Regulatory Control of a Chaotic Nonisothermal CSTR

Jayanta K. Bandyopadhyay, V. Ravi Kumar, and B. D. Kulkarni
Chemical Engineering Div., National Chemical Laboratory, Pune 411 008, India

Open nonlinear chemical systems can show a variety of behavioral patterns depending on the operating values of the parameters and intrinsic system features. In general, for different sets of parameter values, a nonlinear system can operate at a steady state, or perform simple/complex oscillations or even chaotic motions (Doherty and Ottino, 1988). Controlling these systems with a view to operate them under favorable conditions poses considerable challenges. The use of conventional PID control methods (which do not use a mathematical process model) seems to be inadequate, since they perform well only for linear and mildly nonlinear systems. For systems with strong nonlinearity, better methods are needed; in particular, internal model control (IMC) strategies have been studied (García and Morari, 1982; Economou and Morari, 1985; Economou et al., 1986; Calvet and Arkun, 1988; Morari and Zafiriou, 1989; Bequette, 1991; Henson and Seborg, 1991; Kulkarni et al., 1991; Ravi Kumar et al., 1991).

This work deals with the control of a class of nonlinear systems, namely chaotic processes. A chaotic system has a large number of embedded unstable orbits, and a careful choice of one of these orbits for regulatory control may prove to be useful in achieving overall system performance. It is known that, in the control of a chaotic process, stability constraints play an important role, and there exists distinct regions in phase space where only controller action can direct the system toward a desired orbit (Jackson, 1991a,b). An IMC method applicable to a chaotic nonisothermal CSTR incorporating stability considerations has been recently studied for both servo and regulatory control cases (Bandyopadhyay et al., 1992). The simulation studies show that the chaotic CSTR can be dynamically controlled along a chosen system orbit with sufficient accuracy even in the presence of unknown disturbances. It may be clarified at this stage that the method requires dynamic input information of the state variables and their rate of change at fast intervals for the control to be successful. In typical practice, monitoring certain variables like species concentrations is likely to take relatively longer time and implementation of the method may be restrictive, even though it is rigorous.

Correspondence concerning this work should be addressed to B. D. Kulkarni.

For the reasons stated above, it would be desirable to have a method for controlling a chaotic CSTR under less stringent conditions. A possible way out is to redefine the control objectives by stipulating that the process in the act of performing its dynamics need only pass through a few chosen key phase space point values on a chosen orbit. A recent method by Ott et al. (1990) has shown that the unstable periodic orbits of a chaotic attractor can be stabilized by applying computed values of an externally manipulable system parameter on the process and shown its usefulness in controlling a mapping of the Henon type. Mappings can provide a reflection of the process dynamics with reduced dimensionality, in the sense that they can represent the movement of phase space points on a Poincaré section. The method has been studied for the control of a few chaotic systems both theoretically and experimentally (Ditto et al., 1990; Mehta and Henderson, 1991; Peng et al., 1991; Singer et al., 1991; Roy et al., 1992). This study shows that the Poincaré mappings of the chaotic CSTR can be used to identify its periodic orbits and that adequate regulatory control of the process can be achieved on choosing these orbits as the desired system performance. The method is built up for the case of a series reaction in a CSTR known to exhibit chaos, and the applicability of the method is shown by simulations.

Theory

Let us assume that the dynamics of the nonisothermal, irreversible first-order, series reaction $A \rightarrow B \rightarrow C$ in a CSTR are governed by the following differential equations (Kahlert et al., 1981; Calvet and Arkun, 1988):

$$dx_1/dt = 1 - x_1 - Dax_1\exp[x_3/(1+\epsilon x_3)] - d_2 \quad (1)$$

$$dx_2/dt = -x_2 + Dax_1\exp[x_3/(1+\epsilon x_3)] - DaSx_2\exp[\kappa x_3/(1+\epsilon x_3)] - d_3 \quad (2)$$

$$dx_3/dt = -x_3 + DaBx_1\exp[x_3/(1+\epsilon x_3)] - DaB\alpha Sx_2\exp[\kappa x_3/(1+\epsilon x_3)] - \beta(x_3 - x_{3c}) + \beta u_t + d_1 \quad (3)$$

