a Jacobian of $\mathbf{F}$ evaluated at $\mathbf{x}_F(0)$. λ_u and λ_s are unstable and stable eigenvalues, respectively, i.e.

$$|\lambda_u| > 1 > |\lambda_s| \tag{14}$$

Unstable and Stable eigenvectors ρ_u and ρ_s are defined as

$$\mathbf{A}\rho_u = \lambda_u \rho_u$$
$$\mathbf{A}\rho_s = \lambda_s \rho_s \tag{15}$$

and contravariant basis vectors $\mathbf{f}_u$ and $\mathbf{f}_s$ are given by

$$\mathbf{f}_u^T \cdot \rho_u = 1$$
$$\mathbf{f}_s^T \cdot \rho_s = 1 \tag{16}$$
$$\mathbf{f}_u^T \cdot \rho_s = \mathbf{f}_u^T \cdot \rho_s = 0$$

Note that the eigenvalues, eigenvector and the vector $\mathbf{g}$ are experimentally assessable. $\mathbf{A}$ can be expressed by using predefined eigenvalues and eigenvectors

$$\mathbf{A} = [\rho_u \, \rho_s] \begin{bmatrix} \lambda_u & 0 \\ 0 & \lambda_s \end{bmatrix} [\rho_u \, \rho_s]^{-1} \tag{17}$$

The contravariant basis vectors and the eigenvectors have the following property

$$\begin{bmatrix} \mathbf{f}_u^T \\ \mathbf{f}_s^T \end{bmatrix} [\rho_u \, \rho_s] = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{18}$$

or

$$[\rho_u \, \rho_s]^{-1} = \begin{bmatrix} \mathbf{f}_u^T \\ \mathbf{f}_s^T \end{bmatrix}$$

Hence the matrix $\mathbf{A}$ can be written as

$$\mathbf{A} = [\rho_u \, \rho_s] \begin{bmatrix} \lambda_u & 0 \\ 0 & \lambda_s \end{bmatrix} \begin{bmatrix} \mathbf{f}_u^T \\ \mathbf{f}_s^T \end{bmatrix} = (\lambda_u \rho_u \mathbf{f}_u^T + \lambda_s \rho_s \mathbf{f}_s^T) \tag{19}$$

Therefore the linearized difference equation (14) is given by

$$\mathbf{x}_{n+1} - \mathbf{x}_F(u) \approx (\lambda_u \rho_u \mathbf{f}_u^T + \lambda_s \rho_s \mathbf{f}_s^T)[\mathbf{x}_n - \mathbf{x}_F(u)] \tag{20}$$

From the definition of vector $\mathbf{g}$, We can find that

$$\mathbf{x}_F(u) = ug + \mathbf{x}_F(0) \tag{21}$$

Using the equation (21), We have

$$\mathbf{x}_{n+1} \approx u_n g + \mathbf{x}_F(0) + (\lambda_u \rho_u \mathbf{f}_u^T + \lambda_s \rho_s \mathbf{f}_s^T)[\mathbf{x}_n - ug + \mathbf{x}_F(0)] \tag{22}$$

The purpose of this algorithm is to suppress chaotic behavior of $\mathbf{x}_{n+1}$ and let the value stay in the close neighborhood of $\mathbf{x}_F(0)$. We choose control u_n , so that

$$\mathbf{f}_u^T \cdot \mathbf{x}_{n+1} = 0 \tag{23}$$

From equation (22) and equation (23), control input u_n can be expressed in terms of the unstable eingenvalue, the unstable contravarient vectos and $\mathbf{g}$ as

$$u_n = \frac{(1 - \lambda_u)\mathbf{f}_u^T \cdot \mathbf{x}_F(0) + \lambda_u \mathbf{f}_u^T \cdot \mathbf{x}_n}{(\lambda_u - 1)\mathbf{f}_u^T \cdot \mathbf{g}} \tag{24}$$

We impose a constraint on control

$$u_{n,min} < u_n < u_{n,max} \tag{25}$$

When calculated $u_n > u_{n,max}$ or $u_{n,min} > u_n$, We let $u_n = u_{n,max}$ or $u_{n,min} = u_n$. Note that $\mathbf{x}_n$ is on the left term of the eq (24), so control u_n is calculated when the flow of eqs (7) - (9) pierces the surface of section. Usually the return map $\mathbf{F}$ is not explicitly obtained, numerical estimation of eigenvalues, eigenvectors and the vector $\mathbf{g}$ is required to implement the controller.

