Regulation of Lumped Periodic Processes

When a periodic process is disturbed, control action may be necessary to maintain satisfactory performance. Regulating controls to achieve this objective can be synthesized by solving a linear-quadratic optimization problem with periodic coefficients. Generalized proportional and proportional-integral feedback regulators developed in this manner are tested by simulating a cyclic reactor. Very satisfactory control is achieved for 10% step disturbances in reactor feed conditions although the results are sensitive to the choice of manipulated variables.

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SCOPE

Significant recent research interest has been focused on possible advantages of intentional unsteady state processing. Among the potential benefits of periodic operation are increased reactor selectivity (see Bailey, 1974) and enhanced separation (see, for example, Robinson and Engel, 1967; Wilhelm et al., 1968). All previous work, however, has considered only the question of periodic process design: how should some manipulated variable be oscillated to achieve optimum performance? Once a suitable design has been developed, another problem which we call *periodic process regulation* must be resolved: What control manipulations are necessary when the operating cyclic system is disturbed by an unexpected change in its environment? This paper presents one approach to this problem for systems described by ordinary differential equations.

By adopting the objective of maintaining design conditions and assuming that deviations from these conditions are sufficiently small, regulating controls can be synthesized in feedback form by solving a time-varying linear-quadratic optimization problem (see Edgar et al., 1973). Employing this approach, generalized proportional (P) and proportional-integral (PI) regulators are developed.

A continuous-flow stirred tank reactor (CSTR) in which parallel reactions occur is employed to test these regulating controls. In the absence of disturbances, periodic variations in heat flux to the reactor provide greater selectivity for the desired product than can be obtained by steady state operation. Step disturbances in feed conditions can unfavorably alter the reactor's performance. The effectiveness of flow rate or heat flux manipulation in counteracting these upsets is investigated using simulation studies.

CONCLUSIONS AND SIGNIFICANCE

A generalized proportional-integral control employing heat flux as the regulating variable effectively returns the cyclic reaction system to its design specifications following 10% step decreases and increases in feed concentration and temperature. This can be seen by comparing the response with this controller, denoted PI-Heat, to the periodic fluctuations of the reference design (undisturbed) process in Figures 2, 4, and 5. Proportional control using heat flux regulates the reactor almost as well but requires more extreme fluctuations in the manipulated variable as Figure 3 illustrates. Examination of Figures 2, 4, and 5 shows that flow rate is far less effective than heat flux in maintaining reference design conditions. Without a regulating control these disturbances cause significant shifts in the reactor's response.

Therefore the periodic process regulator developed here appears adequate for small disturbances. Although the optimal regulating controller requires a matrix of time-varying gains, only one period of this matrix need be retained in the regulatory memory. Adequate regulation may be feasible with a suboptimal controller employing time-invariant gains. Consequently, control implementation should be straightforward.

Several questions remain for future study. Among the possibilities are adaptive regulators to capitalize on advantageous disturbances and regulators capable of counteracting larger upsets. Figure 6 demonstrates how the performance of the reactor with PI-heat regulator deteriorates following a 30% step decrease in feed conditions.

In this paper we address the problem of regulation of periodic processes. This problem is closely related to that of steady state regulation: in both cases we seek appropriate control responses to upsets in the system's environment. The novel challenge of periodic regulator design derives from the time-varying nature of the undisturbed or reference system. Before undertaking any mathematical analysis of periodic regulators, we must carefully consider suitable control objectives and constraints for this new class of problems.

The processes of interest here have been designed to operate periodically in the absence of disturbances. We shall call the periodic system free from disturbances the *design* or *reference process*. In the reference process, oscillations in the system's state and output are usually forced by time-periodic variations in one or more of the manipulated variables which influence the process. These manipulated variables will be termed the *programmed control variables* since their time dependence is specified as part of the reference process design. Proper choice of the programmed control, which usually operates on an open-loop basis, has been treated extensively in the earlier literature (Marzollo, 1972).

The usual basis for choosing periodic rather than steady state operation for the reference process is improved profit. Among the indirect profit indicators employed in earlier studies are reactor selectivity (Bailey, 1974) and column separation factor (Wilhelm et al., 1968). Ideally, maximum profit should remain the goal for an operating system which is subjected to disturbances. Optimal control theory reveals, however, that controls to achieve the maximum possible profit cannot be specified without knowing in advance what upsets the process will face in the future. Since such information is never available, usual practice is pursuit of an alternative objective—one which is a reasonable compromise between process profit maximization and minimization of the difficulty of control design.

Such an approach is adopted in this work, although not without some reluctance since one major thrust of earlier research in periodic processes was demonstration of the desirability of some disturbances (Douglas, 1967). Development of controllers to capitalize on such upsets but to counteract unfavorable disturbances remains a problem for the future. We shall assume that all disturbances are undesirable. Consequently, the regulators developed here attempt to negate disturbances and to maintain all operating variables at their design values. In contrast to steady state regulation, however, the design values here are periodic functions of time. Thus, we must always try to hit a moving target: the periodic state of the design system.

Design of periodic regulators cannot be divorced completely from development of the reference process. This point is perhaps best illustrated by examining one feature of the example considered in detail below. Suppose that we can manipulate two quantities, say flow rate through a reactor and the heat flux into it, and thus influence the behavior of a process. When seeking the best idealized process, we must not exhaust all degrees of freedom in these manipulated variables. That is, we should not employ both flow rate and heat flux as programming variables and allow them to oscillate over their entire operating ranges in the reference process design. If all manipulated variables fluctuate between their maximum and minimum values in the reference design, the regulator will be severely constrained.

At least two methods of preserving adequate flexibility for the regulating controller may be envisioned. First, some controlling variables can be fixed during the idealized process design but allowed to vary with time in regulator design. That is, some manipulated variables are saved for the sole purpose of regulation. On the other hand, the programming variable can be used both to drive the reference periodic process and to counteract disturbances. In this case, we place artificially tight limits on the control during the reference design phase. This preserves freedom for the regulating control to drive the manipulated variable beyond these limits if necessary.

OPTIMAL FEEDBACK REGULATORS FOR SMALL DISTURBANCES

Most lumped periodic processes can be described by a set of ordinary differential equations

$$\frac{d\mathbf{c}(t)}{dt} = \mathbf{f}(\mathbf{c}(t), \mathbf{y}(t), \mathbf{d}(t), \mathbf{z}(t)) \tag{1}$$

where $\mathbf{c}$ is an n-vector of state variables. $\mathbf{y}$ is an m-vector of programmed control variables. Disturbances are included in the p-dimensional vector $\mathbf{d}$, while the q-vector $\mathbf{z}$ represents those manipulated variables which are employed strictly for regulation.