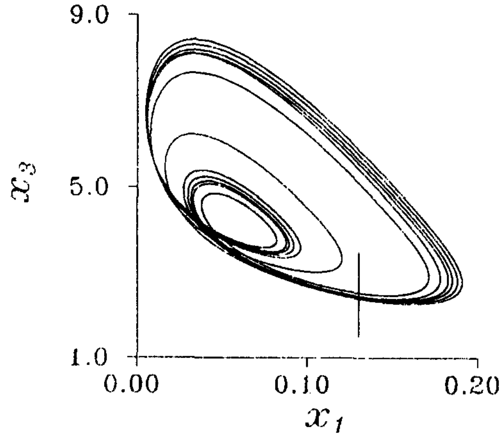

Figure 1. Phase plane plot of the chaotic dynamics with the vertical line showing the chosen Poincaré section.

where the variables x_1, x_2 denote the dimensionless concentrations of species A, B, and x_3 is the dimensionless temperature. The quantity u_t can be viewed as an externally manipulable variable and is a measure of the deviation in the coolant temperature from a reference value x_{3c}. For discussion, we assume that the process operating with $u_t = 0$ implies the system exhibits its open-loop dynamics. The d_i, where $i = 1, 2, 3$, provides for including load disturbances that can affect the process outputs x_i. The other parameters are defined in the notation section. Kahlert et al. (1981) have shown that on considering the individual steps in the series reaction to be endothermic and exothermic, respectively, and for a systematic variation in the value of the parameter β for chosen values of the remaining parameters ($Da = 0.26$, $\epsilon = 0.0$, $S = 0.5$, $\kappa = 1.0$, $B = 57.77$, $\alpha = 0.42$, $x_{3c} = 0.0$, and $u_t = 0.0$), the process typically undergoes a period doubling bifurcation route to chaos. In particular, for the above set of parameter values with $\beta = 7.9999$ calculation of the three system Lyapunov exponents (using the algorithm of Shimada and Nagashima, 1979) clearly showed the maximal Lyapunov exponent to be positive, thereby indicating the presence of chaos. Figure 1 shows the phase plane plot of the chaotic dynamics described by the system for the chosen parameter values. The set of Eqs. 1-3 can also be used to generate a mapping of points as the system trajectories cross a Poincaré section of the phase space, that is, points which cross transversely a plane corresponding to a fixed value of a dependent variable having the same direction of flow. Without any loss in generality let us assume that the dependent variable chosen for studying the Poincaré section mapping is at $x_1 = x_1'$ with $\dot{x}_1 > 0$ (indicated in Figure 1 by the vertical plane).

The trajectories of chaotic processes are dense in certain regions, and in general much of the dynamics of the attractor can be characterized by identifying the periodic orbits within its topology (Lathrop and Kostelich, 1989). We shall therefore identify the periodic orbits for this system by locating the fixed point solutions for the Poincaré mapping. Fixed points on the mapping can be located by plotting the return map of the process: $x_{3,n}$ vs. $x_{3,n+i}$ for $i = 1, 2, \ldots$. The remarkable feature of chaotic attractors is that although the return maps show that the sequence of points crossing the Poincaré section to be chaotic, these points can be localized in a thin band. As an example, curve I in Figure 2a shows the first return map for

