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Optimality and Computational Feasibility in Transient Control: Part I. A Modified Criterion for Optimality

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The notion of optimality with regard to transient control is critically examined with a particular view toward the computational difficulties of solving the optimal control problem, and the arbitrary aspects of the usual objective functions. Realizing a need for effective approximations, a criterion for transient control is developed which requires a minimum of computational effort to apply in practice. Optimality is achieved in an instantaneous sense, and it is argued that overall optimality is well approximated for many cases of practical interest. To demonstrate its use, the criterion is applied to the transient control of a stirred-tank reactor. Numerical examples are given and the results are discussed and compared with those obtained by alternative methods.

The subject of mathematical optimization is intimately tied to the matter of objectives. The very concept of optimality is, in fact, predicated upon the notion that the numerous factors which determine the quality of performance can be combined and properly accounted for by a single performance index. Perhaps maximum net profit is the most meaningful of many possible indicators of optimality, but the formulation of such an index of performance requires a detailed economic analysis involving many factors, some (such as safety) difficult to judge accurately in terms of monetary values. Although performance indices have been devised in this manner (5), the arbitrary quality of the performance index is difficult to eliminate altogether. As more factors are taken into consideration, the objective function becomes unwieldy and of limited usefulness in obtaining practical solutions to the control problem.

Optimization with respect to other indices of performance may be viewed as an expedient means of approximating the condition of maximum profit. For example, it is sometimes required that the system attain a desired state in the minimum possible time (*11, 13*). Although such a strategy is generally compatible with a desire for maximum profits, it is not difficult to conceive of instances where a higher return would result from an increase in the duration of the transient: perhaps the cost of time optimal control is excessive or the product quality is poor. Similarly, minimizing some other performance index, say, mean square deviation of a critical state variable, might more or less approximate maximum profit. It is thus important to bear in mind in comparing various strategies of control that each is based on a somewhat arbitrary measure of effectiveness. Although superficially the object of control may be to minimize rigorously some particular performance index, the index itself must be subjectively formulated. Whether the resulting control is acceptable or not must be determined by the designer. From an engineering point of view the decision on a suitable objective function does not entirely precede the optimization but is, in an important sense, part of it.

These considerations not withstanding some measure of system performance must be chosen. One common form of the optimal control problem is to determine that control policy $\mathbf{u}(t)$ which minimizes the reasonable but of necessity somewhat arbitrary criterion:

$$J[\mathbf{u}(t)] = \int_o^{t_f} \sum_{i=i}^{n} a_i [x_i(t) - x_i^d]^2 \, dt \qquad (1)$$

where the x_i are the system state variables usually related by equations of the form

$$\dot{x}_i = f_i[x_1(t), \ldots, x_n(t); u_1(t), \ldots, u_p(t)]; \quad i = 1, 2, \ldots, n \qquad (2)$$

or in vector notation:

$$\dot{\mathbf{x}} = \mathbf{f}[\mathbf{x}(t); \mathbf{u}(t)] \qquad (3)$$

with initial state $\mathbf{x}^o$ and desired operating state $\mathbf{x}^d$. In addition, it may be required that the system satisfy a set of physically imposed constraints on the control variables of the form

$$(u_j)_{\min} \leqq u_j(t) \leqq (u_j)_{\max}; \quad j = 1, 2, \ldots, p \text{ all } t \geqq 0 \qquad (4)$$

If the system can be adequately described by Equation (3), a large body of relatively well-developed theory can be applied to determine the optimal control strategy. In principle, the problem may be attacked by any of several powerful methods: Pontryagin's maximum principle (*9, 13*), the calculus of variations (*4, 9*), dynamic programming (*2, 11*), or various gradient techniques (*7, 9*). To apply these methods in practice, however, normally requires an enormous amount of computation. A solution by either Pontryagin's maximum principle or the calculus of variations necessitates the simultaneous solution of a set of two-point boundary-value problems, usually nonlinear. The dynamic programming approach effectively avoids the boundary-value problem but may require a great deal of computer time and memory to search out the optimum strategy of control. A similar difficulty is encountered with gradient (hill-climbing) techniques which converge on an extremal solution through a systematic repeated integration of the system equations, each iteration obtaining a better estimate of the optimal control policy.