In the undisturbed process, there are no upsets. Both $\mathbf{d}$ and $\mathbf{z}$ are constant at their reference values $\mathbf{d}_r$ and $\mathbf{z}_r$, respectively. In this situation it is assumed that periodic variations in $\mathbf{y}$

$$\mathbf{y}_r(t) = \mathbf{y}_r(t+\tau) \tag{2}$$

lead to oscillating state variables with period τ:

$$\mathbf{c}_r(t) = \mathbf{c}_r(t+\tau) \tag{3}$$

The subscript r in Equations (2) and (3) denotes the reference periodic process. For the special case of autonomous oscillations, $\mathbf{c}$ oscillates even though all process inputs are time invariant. We should note that the regulator theory developed here also applies in this instance.

Since we seek a regulator for small disturbances, the nonlinear periodic process can be linearized about the design oscillatory state to obtain

$$\frac{d\mathbf{x}(t)}{dt} = \mathbf{A}(t)\mathbf{x}(t) + \mathbf{B}(t)\mathbf{u}(t) \tag{4}$$

The deviation vector $\mathbf{x}$ is the difference between the actual and idealized system state

$$\mathbf{x}(t) = \mathbf{c}(t) - \mathbf{c}_r(t) \tag{5}$$

and $\mathbf{A}(t)$ is a periodic $n \times n$ Jacobian matrix defined by

$$\mathbf{A}(t) = \frac{\partial \mathbf{f}(\mathbf{c}_r(t), \mathbf{y}_r(t), \mathbf{d}_r, \mathbf{z}_r)}{\partial \mathbf{c}} \tag{6}$$

Similarly, $\mathbf{u}$ represents the change of the regulating control from its design value, and its $n \times q$ coefficient matrix $\mathbf{B}(t)$ is a periodic function of time:

$$\mathbf{u}(t) = \mathbf{z}(t) - \mathbf{z}_r \tag{7}$$

$$\mathbf{B}(t) = \frac{\partial \mathbf{f}(\mathbf{c}_r(t), \mathbf{y}_r(t), \mathbf{d}_r, \mathbf{z}_r)}{\partial \mathbf{z}} \tag{8}$$

The same formalism applies when there are no distinct regulating variables and alterations in the programmed control are employed to attempt process regulation. In this situation $\mathbf{u}(t)$ is $\mathbf{y}(t) - \mathbf{y}_r(t)$, and $\mathbf{B}(t)$ is the Jacobian of $\mathbf{f}$ with respect to $\mathbf{y}$, again evaluated at the idealized process conditions. The influence of disturbances is represented here by a nonzero value of the initial perturbation $\mathbf{x}(0)$. This is standard practice in optimal control design for small perturbations (Douglas, 1972, p. 204 and Chapter 9): it is based on the equivalence of any input to a train of impulses. Thus, the response to any input may be viewed as a superposed collection of impulse responses each of which is equivalent to the response of the undisturbed system with an appropriate nonzero initial perturbation.

To achieve satisfactory regulation of the process, $\mathbf{x}$ should be kept small without employing excessively large $\mathbf{u}$ values. To meet this objective we base the regulating controller design on minimizing a quadratic performance index. Still it is not easy to specify the precise form of the objective function for regulation of a periodic process because (1) the disturbed system may return to the idealized system response after a large time T; for example, after a pulse disturbance, (2) the disturbed system may reach a new periodic state after a large time T. This is expected for step disturbances, for example. For the former case, Equation (9) will serve as a satisfactory objective function:

$$J_1 = \frac{1}{2}\int_0^T [\mathbf{x}'(t)\mathbf{Q}\,\mathbf{x}(t) + \mathbf{u}'(t)\mathbf{R}\,\mathbf{u}(t)]dt \qquad (9)$$

where $\mathbf{Q}$ is an $n \times n$ positive semidefinite matrix, $\mathbf{R}$ is a $q \times q$ positive definite matrix, and $'$ denotes transposition. For case (2), however, the following objective function may be more appropriate:

$$J_2 = \frac{1}{2}\int_T^{T+\tau} [\mathbf{x}'(t)\mathbf{Q}\,\mathbf{x}(t) + \mathbf{u}'(t)\mathbf{R}\,\mathbf{u}(t)]dt \qquad (10)$$

Since a good regulator should be capable of handling any type of disturbance, it is important to compare the controllers obtained using the different objective functions J_1 and J_2.

The general structure of the optimal controller for a nonstationary linear system with quadratic performance index is well known (see Athans and Falb, 1966; Edgar et al., 1973). The optimal control can be determined in feedback form

$$\mathbf{u}(t) = -\mathbf{R}^{-1}\mathbf{B}'(t)\mathbf{K}(t)\mathbf{x}(t) \qquad (11)$$

where the $n \times n$ symmetric matrix $\mathbf{K}(t)$ is the solution of the Riccati equation

$$\frac{d\mathbf{K}(t)}{dt} = -\mathbf{K}(t)\mathbf{A}(t) - \mathbf{A}'(t)\mathbf{K}(t) + \mathbf{K}(t)\mathbf{B}(t)\mathbf{R}^{-1}\mathbf{B}'(t)\mathbf{K}(t) - \mathbf{Q} \qquad (12)$$

ON THE PERIODIC *K* MATRIX

The special nature of the periodic regulator problem arises from the periodic coefficients in Equations (11) and (12) and the boundary conditions on $\mathbf{K}$. The latter conditions depend on which objective function is applied. For J_2, a periodic $\mathbf{K}$ matrix is required (see Bailey, 1972).

$$\mathbf{K}(T) = \mathbf{K}(T+\tau) \qquad (J_2) \qquad (13)$$

Use of J_1 apparently gives a different controller since then

$$\mathbf{K}(T) = \mathbf{0} \qquad (J_1) \qquad (14)$$

is necessary to achieve optimal control. In this context it is instructive to review related theory for time-invariant systems.

Kalman (1960) has shown that in the case of a stationary system, the assumption of controllability and absence of terminal cost implies $\lim_{T\to\infty} \mathbf{K}(t) = \mathbf{K}_0$, where $\mathbf{K}_0$ is a unique constant matrix obtained from the steady state Riccati equation.