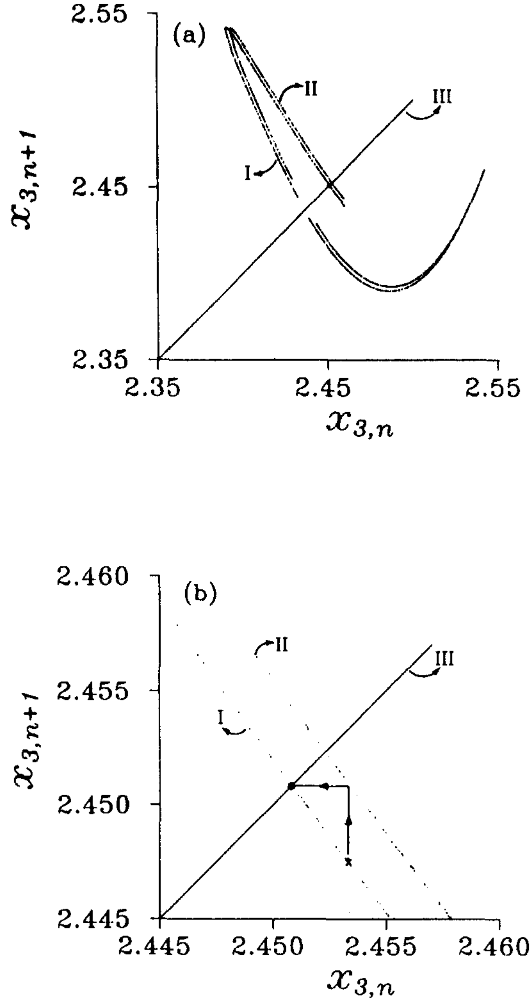

Figure 2. a) Period-1 return map; b) magnified map in the region of $x_{3,s}^{(1)}$. Curve I, $u_t = 0.0$; Curve II, $u_t = 0.001$; Curve III, bisectrix; (·), $x_{3,s}^{(1)}$; (×), $x_3^{(1)}$.

the chaotic system with the manipulable variable $u_t = 0$. Notably, the set of points in the neighborhood of an intersection with the bisectrix (see Figures 2a and 2b) shows linearity. This facilitates location of the period-1 fixed point solution on the Poincaré section, where $x_{3,n} = x_{3,n+1}$ by a least-squares fit of the mapping in the linear region and then solving for its intersection with the bisectrix. Let the location of the fixed point be $x_{3,s}^{(1)}$ (see Figure 2b). By a similar analysis from return maps of higher values of $i = 2, 3, \ldots$ we can identify fixed points $x_{3,s}^{(i)}$ in phase space with period-2 and higher periodicity crossing the Poincaré section. Note that a number of period-i cycles can exist on a Poincaré section, but we assume that in the neighborhood of a fixed point the mapping is single valued.

Notably, for a small change in the value of the manipulable variable from the open-loop setting of $u_t = 0$ to u_t', the linear section shifts only in phase space, that is, retains its original slope (see Figure 2b; compare curves I and II). This feature allows us to locate a specific phase point $x_3^{(i)}$ such that for a perturbation of the process to u_t', the system at $x_3^{(i)}$ is directed toward the desired fixed point $x_{3,s}^{(i)}$ for its next return to the Poincaré section. The location of the $x_3^{(1)}$ for the first return map is marked in Figure 2b. The shift corresponding to

$\Delta x_3^{(i)} = x_{3,s}^{(i)} - x_3^{(i)}$ can be used to quantify the system sensitivity to small parametric variations in the entire linear region close to $x_{3,s}^{(i)}$ by estimating the sensitivity coefficient g_i for the period-i cycle and is given by:

$$g_i = \Delta x_3^{(i)} / u_t' \tag{4}$$

From the knowledge of g_i it is possible to build a control algorithm for regulating the process on a period-i orbit and is discussed below.

The process dynamics monitored as $x_{3,n}$ will at some time visit the Poincaré section in the linear region around $x_{3,s}^{(i)}$. The values for the controller output $u_{t,n}^{(i)}$ to be implemented at the nth intersection of the Poincaré plane for a deviation $(x_{3,s}^{(i)} - x_{3,n})$ and a known sensitivity coefficient g_i can be calculated for every n by:

$$u_{t,n}^{(i)} = (x_{3,s}^{(i)} - x_{3,n}) / g_i \tag{5}$$

It is noted that the controller action $u_{t,n}^{(i)}$ needs to be implemented at every ith intersection of the plane. A specific controller output $u_{t,n}^{(i)}$ alters the process operating conditions such that the $(n+i)$th crossing on the Poincaré section will be closer to $x_{3,s}^{(i)}$. At this time, a new value of the controller output is calculated and implemented taking care of initializing $n = n + i$ at every step. Repeated application of the procedure leads to conditions when the process stabilizes itself at the desired period-i orbit (since, $x_{3,n} \approx x_{3,s}^{(i)}$). We also caution, however, that applying the control when the trajectory enters the linear regime but is still far from $x_{3,s}^{(1)}$ can result in stabilizing the system at some other existing periodic orbit. From an alternative viewpoint, Eq. 5 can be regarded as proportional feedback control with $1/g_i$ as a proportionality constant and Eq. 4 as a Euler approximation (see, for example, Goodwin and Sin, 1984; Mareels et al., 1992).