In view of the foregoing, it would seem reasonable to seek simpler methods of arriving at a control policy, perhaps sacrificing some degree of optimality for the sake of easing the computations. An important step in this direction was suggested by Rosenbrock (*12*), who considered the plausibility of utilizing control to achieve an instantaneous rather than an overall optimum. He was able to develop necessary and sufficient conditions corresponding to the maximum instantaneous rate of decrease of a disturbance function associated with a linearized model of a distillation column, but excepting a rather restrictive set of circumstances, no attempt was made to translate the conditions into explicit control requirements. Since the method calls for matching areas enclosed by two curves which may repeatedly intersect, it would seem a difficult task to obtain a general control criterion corresponding to Rosenbrock's instantaneous optimum. The need for such near-optimal schemes was recognized also by Grethlein and Lapidus (*6*), who formulated a predictor-controller which will be compared and contrasted to this research in the following.

Yet another approach to near optimization was studied in detail for a chemical engineering extraction application by Koepcke and Lapidus (*8a*). By using a Liapunov function as a measure of system deviation, these authors developed the argument that "the optimum control vector is that **u** which makes [the change in the Liapunov function] the most negative." This method has the merit of giving a control system guaranteed to be stable, but the price of this guarantee is a considerable (unknown) degree of conservatism. Again, an arbitrary condition has been included: that the objective function be sufficient (not necessary) to assure stability. To be sure this is not an unreasonable requirement but for practical results it is not necessary to limit the design so narrowly. In releasing the constraint that the deviation measure be a Liapunov function, the entire class of sign indefinite changes is allowed, and the relative ease in forming J permits the treatment of otherwise impractical nonlinear functions.

The matter of stability thus remains in theory an open question, since it is neither guaranteed by a Liapunov function integrand as in Koepcke and Lapidus nor, as in Kalman and Bertram (*8*), by a Liapunov integral; however, as emphasized by the latter authors, and shown in the numerical results of this study, many optimum systems will in fact be stable. This point must be checked in each case.

A CRITERION FOR TRANSIENT CONTROL

The approach to be considered is limited to systems of a slightly more restrictive form than Equation (2); that is, let the dynamics of the controlled system be described by n equations of the form

$$\dot{x}_i = u_1 f_{i1} + u_2 f_{i2} + \ldots + u_p f_{ip} + g_i; \quad i = 1, 2, \ldots, n \qquad (5)$$

where $f_{i1}, f_{i2}, \ldots, f_{ip}$ and g_i are any continuous linear or nonlinear functions of the state variables $x_1(t)$, $x_2(t)$, $\ldots$, $x_n(t)$. Equations (5) are applicable whenever the system is linear with respect to the chosen control variables; it may be written in vector notation as

$$\dot{\mathbf{x}} = \mathbf{F}\mathbf{u} + \mathbf{g} \qquad (6)$$

The difference between the instantaneous state of the system and its desired state may be expressed by defining a deviation vector $\mathbf{y}(t)$ as

$$\mathbf{y}(t) = \mathbf{x}(t) - \mathbf{x}^d \qquad (7)$$

Consider a positive definite scalar function E of the quadratic form

$$E = \mathbf{y}^T \mathbf{A}\, \mathbf{y} \qquad (8)$$

where $\mathbf{A}$ is a symmetric matrix of constants of order n with element a_{ij}. It is desired to obtain a criterion by which the elements of $\mathbf{u}$ may be set according to the instantaneous state of the system such that the time derivative $\dot{E}$ will always take on its minimum possible value. The physical interpretation of such a criterion will be examined in the ensuing discussion. Since $\mathbf{A}$ is symmetric, the time derivative of E is given by

$$\dot{E} = 2\, \mathbf{y}^T \mathbf{A}\, \dot{\mathbf{y}} \qquad (9)$$

and by substituting for $\mathbf{y}$ and $\dot{\mathbf{y}}$ from Equations (6) and (7)

$$\dot{E} = \mathbf{b}^T \mathbf{u} + \phi \qquad (10)$$

where $\mathbf{b} = 2\, \mathbf{F}^T \mathbf{A}\, \mathbf{y}$ ($\mathbf{b}$ is a p vector), and $\phi = 2\, \mathbf{y}^T \mathbf{A}\, \mathbf{g}$ (ϕ is a scalar). Expansion of Equation (10) yields

$$\dot{E} = b_1 u_1 + b_2 u_2 + \ldots + b_p u_p + \phi \qquad (11)$$

It is evident from Equation (11) that a minimum instantaneous $\dot{E}$ is obtained by setting

$$\begin{aligned} u_j &= (u_j)_{\max} \text{ whenever } b_j < 0 \\ u_j &= (u_j)_{\min} \text{ whenever } b_j > 0 \end{aligned} \quad ; j = 1, 2, \ldots, p \qquad (12)$$