In an analogous fashion, intuition as well as our computational experience suggests that as the final time T in the transient response objective function J_1 grows large for the nonstationary system with periodic coefficients, the gain matrix is periodic with period τ over most of the interval $[0, T]$. Thus if we integrate the Riccati equation backwards in time from T starting with $\mathbf{K}(T) = 0$, a periodic $\mathbf{K}$ matrix rapidly evolves.

Consequently, an excellent approximation to the optimal control can be obtained by extending the periodic gain matrix obtained for small times over the entire interval. Thus, the periodic gain matrix over the interval $[0, \tau]$:

$$\mathbf{K}(0) = \mathbf{K}(\tau) \qquad (15)$$

is extended according to

$$\mathbf{K}(t) = \mathbf{K}(t+\tau) \qquad (16)$$

for $t > \tau$. This approximate control has the advantage that only one period of the time-varying gain matrix need be stored in the controller memory.

Besides providing an excellent approximation to the optimal $\mathbf{K}$ for the transient response problem (case 1), the periodic $\mathbf{K}$ function just described satisfies all necessary conditions for the alternate problem of controlling a periodic response of the disturbed process (case 2). Thus, we see that the same feedback controller should meet the objectives for both of these cases. Such insensitivity to the mathematical formulation of the control objective and the need to store $\mathbf{K}$ and other required matrices only over a limited time interval are fortunate properties of the periodic process regulation problem.

Limited results on existence and uniqueness of the regulating controller just described are available. Sufficient conditions for existence of a periodic $\mathbf{K}$ matrix satisfying Equations (12) and (15) are stated in Bittanti, Locatelli, and Maffezoni (1971) and related by Chang (1972). Sanchez (1969) provides a sufficient condition for existence of one and multiple periodic solutions for the scalar case ($n = 1$). In the instance of $\mathbf{Q} = \mathbf{0}$ the explicit solution of the nonstationary Riccati equation (12) provided by Porter (1967) can be utilized to develop an algebraic equation for the proper initial condition $\mathbf{K}(0)$ leading to a periodic solution. Existence and uniqueness of a periodic $\mathbf{K}$ matrix then follows directly from existence and uniqueness of solutions of the algebraic equation. This matrix equation has the same form as the Liapunov matrix equation for which powerful solution techniques are available (Beavers and Dennman, 1973). Since we shall deal with nonzero $\mathbf{Q}$ matrices and the available theory for such cases is relatively weak, we shall proceed under the assumption that a satisfactory periodic solution to the Riccati equation exists. In the many chemical process examples we have investigated, there has been no difficulty in obtaining a approximately periodic $\mathbf{K}$ matrix by numerically integrating (12) backwards in time over a sufficiently large time interval.

Figure 1 provides a schematic illustration of implementation of this regulator. From the reference periodic process, which is in general nonlinear, the periodic Jacobian matrices $\mathbf{A}(t)$ and $\mathbf{B}(t)$ as well as the reference periodic state $\mathbf{c}_r(t)$ are determined. The matrix Riccati equation is then integrated until a periodic $\mathbf{K}(t)$ is obtained. Of course this calculation can be done off-line: only one period of the reference state $\mathbf{c}_r(t)$ and feedback gain $-\mathbf{R}^{-1}\mathbf{B}'(t)\mathbf{K}(t)$ must be stored in the memory of the on-line regulating controller. As shown in Figure 1, this controller acts on the deviation $\mathbf{x}(t)$ of $\mathbf{c}(t)$ from $\mathbf{c}_r(t)$ to give the deviation $\mathbf{u}(t)$ in the regulating control. This input, combined with the influences of the programmed periodic control $\mathbf{y}(t)$ and any disturbances $\mathbf{d}(t)$, determine the subsequent changes in the actual system state $\mathbf{c}(t)$.

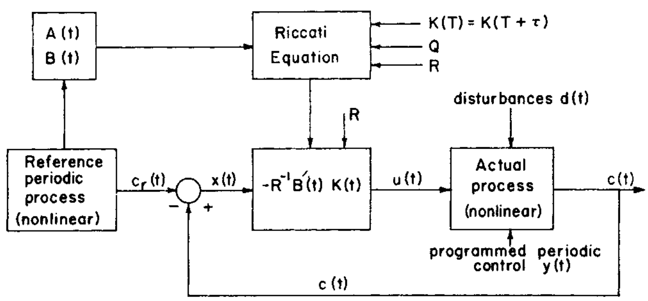

Fig. 1. Schematic diagram illustrating implementation of a feedback regulator for a periodic process.

GENERALIZED PROPORTIONAL-INTEGRAL REGULATOR

The feedback control law of Equation (11) may be viewed as a multivariable proportional controller with time-varying gains. Following the approach of Puri (1965) as later applied in several other control studies (see O'Connor and Denn, 1972) a generalized proportional-integral regulator can be developed for periodic processes. Derivation of such a control begins by including quadratic terms in the derivative of $\mathbf{u}$ $(= \dot{\mathbf{u}}(t))$ in the performance index. Thus, for case 2 discussed above where the disturbed system response is eventually periodic, it is necessary to minimize

$$J_2 = \frac{1}{2}\int_T^{T+\tau} [\mathbf{x}'(t)\mathbf{Q}\,\mathbf{x}(t) + \dot{\mathbf{u}}'(t)\mathbf{R}\,\dot{\mathbf{u}}(t)]dt \quad (17)$$

where $\mathbf{Q}$ and $\mathbf{R}$ have the properties stated in the previous section.