CONTROLLING CHAOS

We choose the ratio of species A to species B in the feed, γ_2 as the manipulatable parameter. We let $\gamma_2 = \bar{\gamma}_2 + u$, and change slightly control u around nominal value $\bar{\gamma}_2$. The control u is not required to change in wide range. To implement the chaos controller the eigenvalues and the eigenvectors should be obtained in the close neighborhood of desired fixed point. Period 2 return map of the system has one fixed point. The map slightly moves as γ_2 changes from 4.200 to 4.201 and 4.202 for both variable x_2 and x_3 (See (a) (b) and (c) in **Fig. 4** and **Fig. 5**). Furthermore near the fixed point, which is the intersection with bisectrix, the set of points shows linearity as shown in **Fig. 6**. The fixed point at $u = 0$ and 0.002 are approximately $\mathbf{x}_F(0) = [0.3006\ 0.03365]^T$ and $\mathbf{x}_F(0.002) = [0.2997\ 0.033704]^T$. The vector $\mathbf{g}$ evaluated at $\mathbf{x}_F(0)$ is $[-0.450\ -0.027]^T$. The eigenvalues and the eigen vectors of the map of $u_o = 0$ near fixed point were $\lambda_u = -2.146$, $\lambda_s = 0.999$, $\rho_u = [-0.997\ -0.074]^T$ and $\rho_s = [-0.994\ -0.111]^T$. Unstable contravariant vector is $\mathbf{f}_u = [-3.002\ 26.803]^T$. Then the controller of eq (23) is

$$u_n = \frac{0.62932\times10^{-4} + [6.4444\ \ -57.536]\begin{bmatrix} x_{2,n} \\ x_{3,n} \end{bmatrix}}{-1.97} \tag{26}$$

and we let $u_{n,max}$ and $u_{n,min}$ as 0.002 and - 0.002, respectively. The control u_n is calculated every even piercing time at the surface section. After the orbit of system (7) - (9) shows post transient response, we attempt to control chaos. After $\tau = 146$ the controller is let active. Just after the controller become active, the calculated value of the control in eq (26) is not in between constraint imposed, so the controller output u_n shows $u_{n,max}$ or $u_{n,min}$. After τ becomes greater than 156, the controller output shows the values between $u_{n,max}$ and $u_{n,min}$. $x_{2,n}$ and $x_{3,n}$ converges to two fixed points and continue to stay in the close neiborhood of the points. The system does not have any fixed point in period 1 return map as shown in **Fig. 3**, it is impossible to apply the map based control to let the system be period 1 orbit. The controller output is sensitively dependent on the vector $\mathbf{g}$, the value should be carefully evaluated.

CONCLUSIONS

It is shown that chaotic Autocatalytic CSTR is controllable by using the Poincare map based control algorithm. The algorithm does not necessarily require

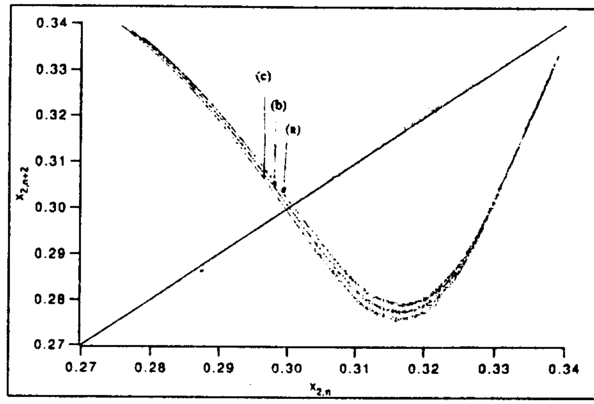

Fig. 4 Period 2 return map of x_2,
(a) $\gamma_2 = 4.200$, (b) $\gamma_2 = 4.201$, (c) $\gamma_2 = 4.202$.

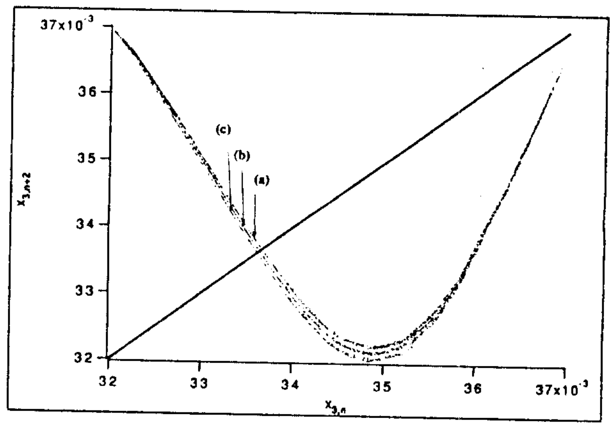

Fig. 5 Period 2 return map of x_3,
(a) $\gamma_2 = 4.200$, (b) $\gamma_2 = 4.201$, (c) $\gamma_2 = 4.202$.