The resulting control policy will thus be of the relay or bang-bang type, a result expected from prior applications of the maximum principle (*13*). The possibility of singu-

lar control (values of u sustained for a finite period between the limits) that arises from application of the maximum principle is not a practical concern in this case, for it may be seen from Equation (11) that there is no advantage to the objective in a sustained $b_j = 0$. The switching points for each u_j do, however, correspond to the instantaneous conditions $b_j = 0$. An expression for each b_j can be obtained by expanding the defining matrix equation $\mathbf{b} = 2\,\mathbf{F}^T\mathbf{A}\,\mathbf{y}$:

$$b_j = 2\sum_{k=1}^{n}\sum_{i=1}^{n} f_{ij}(\mathbf{x})\, a_{ki}\, y_k;\ j = 1, 2, \ldots, p \qquad (13)$$

In applying this criterion the quadratic E function may be associated with a family of surfaces $E = c$, $c \geq 0$, the nature of which depends on the choice of the A matrix. It is difficult to attach physical significance to the surfaces generated by many otherwise acceptable A matrices. One possibility, however, which is amenable to a meaningful interpretation is to set all off-diagonal elements equal to zero so that by Equation (8), E is given as

$$E = a_1y_1^2 + a_2y_2^2 + \ldots + a_ny_n^2;\ \text{all } a_i \geq 0 \qquad (14)$$

where the double subscript formerly used to specify the elements of A is no longer necessary, that is, $a_i = a_{ii}$. For this special case, the b_j of Equation (12) is given by the single summation

$$b_j = 2\sum_{i=1}^{n} f_{ij}(\mathbf{x})\, a_i\, y_i \qquad (15)$$

The details of the necessary computation are outlined in the Appendix.

As an illustration in two dimensions, the contours of constant E for $a_1 = a_2 = 1$ are a family of circles about the desired state. At any point in the x_1, x_2 plane, E is a measure of the Euclidian distance from the given state to the desired state (x_1^d, x_2^d). By continuously making $\dot{E}$ as negative as possible, the rate of motion toward (x_1^d, x_2^d) is always at a maximum, or if away from the desired point, it is always as small as possible. However, since the variables x_1 and x_2 may in fact be fundamentally unlike, for example, temperature and concentration, it becomes necessary to weight the terms appropriately by including the factors a_1 and a_2, the contours of constant E becoming a family of concentric ellipses. These constants should also be chosen so as to account for the relative importance of x_1 and x_2 in the analysis, but again the choice of weighting constants is of necessity somewhat arbitrary. With regard to steepest ascent methods for static optimization problems, a lucid description of the effect of weighting constants is given by Wilde (*14*). The general n dimensional case may be interpreted analogously.

A clearer picture of the nature of this approach is obtained when the control policy required to minimize instantaneously $\dot{E}$ is compared with that required to minimize the integral performance index of Equation (1). The integrand of Equation (1) is exactly the E function of Equation (14), so that

$$J = \int_o^{t_f} E\, dt \qquad (16)$$

The control policy $\mathbf{u}_{opt}$ may be interpreted as the control which minimizes J, the area under the $E(t)$ curve. In contrast, the criterion of Equation (12) leads to a response in which the associated value of E is always forced to decrease as fast as possible or increase as slowly as possible. The $\mathbf{u}(t)$ which obtains this goal may differ from the $\mathbf{u}_{opt}(t)$ required to minimize J. It may, for example, be wiser at certain times to decrease E more slowly than is possible in order to permit an even faster decrease at other times, thus obtaining a lesser area under the E versus t curve. Such a possibility is not taken into account when $\dot{E}$ is instantaneously minimized. It is not difficult to envision instances where the inability of the control scheme to reckon with the long-range effect of control decisions could result in an unsatisfactory or even unstable control system. Nevertheless, it will be shown that the simpler control criterion can provide satisfactory control for systems of practical interest. Each potential application must be examined individually.