Minimization of J_2 in Equation (17) subject to condition (4) and a given value of $\mathbf{x}(0)$ is achieved as in previous investigations by transforming this optimization problem into the form considered earlier. To this end, $\dot{\mathbf{u}}$ is viewed as the control, and the state is augmented by a q-vector $x^{\neq}$ which is made identical to $\mathbf{u}$ by setting

$$\mathbf{x}^{\neq}(0) = \mathbf{u}(0) \quad (18)$$

and

$$\frac{d\mathbf{x}^{\neq}(t)}{dt} = \frac{d\mathbf{u}(t)}{dt} \overset{\Delta}{=} \tilde{\mathbf{u}}(t) \quad (19)$$

Now from Equations (4) and (19), the augmented $(n + q)$-dimensional state vector $\mathbf{x}$ from Equations (4) and (19)

$$\tilde{\mathbf{x}} \overset{\Delta}{=} \begin{bmatrix} \mathbf{x} \\ \mathbf{x}^{\neq} \end{bmatrix} \quad (20)$$

satisfies the linear ordinary differential equation

$$\frac{d\tilde{\mathbf{x}}(t)}{dt} = \tilde{\mathbf{A}}(t)\,\tilde{\mathbf{x}}(t) + \tilde{\mathbf{B}}(t)\,\tilde{\mathbf{u}}(t) \quad (21)$$

where

$$\tilde{\mathbf{A}}(t) = \begin{bmatrix} \mathbf{A}(t) & \mathbf{B}(t) \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \quad (22)$$

and

$$\tilde{\mathbf{B}}(t) = \begin{bmatrix} \mathbf{0} \\ \mathbf{I} \end{bmatrix} \quad (23)$$

Moreover minimization of J_2 given in Equation (17) is equivalent to minimizing

$$\tilde{J}_2 = \int_T^{T+\tau} [\tilde{\mathbf{x}}'(t)\tilde{\mathbf{Q}}\,\tilde{\mathbf{x}}(t) + \tilde{\mathbf{u}}'(t)\tilde{\mathbf{R}}\,\tilde{\mathbf{u}}(t)]dt \quad (24)$$

The problem of minimizing $\tilde{J}_2$ with respect to $\tilde{\mathbf{u}}(t)$ is formally equivalent to that considered earlier for derivation of the multivariable proportional regulator. Therefore, the solution given for that controller may be applied to the augmented problem posed here. The result is the periodic analog of a multivariable PI control for stationary systems. Since all of the previous comments concerning different objective functions, boundary conditions, existence and uniqueness also carry over immediately to the PI regulator problem, we may now consider application of these two regulators to lumped chemical processes.

EXAMPLE REFERENCE SYSTEM: A PERIODIC CSTR

In order to test the regulators derived above, we shall consider a continuous flow stirred-tank reactor (CSTR) in which the parallel reactions

$$S \rightarrow P_1 \quad (25.1)$$

$$S \rightarrow P_2 \quad (25.2)$$

occur. This system has already been analyzed in detail (Bailey et al., 1971; Matsubara et al., 1973) with the result that periodic fluctuations in reactor temperature can improve selectivity relative to steady state operation. While some minor modifications to encompass disturbances and process regulations are necessary, the model employed here is essentially the same as the one presented by Bailey et al. (1971).

$$\frac{dc_1(t)}{dt} = z(t)[d_1(t) - c_1(t)] - a_1c_1^{\alpha}(t)\exp[-1/c_4(t)] - a_2c_1(t)\exp[-\delta/c_4(t)] \quad (26.1)$$

$$\frac{dc_2(t)}{dt} = -z(t)c_2(t) + a_1c_1^{\alpha}(t)\exp[-1/c_4(t)] \quad (26.2)$$

$$\frac{dc_3(t)}{dt} = -z(t)c_3(t) + a_2c_1(t)\exp[-\delta/c_4(t)] \quad (26.3)$$

$$\frac{dc_4(t)}{dt} = z(t)[d_2(t) - c_4(t)] + y(t) \quad (26.4)$$

Here c_1, c_2, and c_3 are the dimensionless concentrations of S, P_1, and P_2, respectively. We shall assume that P_1 is the desired reaction product and that P_2 is waste. The dimensionless reactor temperature is c_4 while z is the dimensionless flow rate through the reactor. Flow rate will be considered here only as a potential regulating variable: it is therefore held constant during design of the reference system. Disturbances enter this system through either dimensionless feed reactant concentration (d_1) or feed temperature (d_2). The dimensionless heat flux y, although serving as the programmed control, can also be employed for process regulation. This is achieved by modification of the reference periodic program for $y(t)$ as explained below Equation (8).

In previous investigations of reference system ($z_r = d_{1r} = 1$, $d_{2r} = 0$) optimization, the objective was maximization of time-average production $P1A$ which in dimensionless terms is

$$P1A = \frac{1}{\tau}\int_0^{\tau} c_2(t)\,dt \quad (27)$$

If the system is characterized by the following dimensionless parameters

$$\alpha = 2 \qquad \delta = 0.55$$
$$a_1 = 10{,}000 \quad a_2 = 400 \quad (28)$$

and the programming control is constrained during reference process design by

$$0.049 = u_{\min} \leq y(t) \leq u_{\max} = 0.449 \quad (29)$$

the greatest P_1 production attainable by steady state reactor operation is $P1A = 0.0846$. On the other hand, if the heat flux cycles between its upper and lower design limits according to Equation (2) and

$$u(t) = \begin{cases} u_{\max} & 0 \leq t < 0.2 \\ u_{\min} & 0.2 \leq t < 1.2 \end{cases} \quad (\tau = 1.2) \quad (30)$$

then the resulting periodic reactor gives more desired product: $P1A = 0.0927$. This periodic process will be taken as the reference system in computational evaluation of our proportional and proportional-integral regulators.

Table 1. Regulating Control Specifications and Nomenclature for the CSTR Example

	$\mathbf{Q}$	$\mathbf{R}$	$\tilde{\mathbf{Q}}$	$\tilde{\mathbf{R}}$	Designation
Proportional controller using flow rate changes as regulating control	$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$	1/5			P-flow
Proportional controller using changes in heat flux program as regulating control	$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$	1/5000			P-heat
Proportional plus integral controller using flow rate changes as regulating control			$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	1/100	PI-flow
Proportional plus integral controller using changes in heat-flux program as regulating control			$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	1/5000	PI-heat
Proportional plus integral controller using changes in heat-flux program as regulating control			$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$	1/5000	PI-heat II

REGULATOR EVALUATION PROCEDURE

We have investigated the performance of both types of regulators for a variety of disturbances in feed conditions, including sinusoidal, random, and step changes. These simulations reveal that step changes provide the most severe test of the control system: any design which satisfactorily meets a step disturbance performs adequately in other situations. Consequently we shall consider here the two disturbances labeled A and B below:

A Disturbance: 10% step decrease in inlet reactant concentration and temperature ($d_1(t) = 0.9$, $d_2(t) = -0.1$ for $t > 0$).

B Disturbance: 10% step increase in feed reactant concentration and temperature ($d_1(t) = 1.1$, $d_2(t) = .1$ for $t > 0$).