It may be observed that the application of the method does not pose any problem in real-life when the set of model Eqs. 1-3 for the process are not available and process load disturbances are absent for the g_i's can be ascertained from the return maps of monitored experimental data.

Results and Discussion

For the purpose of illustrating the control algorithm we shall present the simulation results for stabilizing the period-1 and period-2 cycles and also the control performance in the presence of an unknown load disturbance for the nonisothermal CSTR. In this study, the physical process is assumed to follow the model Eqs. 1-3 and the process dynamics obtained by numerically integrating them for the set of parameter values indicated earlier. The method of Henon (1982) was simultaneously applied during integration to obtain the Poincaré maps at $x_1' = 0.13$.

We shall first discuss the case of controlling the system at a period-1 cycle. As discussed earlier, Figure 2a shows the first return plot for the open-loop temperature behavior (curve I), and the intersection of the bisectrix (curve III) with this map shows that the fixed point solution $x_{3,s}^{(1)}$ is unique. For a small change in the manipulable variable to $u_t = 0.001$, the resultant map (curve II) shifts slightly but distinctly from curve I with the desired linearity conditions in the region of the fixed point

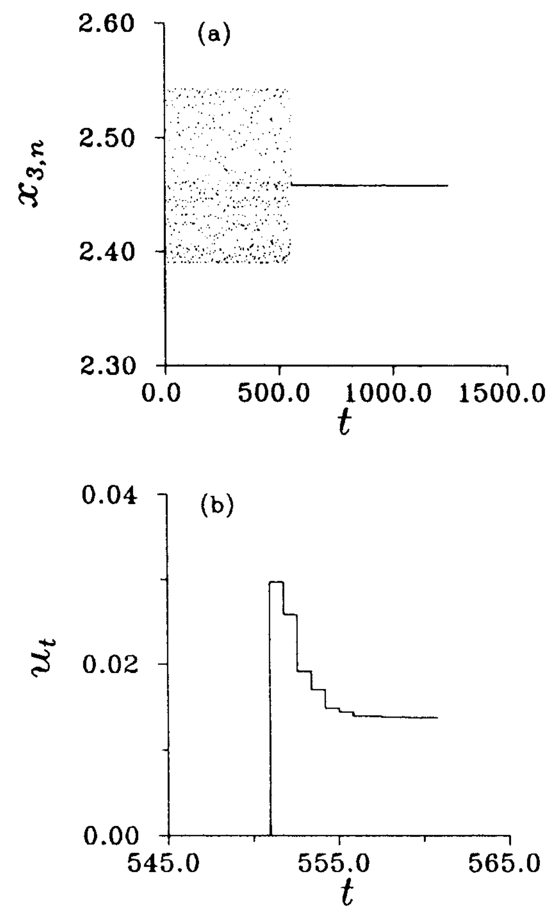

Figure 3. a) Period-1 control performance; b) dynamic controller output.

$x_{3,s}^{(1)}$ retained. In fact, both of the plots show linearity for a wide range in $x_{3,n}$. Figure 2b shows the return map around the region $x_{3,s}^{(1)}$ on magnification. A linear least-squares fit to curve I followed by solving for its intersection with the bisectrix (curve III) yields the value for the fixed point solution $x_{3,s}^{(1)} = 2.45075$ for the period-1 cycle. Also, the intersection point of curve I with a perpendicular drawn from $x_{3,s}^{(1)}$ on curve II gives the value of $x_3^{(1)} = 2.45339$, whose knowledge is essential to calculate a value for the sensitivity coefficient g_1 by Eq. 4. For this case, a value of $g_1 = 2.64$ was obtained. The results of attempting to control the process at a period-1 cycle is shown in Figures 3a and 3b. Figure 3a shows the time variation of the dependent variable x_3 as it intersects sequentially with the Poincaré section: $x_{3,n}$, $n = 1, 2, \ldots$ Care was taken to eliminate the initial transients so that the chaotic attractor localized itself on its associated manifold and after the completion of this step t was reset to zero. Additionally, the simulation procedure allowed the system to perform its open-loop dynamics until $t = 550$. Controls were initiated soon after the system finds itself in the neighborhood of $x_{3,s}^{(1)}$ which occurred in a few integration steps. Figure 3a clearly shows that the system stabilizes at the chosen period-1 orbit, and the controller outputs (calculated using Eq. 5) which can achieve this task is shown in Figure 3b. Note that during the time lapse between nth and $n+i$th intersection, maintaining the controller output at a constant value of $u_{t,n}^{(i)}$ did not affect the control performance. Therefore, in-between the time interval of $550 < t < 560$, the