APPLICATION TO A STIRRED REACTOR

Consider a simple model of a stirred-tank reactor described by one heat balance and one material balance:

$$\frac{dT}{dt} = \frac{q}{V}T_o - \frac{q}{V}T - \frac{\Delta H}{\rho C_p}r - \frac{UA_r}{\rho C_pV}(T - T_c)$$
$$\frac{dc}{dt} = \frac{q}{V}c_o - \frac{q}{V}c - r \qquad (17)$$

The control variables are the heat transfer coefficient U and the feed flow rate q, limited in range by

$$U_{min} \leq U \leq U_{max}$$
$$q_{min} \leq q \leq q_{max} \qquad (18)$$

The choice of U as a control variable is primarily for the sake of simplicity. It has been shown (*1*) that U may be regarded as a good first approximation to an algebraic function of the cooling water flow rate. By writing the system equations in the form of Equation (5)

$$\dot{x}_1 = u_1f_{11} + u_2f_{12} + g_1$$
$$\dot{x}_2 = u_2f_{22} + g_2 \qquad (19)$$

where

$$x_1 = T,\ x_2 = c,\ u_1 = U,\ u_2 = q$$

and

$$f_{11} = \frac{A_r}{\rho C_pV}(T_c - x_1)$$
$$f_{12} = \frac{1}{V}(T_o - x_1)$$
$$f_{22} = \frac{1}{V}(c_o - x_2) \qquad (20)$$
$$g_1 = -\frac{\Delta H}{\rho C_p}r$$
$$g_2 = -r$$

By using the results of the last section [Equations (12) and (15)], the control criterion for u_1 is

$$u_1 = (u_1)_{max} \equiv U_{max} \text{ whenever } b_1 = 2f_{11}a_1(x_1 - x_1^d) < 0$$
$$u_1 = (u_1)_{min} \equiv U_{min} \text{ whenever } b_1 > 0 \qquad (21)$$

and for u_2

$$u_2 = (u_2)_{max} \equiv q_{max} \text{ whenever } b_2 < 0$$
$$u_2 = (u_2)_{min} \equiv q_{min} \text{ whenever } b_2 > 0 \qquad (22)$$
$$b_2 = 2\,[f_{12}\,a_1\,(x_1 - x_1^d) + f_{22}\,a_2\,(x_2 - x_2^d)]$$

RESULTS OF CONTROL

To demonstrate the performance of the proposed control scheme, two numerical examples will be considered.

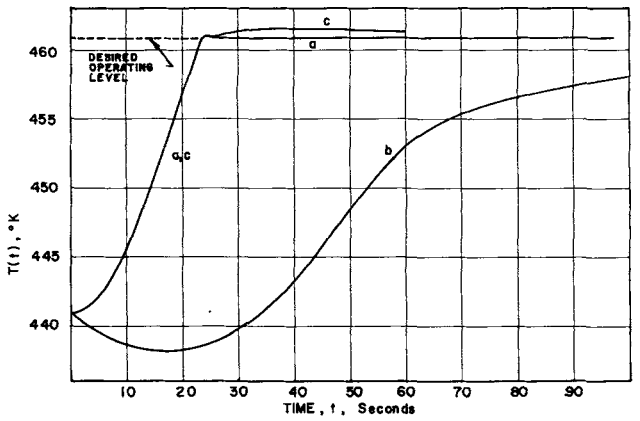

Fig. 1. Transient temperature responses of a stirred reactor. (*a*) Control with unlimited switching. (*b*) No control. (*c*) Control with limited switching.