It should be mentioned here that, while there are optimal design procedures which incorporate the influences of step disturbances (see Edgar et al., 1973), these were not explored because our present goal is a feedback regulator for any disturbance.

After investigating the effect of these disturbances in the absence of a regulating controller, the regulated system response was determined for a variety of control designs. Table 1 summarizes the design parameters, that is, the **Q** and **R** weighting matrices, for a number of different regulators whose designations are also given. Notice that, with the exception of the PI-heat II control, effort is concentrated on regulating the effluent product concentrations c_2 and c_3. This is accomplished by choosing **Q** or $\tilde{\mathbf{Q}}$ weighting matrices so that only $(c_2)^2$ and $(c_3)^2$ appear in the objective functions J or $\tilde{J}$.

A more difficult problem is suitable choice of R, which is a scalar since u is one-dimensional in all cases that are reported here. R must be chosen large enough to prevent excessive excursions of the regulating variable. On the other hand, R must not be so large that control action is overinhibited and insufficient regulating action is applied. We had little difficulty in determining acceptable values for R by trial and error. Although more systematic procedures have been proposed (Edgar et al., 1973), they are quite involved and appear to offer minimal advantages for this example.

Since it is not feasible to illustrate graphically the behavior of the reactor for all combinations of disturbances and regulator, it is convenient to introduce several quantitative indices of the system's performance. We shall employ the following:

$$P1A \triangleq \frac{\int_T^{T+\tau} z(t)\, c_2(t)\, dt}{\int_T^{T+\tau} z(t)\, dt} \tag{31}$$

$$\mathrm{DEV} \triangleq \int_T^{T+\tau} [x_1^2(t) + x_2^2(t) + x_3^2(t) + x_4^2(t)]\, dt \tag{32}$$

$$\mathrm{ERR} \triangleq \int_0^{T} [x_1^2(t) + x_2^2(t) + x_3^2(t) + x_4^2(t)]\, dt \tag{33}$$

In all of these quantities, T represents a time duration sufficiently long to permit the disturbed system to reach a periodic state. An eventual periodic state can be expected here since the disturbances are constant for $t > 0$. Thus, $P1A$ is the average amount of desired product formed. This quantity provides a measure of how well the regulating control maintains the design objective of maximum $P1$ production. DEV indicates how well the periodic behavior of the disturbed system with regulation approximates the design periodic state. ERR shows roughly how the system behaves in the transient period between imposition of the disturbance and achievement of a new periodic state. In the absence of disturbances, ERR provides a measure of the efficiency of start-up: All simulations were initiated with $c_i(0) = 0$ ($i = 1, 2, 3, 4$), and periodic conditions were achieved very accurately after twelve to sixteen cycles.

SIMULATION RESULTS

Table 2 summarizes many features of the periodic reactor when subjected to the A-disturbance. As comparison of the reference data with the results for no regulation reveals, a 10% step decrease in reactant concentration and feed temperature essentially stops $P1$ production. The need for a regulating control is evident. The third through sixth rows of Table 2 illustrate that all four feedback regulation schemes considered here substantially increase formation of the desired product and also decrease the differences in other state variables from their reference trajectories.

However, heat flux is a much more effective regulating variable than flow rate. This is apparent from Table 2 and from the desired product concentration cycle shown in Figure 2. While flow rate fluctuations influence all state variables directly, the heat flux directly enters only the reactor's energy balance. Thus, for heat flux regulation the reactor's temperature, which is the dominant variable determining selectivity, is kept in line while the other state variables are not influenced directly. This suggests that sensitivity studies might provide useful guidelines in choosing regulating variables for other situations. Another difference between flow rate and heat flux is the latter's role as the programming variable. With heat flux also used as the regulating variable, the reference program is modified to

TABLE 2. PERFORMANCE CRITERIA FOR THE UNDISTURBED REFERENCE SYSTEM AND THE REACTOR WITH 10% DECREASE IN FEED TEMPERATURE AND REACTANT CONCENTRATION. ALL ROWS EXCEPT THE FIRST REFER TO THE DISTURBED REACTOR

	P1A	ERR	DEV
Reference (undisturbed)	0.0927	0.8166	0.0000
No regulation	0.7×10^{-6}	8.4234	1.1620
P-flow	0.0499	1.7594	0.1036
PI-flow	0.0599	2.0880	0.0218
P-Heat	0.0837	0.6494	0.0093
PI-heat	0.0843	0.3690	0.0061
PI-heat II	0.0793	0.3340	0.0052

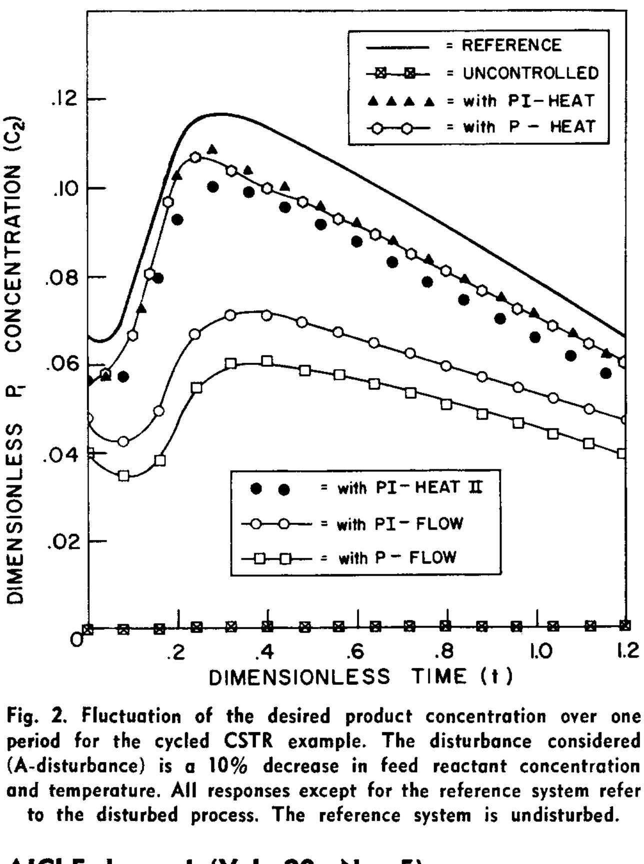

Fig. 2. Fluctuation of the desired product concentration over one period for the cycled CSTR example. The disturbance considered (A-disturbance) is a 10% decrease in feed reactant concentration and temperature. All responses except for the reference system refer to the disturbed process. The reference system is undisturbed.