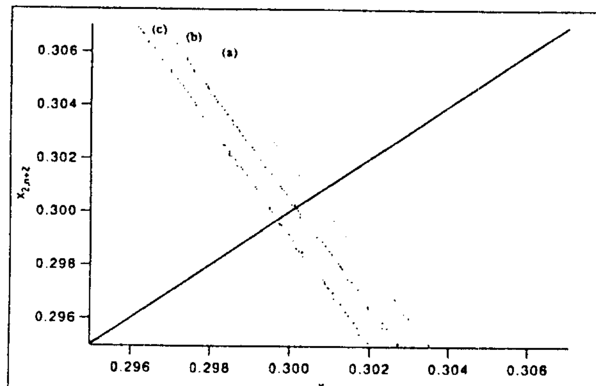

Fig. 6 Period 2 return map around fixed point of x_2,
(a) $\gamma_2 = 4.200$, (b) $\gamma_2 = 4.201$, (c) $\gamma_2 = 4.202$.

detailed dynamical equation, but only experimentally obtained eigenvalues and eigenvalues of the return map in the vicinity of fixed point and the vector **g** which is assessable based on the observation of fixed point movement by small perturbations of the control parameter. In this study, stable period 2 orbit is successfully obtained in the normal chaotic chemical process.

NOTATION

A	Jacobian of F
C_A, C_B, C_D	concentrations in the reactor and outlet flow of species A, B and D
C_{A0}, C_{B0}, C_{D0}	inlet concentration of species A, B and D
D_{a1}	Damkohler number for species A
D_{a2}	Damkohler number for species B
D_{a3}	Damkohler number for species D
f_s, f_u	stable and unstable contravariant vector
F	map on the poincare section
g	fixed point movement vector
k_1, k_2, k_3	reaction rate constant
Q	flow rate
t	time
u, u_n	control input and control input at n th piercing
u_0	nominal value of control input
u_{min}, u_{max}	maximum and minimum value of the controller output
V	reactor volume
x_1	dimensionless concentration of species A
x_2	dimensionless concentration of species B
x_3	dimensionless concentration of species D
x_F	fixed point of map F
x_n	n th value of the map F

Greek letters

γ_1	ratio of species A to B in the inlet flow
γ_2	ratio of species D to B in the inlet flow
γ_A, γ_C, γ_D	reaction rate of species A, C and D
λ_s, λ_u	stable and unstable eignevalues of F
ρ_s, ρ_u	stable and unstable eigenvectors
τ	dimensionless time

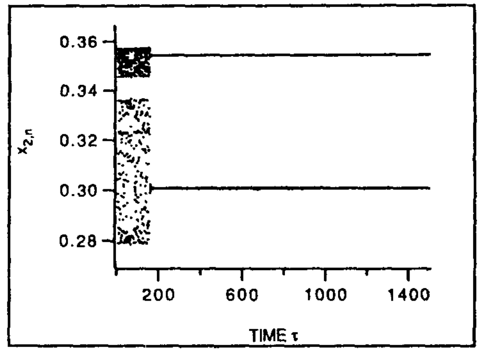

Fig. 7 Time series data of $x_{2,n}$, controller is active after $\tau = 146$.

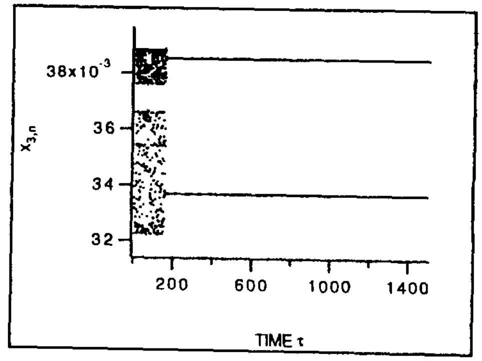

Fig. 8 Time series data of $x_{2,n}$, controller is active after $\tau = 146$.

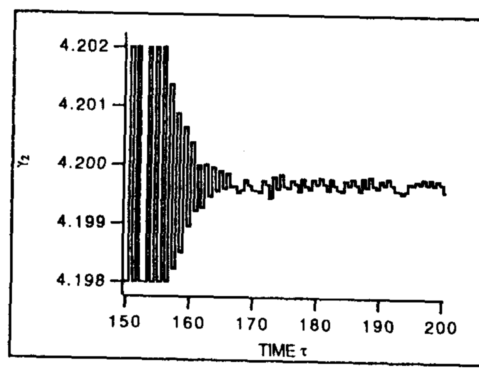

Fig. 9 Time series of γ_2.

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