With Equation (17) as a description of the system dynamics, the reaction rate term r is assumed (in order to provide concrete examples) to be a first-order Arrhenius expression:

$$r = N\,c \exp\,(-Q/T) \tag{23}$$

The parameters are given as follows:

N	$= 7.86 \times 10^{12}$ sec.$^{-1}$	C_p	$= 1.0$ cal./(g.)(°K.)
Q	$= 14{,}090$°K.	ρ	$= 0.001$ g./cc.
A_r	$= 10$ sq.cm.	T_o	$= 350$°K.
V	$= 1{,}000$ cc.	T_c	$= 340$°K.
c_o	$= 6.5 \times 10^{-6}$ g.-moles/cc.	ΔH	$= -27{,}000$ cal./g.-mole

(24)

Letting the control variables U and q assume steady state values of

$$(u_1)_{ss} = U_{ss} = 5.0 \times 10^{-4} \text{ cal./(sq.cm.)(sec.)(°K.)}$$
$$(u_2)_{ss} = q_{ss} = 10 \text{ cc./sec.} \tag{25}$$

one obtains the steady state solution of Equation (17) given by

$$(x_1)_{ss} = T_{ss} = 460.91\text{°K.}$$
$$(x_2)_{ss} = c_{ss} = 1.531 \times 10^{-7} \text{ g.-moles/cc.} \tag{26}$$

The conditions of Equation (26) represent the desired state of the process. The initial state of the process is given as

$$x_1^\circ = T(0) = 440.91\text{°K.}$$
$$x_2^\circ = c(0) = 3.531 \times 10^{-7} \text{ g.-moles/cc.} \tag{27}$$

These parameter values were chosen to allow a direct comparison of the results with the numerical example presented in the work of Grethlein and Lapidus (*6*). For the same reason, the E function weighting factors a_1 and a_2 are given the respective values 10^{-4} and 10^{12}, and for the moment it is supposed that the feed flow rate must remain constant at $q = q_{ss} = 10$ cc./sec. and that U may be varied as desired between the limits $0 \leq U \leq 8.0 \times 10^{-4}$ cal./(cc.)(sec.)(°K.). By so doing, q is effectively eliminated as a control variable, leaving U as the solitary means of control.

Following Equation (21), the initial value of $b_1 = +0.4036$, and the corresponding control setting for u_1 is therefore $u_1 = U_{\min}$ at $t = 0$. This result is physically reasonable: minimum cooling is required at first in order to more quickly increase the reaction temperature. Throughout the transient, the computer-controller acts at increments of Δt real time units to evaluate the sign of b_1 and accordingly to set the control variable either to $U_{\min}$ or to $U_{\max}$ for the following increment. In this manner the controlled system response shown in Figures 1 to 3 (curve *a*) is obtained for increments of $\Delta t = 0.05$ sec. To satisfy the criterion, the control setting for the first 23.70 sec. of the transient must be maintained at $u_1 = U_{\min}$. At 23.70 sec., the calculated value of b_1 is negative, thereby requiring a switch in control setting to $u_1 = U_{\max}$. The next switch in control occurs at $t = 25.65$ sec., where again $b_1 > 0$, requiring that $u_1 = U_{\min}$. From this point on, u_1 begins switching ("chattering") back and forth between $U_{\max}$ and $U_{\min}$, the sign of b_1 changing with nearly every evaluation. The value of the integral J remains unchanged (to five significant figures) at 1.8469 after the first 30 sec. of the transient.

With no control at all, that is, letting $U = U_{ss}$ throughout the transient, a numerical integration of the system equations [Equations (17) or (19)] yields the response shown in Figures 1 to 3 as curves *b*. Also shown in the figures is a plot of the E function vs. time. It is interesting to note that early in the transient the process exhibits a tendency to move away from rather than toward the desired steady state. The result is a temporarily positive slope of $E(t)$, showing that this function could not have been used as a Liapunov function. For the uncontrolled response, the transient is essentially complete after 150 sec. of real time and to a good approximation $J = 11.604$. Comparison of the J values shows clearly that the

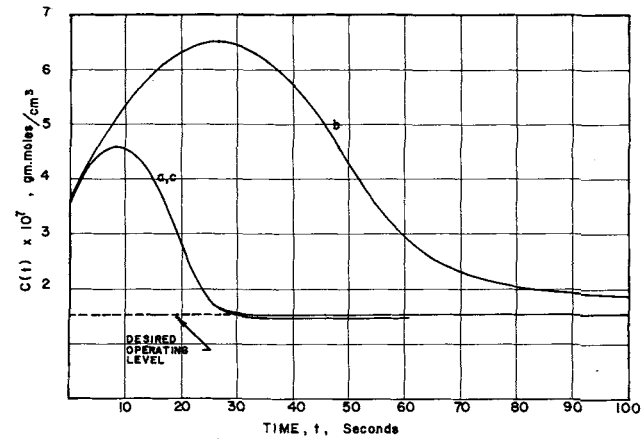

Fig. 2. Transient concentration responses of a stirred reactor. (*a*) Control with unlimited switching. (*b*) No control. (*c*) Control with limited switching.