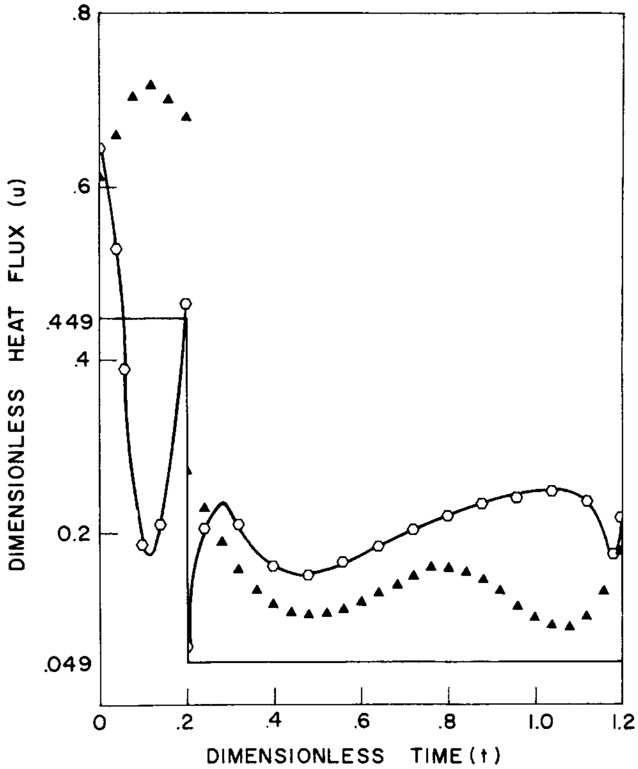

Fig. 3. One period of the heat flux control variable for the reference design periodic reactor and the disturbed reactor with proportional (P) and proportional-integral (PI) regulators. (A-disturbance; same legend as Figure 2).

meet the disturbance. Consequently, the variable manipulated in the reference system design provides a reasonable first guess for the variable of choice in process regulation.

Regardless of the choice of manipulated variable for this example, the PI algorithm provides more satisfactory control than the P version. The data in Table 2 and Figure 2 support this conclusion and show that the PI-heat regulator almost completely eliminates offset from the disturbed system. In order to appreciate fully the advantages of the PI regulator, the heat flux fluctuations dictated by the P and PI modes are given in Figure 3. Notice that the PI control action is substantially smoother and therefore involves less wear on control components.

Another interesting finding of our simulations which is not immediately apparent from the tabulated criteria in Table 2 is the influence of the $\tilde{Q}$ matrix on the PI-heat regulator's performance. As mentioned earlier, the PI heat control concentrates on keeping the two product concentrations close to their reference values. PI-heat II, on the other hand (See $\tilde{Q}$ in Table 1), attempts to minimize deviations in all four state variables by including all of their squares in the performance index. The numbers in Table 2 indicate that PI-heat II does better than PI-heat control from this standpoint: DEV is smaller in the former case. However, better control of the product concentrations is obtained by ignoring reactant and temperature fluctuations in the objective function. Thus, the PI-heat control gives a larger value for $P1A$ and maintains P_2 concentration closer to the design value. Figures 2 and 4 provide additional illustration of these features for the two regulators.

Several different phenomena appear when the disturbance has the opposite sign. In Table 3 are the parameters which characterize the reactor after the feed temperature and reactant concentration have increased 10% from their reference values. Here the average amount of desired prod-

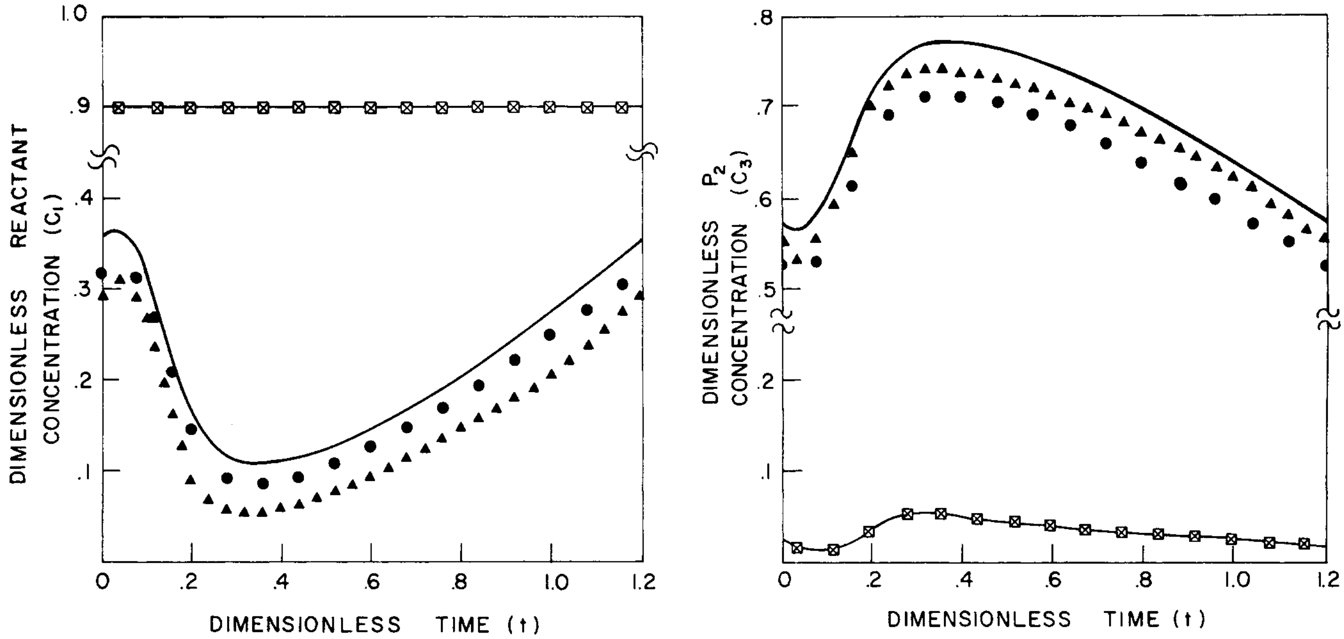

Fig. 4. Cycles of the reactant and waste product concentrations for different control design parameters. (A-disturbance; same legend as Figure 2).

uct $P1$ formed is increased by the disturbance so the need for regulation is questionable. If in addition we consider the average production $P2A$ of waste product

$$P2A \triangleq \frac{\int_T^{T+\tau} z(t) c_3(t) dt}{\int_T^{T+\tau} z(t) dt} \tag{34}$$

a possible motivation for a regulating control emerges. As a result of the B-disturbance, the reactor produces far more waste.