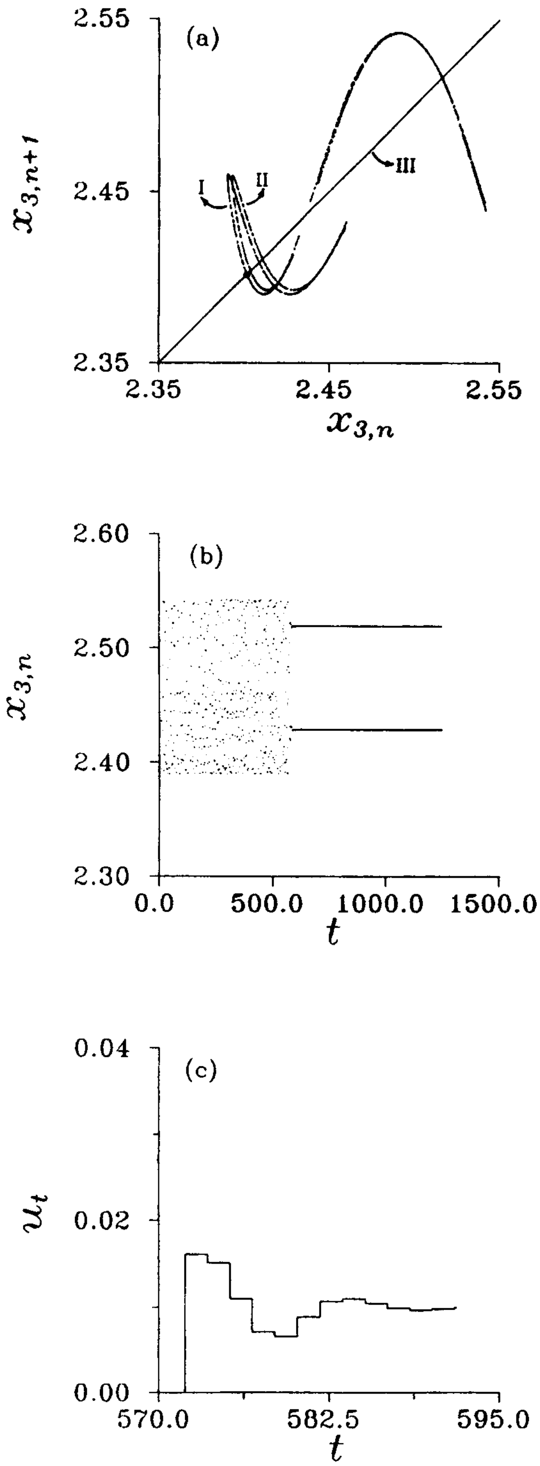

Figure 4. a) Period-2 return map: curve I, $u_t = 0.0$; curve II, $u_t = 0.001$; curve III, bisectrix; (·), $x_{3,s}^{(2)}$; b) period-2 control performance; c) dynamic controller output.

controller is seen to adjust the value of $u_{t,n}^{(1)}$ stagewise at every intersection of the Poincaré section. This result also suggests that the procedure can allow sufficient time intervals in-between implementing controller outputs. It may be also observed that in the stabilized region a finite value of $u_{t,n}^{(1)}$ is continuously implemented.