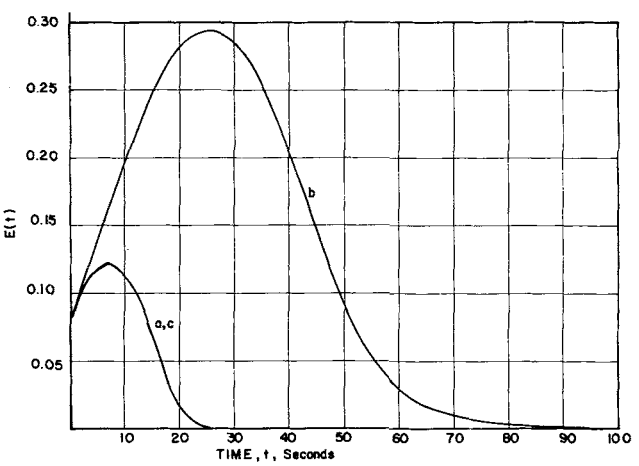

Fig. 3. The E function vs. time. (*a*) Control with unlimited switching. (*b*) No control. (*c*) Control with limited switching.

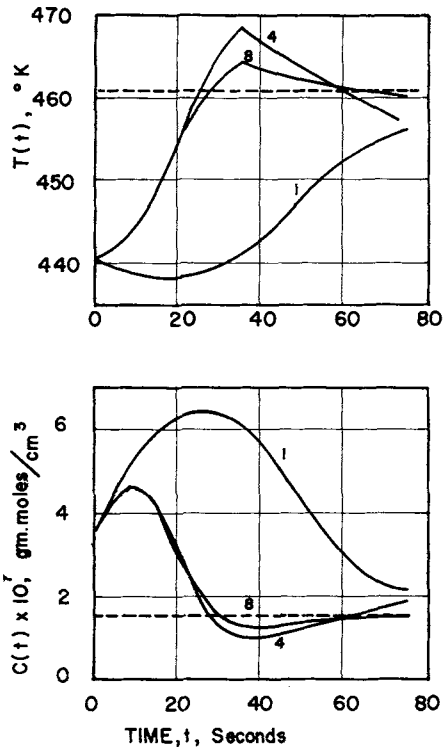

Fig. 4. Transient response by method of Ho and Brentani after first, fourth, and eighth iterations. Numbers of iterations are shown on plots. Broken line represents desired operating level.

computer-controller scheme appreciably improves the system performance.

LIMITED SWITCHING

Since E is an instantaneous measure of the difference between the actual and desired system states, it is reasonable to expect that the value of E will become very small as the transient nears the final time t_f. Noting that E is in fact the integrand of the integral performance index [Equation (16)] the value of J would therefore not be affected significantly by E during the latter portion of the transient (so long as E remains small). If the desired state is a stable steady state, it follows that it may often be possible to set each $u_j = (u_j)_{ss}$ near the end of the transient with little loss of optimality.

When this is indeed possible, a final switch of the control variables to their steady state values eliminates undesirable chatter, for it is apparent that unless the control variables are allowed to assume their steady state values the system will begin chattering as an effort is made to maintain the desired state. This is a well-known phenomenon of bang-bang control systems (3). The desired state will necessarily be attained when the control variables are given their steady state values, provided of course, that the desired state is an asymptotically stable steady state.

An additional criterion is needed for determining the time of final switching to $(u_j)_{ss}$. One such criterion is simply to allow each control variable to switch between extremes a specified number of times [by Equation (12)] with a subsequent and final switch to $(u_j)_{ss}$. The results of Siebenthal and Aris (13) and Grethlein and Lapidus (6) suggest that for a single control variable only one switch is likely to occur until perhaps very near the end of the transient. The first of these investigations is based on rigorous optimization by using Pontryagin's maximum principle.