By adding a regulator we expect to reduce $P2A$ closer to the reference value, and this hypothesis is borne out by the results given in Table 3. Examination of the $P1A$ values reveals an unexpected reward of regulating control: production of P_1 is increased when a regulator is added! In the case of the PI-flow controller, 51% more of the desired product is made than with no control. Choice between the PI-flow and PI-heat regulators would depend on the relative value and cost of $P1$ and $P2$ since the PI-heat control gives less of both. This example reveals the potential importance of designing feedforward and/or adaptive process regulators to capitalize on certain disturbances. Nevertheless, the PI-heat control designed using the approach described above performs satisfactorily for both positive and negative disturbances to our example reactor.

In concluding this review of our simulation studies we should note from Table 3 that again the PI-heat regulator reduces the offset as indicated by DEV almost to zero. This attribute of the PI-heat control is clearly exhibited in Figure 5.

SUBOPTIMAL REGULATORS WITH TIME-INVARIANT GAINS

Implementation of the regulating controls discussed above should not be difficult because the gain matrices, while time-varying, are periodic. Still, it is important to consider regulators with constant gains. Controllers of this class require far less hardware and include classical feedback controls as a subcase.

TABLE 3. INFLUENCE OF REGULATING CONTROL ON SELECTIVITY AND OTHER MEASURES OF PERFORMANCE FOR THE CYCLIC REACTOR FOLLOWING A 10% STEP INCREASE IN FEED TEMPERATURE AND REACTANT CONCENTRATION. ALL ROWS EXCEPT THE FIRST ARE FOR THE DISTURBED PROCESS

	P1A	P2A	ERR	DEV
Reference (undisturbed)	0.0927	0.6923	0.8166	0.0000
No regulation	0.0945	0.9728	1.3185	0.1573
PI-flow	0.1433	0.8518	4.2158	0.0580
PI-heat	0.0955	0.7023	0.2916	0.0098

We have examined the performance of three different suboptimal regulators for the CSTR example considered above. In all cases, heat flux was employed as the regulating variable, and only the proportional mode was examined. The first constant gain controller, which will be denoted MA, is a multivariable proportional controller described by

$$\mathbf{u}(t) = -\mathbf{M}\,\mathbf{x}(t) \tag{35}$$

where the constant matrix $\mathbf{M}$ is the time-average of the varying gain in the optimal control of Equation (11):

$$\mathbf{M} \triangleq \frac{1}{\tau} \int_0^\tau \mathbf{R}^{-1}\,\mathbf{B}'(t)\,\mathbf{K}(t)\,dt \tag{36}$$

Recalling that y is the dimensionless heat-flux into the CSTR, classical proportional feedback controllers have the form

$$y(t) = -K_c\,x_i(t) \tag{37}$$

Two different versions of this form were tested. First, taking $x_i = x_2$, errors in the desired product concentration were used to drive control action. This control, which will be abbreviated CLAS 2, differs from CLAS 4 where temperature deviations motivate regulation (x_i in Equation (37) $= x_4$). In tests of these controllers K_c was adjusted for best results by trial and error.

Table 4 reveals how these suboptimal regulators compare with the optimal regulator for a 10% step decrease

Table 4. Comparison of Three Suboptimal Constant-Gain Controllers with the Optimal Varying Gain Regulator for a 10% Step Decrease in Feed Temperature and Reactant Concentration

	P1A	P2A	ERR	DEV	DEV 23
Reference (undisturbed)	0.0927	0.6923	0.8166	0.000	0.000
No regulation	0.7×10^{-6}	0.00034	8.4234	1.1620	0.5843
Optimal P-heat	0.0837	0.6790	0.6494	0.0093	0.0002
MA	0.0792	0.6804	0.6510	0.0088	0.00036
CLAS 2 ($K_c = 5$)	0.0764	0.430	0.5514	0.1140	0.0779
CLAS 4 ($K_c = 9$)	0.0775	0.5640	0.5952	0.0202	0.01826