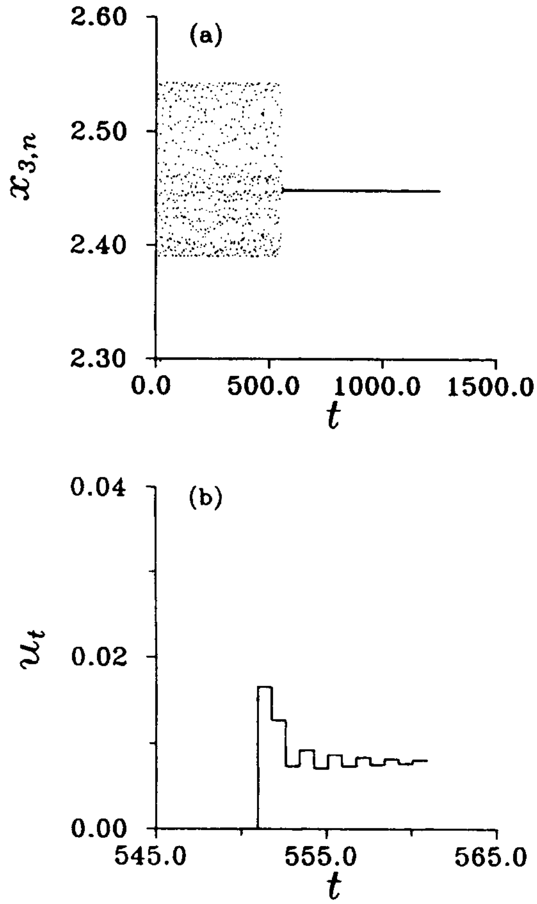

Figure 5. a) Period-1 control performance with load disturbance $d_1 = 0.01$; b) dynamic controller output.

For the case of the period-2 cycle, the return map as seen in Figure 4a shows three possible fixed point solutions $x_{3,s}^{(2)}$. In all the cases, the linearity and shift with respect to the small change in u_t is seen. For brevity, we shall only present the results of attempting to control at one of these cases, namely, the fixed point solution of $x_{3,s}^{(2)} = 2.4218$ (see Figures 4b and 4c). Figure 4b shows every intersection to the Poincaré plane and indicates that in the stabilized regime the system passes successively on its second return through $x_{3,s}^{(2)}$ while stabilizing the odd intersections. Finally, Figures 5a and 5b show the control performance in the presence of an unknown load disturbance on the system for the period-1 cycle studied earlier (Figure 3). The simulation of the process to obtain the Poincaré map was carried out assuming $d_1 = 0.01$, $d_2 = d_3 = 0$. The analysis validates the linearity characteristics for both the load-free and the disturbance return maps. As intuitively expected it is seen that in this case the time taken to achieve control is significantly higher when compared with controlling the period-1 cycle in the absence of a load disturbance.

In summary, a possible method for the regulatory control of a chaotic CSTR on its unstable periodic orbits has been discussed. The method is seen to be efficient although it requires an initial standardization of the process response to a perturbation in the manipulative variable.

Notation

B = dimensionless adiabatic temperature rise
d_1, d_2, d_3 = load disturbance terms in Eqs. 1-3
Da = Damköhler number
g_i = sensitivity coefficient for the period-i orbit defined by Eq. 4
S = ratio of the rate constants for the series reaction
u_t = manipulable control variable
$u_{t,n}^{(i)}$ = controller output for stabilizing the period-i orbit defined by Eq. 5
x_1 = dimensionless concentration of species A
x_2 = dimensionless concentration of species B
x_3 = dimensionless temperature
x_{3c} = reference value for the dimensionless coolant temperature
$x_{3,s}^{(i)}$ = fixed point for the period-i orbit

Greek letters

α = ratio of heat effects for the series reaction
β = dimensionless heat-transfer coefficient
ϵ = dimensionless activation energy
κ = ratio of activation energies for the series reaction