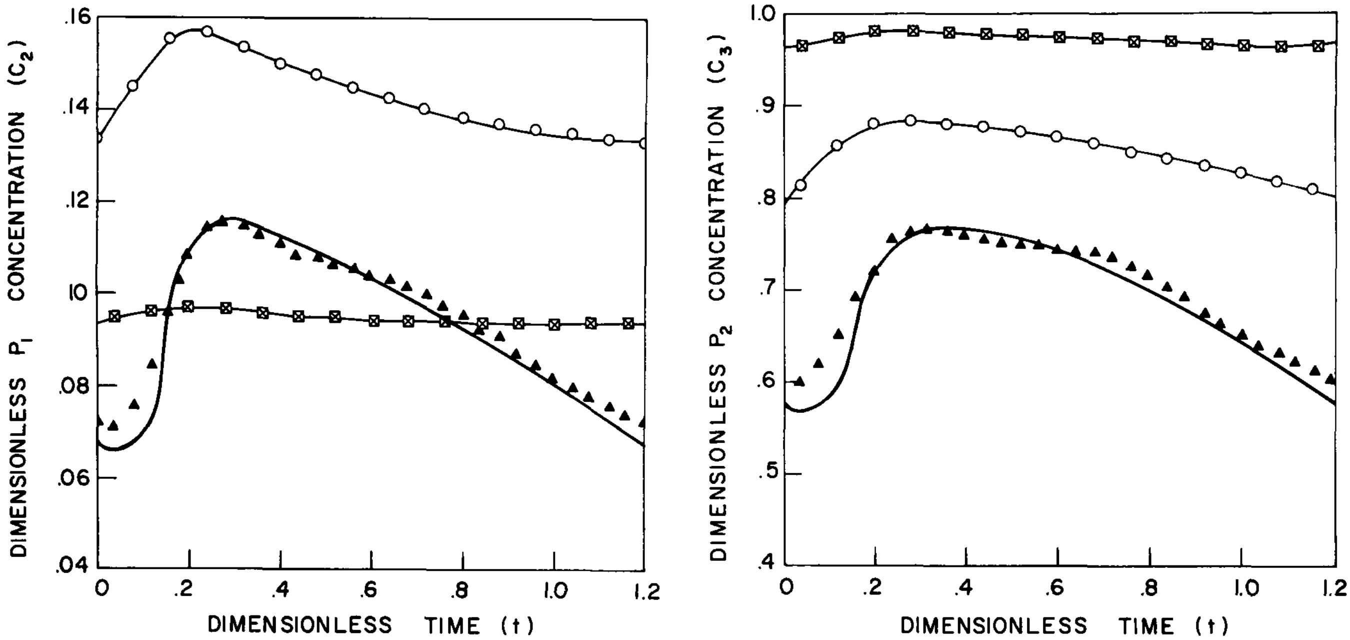

Fig. 5. Following a 10% increase in feed temperature and reactant concentration, the desired and waste product concentrations oscillate as illustrated. (Same legend as Figure 2.)

in feed temperature and reactant concentration. In general, the optimal regulator outperforms the constant gain controls although an apparent anomaly in Table 4 requires additional comment.

Although the averaged multivariable regulator *MI* gives a smaller value for DEV than the optimal control P-HEAT, the latter control was designed to minimize x_2 and x_3 fluctuations without concern for x_1 and x_4 errors. Comparison of DEV23, defined by

$$\text{DEV23} \triangleq \int_{T}^{T+\tau} [x_2^2(t) + x_3^2(t)]dt \tag{38}$$

shows that, as expected, the optimal control does best at meeting its objective.

Considering requisite control effort and quality of regulation, the multivariable averaged suboptimal control is the best of the constant-gain controls explored for this example. It does almost as well as the optimal control. We can expect intuitively, however, that the performance of any control procedure will vary significantly from system to system. Consequently, the comparisons evident for our CSTR example may not carry over to all other lumped systems. For this reason, examination of several regulation strategies should be undertaken for each specific problem.

CLOSING REMARKS

At the outset of our regulator derivation, small deviations from the reference periodic process were assumed. Consequently, the regulators developed here cannot be expected to perform so well when large disturbances buffet the process. Our simulations for a 30% decrease in feed temperature and concentration confirm this limitation (see Figure 6). To date, our efforts to obtain regulators for large disturbances have been unsuccessful. Among the candidate controllers considered was a periodic generalization of Luyben's nonlinear feedforward control (Luyben, 1968; Liaw, 1973).

Several potentially important periodic separation processes are described by partial differential equations and consequently lie beyond the scope of this work. In a later publication, we will discuss regulators for distributed periodic systems using continuous parametric pumping (Chen et al., 1972) as an example.

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NOTATION

a_1, a_2 = kinetic parameters
$\mathbf{A}$ = state coefficient matrix in linearized model
$\tilde{\mathbf{A}}$ = augmented state coefficient matrix; see Equation (22)
$\mathbf{B}$ = control coefficient matrix in linearized model

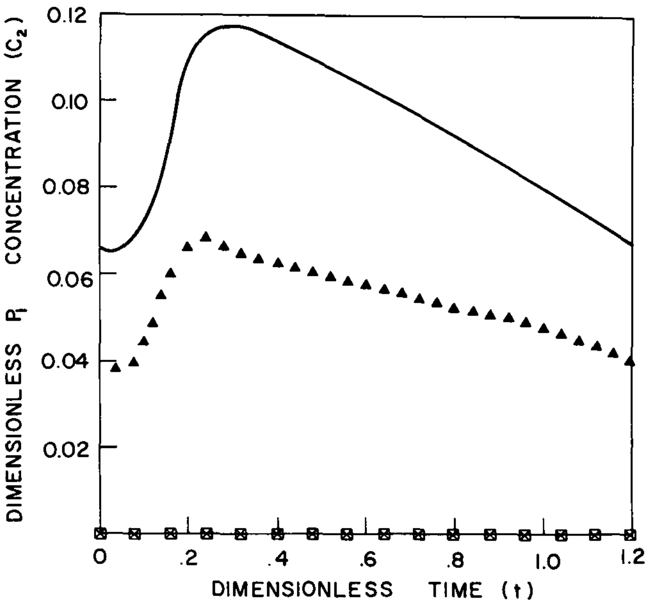

Fig. 6. The PI-regulator fails to maintain the design output of desired product following a 30% step decrease in inlet reactant concentration and temperature (same legend as Figure 2.)

$\tilde{\mathbf{B}}$ = augmented control coefficient matrix; see Equation (23)
c = state vector
c_1 = dimensionless S concentration in example
c_2 = dimensionless P_1 concentration in example
c_3 = dimensionless P_2 concentration in example
c_4 = dimensionless temperature in example
d = disturbance vector
d_1 = dimensionless feed concentration disturbance to CSTR
d_2 = dimensionless feed temperature disturbance for cyclic reactor example
DEV defined in Equation (32)
DEV 23 defined in Equation (38)
ERR defined in Equation (33)
f = function specifying state time derivative
I = identity matrix
J_1 = objective function for short-lived disturbances; see Equation (9)
J_2 = objective function for sustained disturbances; see Equation (10)
K_c = proportional gain
K = solution of Riccati Equation (12)
M = constant gain matrix defined in Equation (36)
P_1, P_2 = desired and waste reaction products, respectively
$P1A$, $P2A$ = time-average production of P_1 and P_2, respectively
Q, $\tilde{\mathbf{Q}}$ = weighting factor for state deviation in P-control, PI-control respectively. See Equations (9) and (24)
R = scalar control deviation weighting factor in example
R, $\tilde{\mathbf{R}}$ = weighting matrices for control deviation in P-control, PI control, respectively
S = reactant
t = time
T = a time large compared to the system's characteristic response time
u = control deviation; see Equation (7)
x = state deviation; see Equation (5)
y = dimensionless heat flux for CSTR problem
y = programmed control
z = dimensionless flow rate in CSTR example
z = regulating control

Greek Letters

α = order of the reaction $R \rightarrow P_1$
δ = dimensionless activation energy
τ = dimensionless period

Subscripts

$(\ )_r$ denotes conditions pertaining to the (undisturbed) reference periodic process

Superscripts

$(\ )'$ = matrix transpose
$(\dot{\ })$ = time derivative

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