Literature Cited

Bandyopadhyay, J. K., V. Ravi Kumar, B. D. Kulkarni, and P. B. Deshpande, "On Dynamic Control of Chaos: A Study With Reference to a Reacting System," *Phys. Lett A.*, **166**, 197 (1992).
Bequette, B. W., "Nonlinear Control of Chemical Processes—A Review," *Ind. Eng. Res.*, **30**, 1391 (1991).
Calvet, J. P., and Y. Arkun, "Feedforward and Feedback Linearization of Nonlinear Systems and its Implementation Using Internal Model Control," *Ind. Eng. Chem. Res.*, **27**, 1822 (1988).
Ditto, W. L., S. N. Rauseo, and M. L. Spano, "Experimental Control of Chaos," *Phys. Rev. Lett.*, **65**, 3211 (1990).
Doherty, M. F., and J. M. Ottino, "Chaos in Deterministic Systems: Strange Attractors, Turbulence, and Applications in Chemical Engineering," *Chem. Eng. Sci*, **43**, 139 (1988).
Economou, C. G., and M. Morari, "Newton Control Laws for Nonlinear Controller Design," *Proc. IEEE Cong. on Decision and Control*, Ft. Lauderdale, 1361 (1985).
Economou, C. G., M. Morari, and B. O. Palsson, "Internal Model Control-5. Extension to Nonlinear Systems," *Ind. Eng. Chem. Process Des. Dev.*, **25**, 403 (1986).
Garćia, C. E., and M. Morari, "Internal Model Control: 1. A Unifying Review and Some New Results," *Ind. Eng. Chem. Process Des. Dev.*, **21**, 308 (1982).
Goodwin, G. C., and K. S. Kin, *Adaptive Filtering, Prediction and Control*, Prentice Hall, Englewood Cliffs, NJ (1984).
Henon, M., "On the Numerical Computation of Poincaré Maps," *Physica D*, **5**, 412 (1982).
Henson, M. A., and D. E. Seborg, "An Internal Model Control Strategy for Nonlinear Systems," *AIChE J.*, **37**, 1065 (1991).
Jackson, E. A., "Controls of Dynamic Flows With Attractors," *Phys. Rev. A.*, **44**, 4839 (1991a).
Jackson, E. A., "On the Control of Complex Dynamic Systems," *Physica D*, **50**, 341 (1991b).
Kahlert, C., O. E. Rossler, and A. Varma, "Chaos in a Continuous Stirred Tank Reactor with Two Consecutive First-Order Reactions, One Exo-, One Endothermic," *Springer Ser. Chem. Phys.*, **18**, 355 (1981).
Kulkarni, B. D., S. S. Tambe, N. V. Shukla, and P. B. Deshpande, "Nonlinear pH Control," *Chem. Eng. Sci.*, **46**, 995 (1991).
Lathrop, D. P., and E. J. Kostelich, "Characterization of an Experimental Strange Attractor by Periodic Orbits," *Phys. Rev. A*, **40**, 4028 (1989).
Mehta, N. J., and R. M. Henderson, "Controlling Chaos to Generate Aperiodic Orbits," *Phys. Rev. A.*, **44**, 4861 (1991).
Morari, M., and E. Zafiriou, *Robust Process Control*, Prentice-Hall, Englewood Cliffs, NJ (1989).
Mareels, I. M. Y., H. B. Penfold, and R. J. Evans, "Controlling Nonlinear Time Varying Systems via Euler Approximations," *Automatica*, **28**, 681 (1992).
Ott, E., C. Grebogi, and J. A. Yorke, "Controlling Chaos, *Phys. Rev. Lett.*, **64**, 1196 (1990).
Peng, B., V. Petrov, and K. Showalter, "Controlling Chemical Chaos," *J. Phys. Chem.*, **95**, 4957 (1991).
Ravi Kumar, V., B. D. Kulkarni, and P. B. Deshpande, "On the Robust Control of Nonlinear Systems," *Proc. R. Soc. Lond. A*, **433**, 711 (1991).
Roy, R., T. W. Murphy, Jr., T. D. Maier, Z. Gills, and E. R. Hunt, "Dynamical Control of a Chaotic Laser: Experimental Stabilization of a Globally Coupled System," *Phys. Rev. Lett.*, **68**, 1259 (1992).
Shimada, I., and T. Nagashima, "A Numerical Approach to Ergodic Problem of Dissipative Dynamical Systems," *Prog. Theor. Phys.*, **61**, 1605 (1979).
Singer, J., Y-Z Wang, and H. H. Bau, "Controlling a Chaotic System," *Phys. Rev. Lett.*, **66**, 1123 (1991).

Manuscript received Apr. 23, 1992, and revision received Sept. 14, 1992.

Errata

In the article titled "Circulation Model for Absorption and Dispersion in Cocurrent Bubble Columns" (Vol. 39, Feb. 1993, p. 224) by R. G. Rice, N. W. Geary, and L. F. Burns, the following corrections are made:

- In the table of contents (the fourth title on the front cover), "Adsorption" should be replaced by "Absorption."

- Lefthand side of Eq. 59 should read $1/t_\theta^*$, not t_θ^*.

- An important reference was not included: M. H. I. Baird and coworkers (*Can. J. of Chem. Eng.*, **54**, 540, 1976) were apparently the first to use an acid-base method to assess axial dispersion. They used ammonia in HCl, whereas Rice and Littlefield (1987) used sodium hydroxide in HCl.