By applying this strategy to the example at hand, the control policy and transient performance are identical with the previous case until the second switching time for u_1, which occurs at $t = 25.65$ sec. At this point, however, u_1 switches to the steady state value U_{ss} for the remainder of the transient. As a result, the response overshoots the desired state by a small amount as shown in Figures 1 to 3, curves *c*. In terms of the integral performance index, the sacrifice is slight: after 60 sec. $J = 1.8486$. In comparison with the uncontrolled J value of 11.604, it is apparent that two switches, $U_{\min}$ to $U_{\max}$ to U_{ss}, provide very nearly as much improvement in system performance as the scheme allowing an unlimited number of switches.

COMPARISONS WITH OTHER APPROACHES

It is appropriate to compare the above results with those of Grethlein and Lapidus and with those obtained by one of the integral optimization techniques, a gradient method proposed by Ho and Brentani (7).

In the first of these references, the control policy is chosen at discrete times by comparing predicted responses of the system for three alternative policies over the interval to follow. On the one hand, a long sampling period is desirable in order that the effect of various control decisions can be foreseen over the largest possible time interval. On the other hand, the decisions are binding over the entire sampling period and the control setting cannot be altered between two sampling points, even if a better response would result. Regardless of the choice of sampling period, $(3)^p$ complete integrations of the system equations are required to determine the control policy for p control variables.

As a compromise, Grethlein and Lapidus chose a ½-sec. sampling period and found that the control policy should consist of minimum cooling ($u_1 = U_{\min}$) for the first 24.0 sec., maximum cooling ($u_1 = U_{\max}$) for the next 3 sec., and intermediate control settings for the remainder of the transient (about 5 sec.). Thus for the first

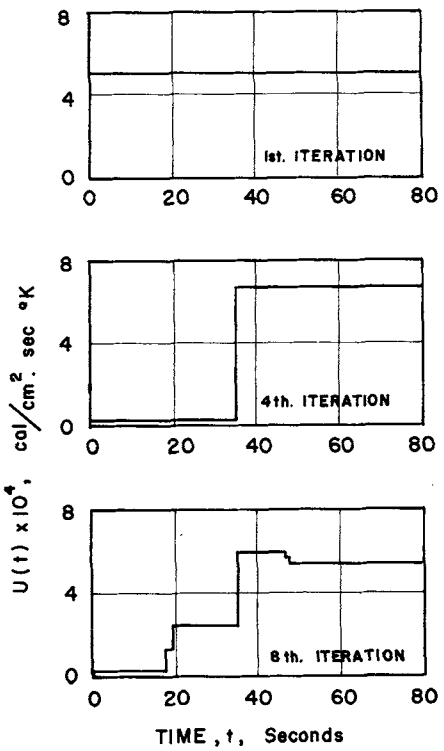

Fig. 5. Control policies which correspond to first, fourth, and eighth iterations for gradient solution.

23.70 sec., that is, until the first switch is required by the E function criterion, the control policies and transient responses are identical by the two methods. It is apparent from Figures 1 to 3 (curves a) that slight differences in switching from that point on affect only the tail-end of the transients and do not contribute greatly to the overall performance. The corresponding J values are 1.8527 from reference 6 and 1.8469 by the E function approach.

By applying the approach of Ho and Brentani (7) to the problem at hand, the control policy is sought which rigorously minimizes the integral performance index. The total transient period, taken as 75 sec., is divided into ½-sec. intervals and, as an initial guess, u_1 is set equal to U_{ss} throughout the transient. By the iterative process described in detail in the reference cited, the values of u_1 over each ½-sec. interval are repeatedly modified, with each iteration corresponding to a lesser value of J. The results after the first, fourth, and eighth iterations are shown in Figures 4 and 5.

The effectiveness of each iteration can perhaps best be expressed in terms of the corresponding values of J. By letting J_i denote the value of J for the i^{th} iteration

$$\begin{aligned} J_1 &= 11.6 & J_5 &= 2.08 \\ J_2 &= 4.48 & J_6 &= 2.03 \\ J_3 &= 2.33 & J_7 &= 2.00 \\ J_4 &= 2.13 & J_8 &= 1.98 \end{aligned} \qquad (28)$$

After eight iterations it was felt that the reduction in J per iteration was insufficient to warrant further computation. From the general trend of values for J_i, it appears unlikely in this example that the gradient technique would converge to a control policy for which the associated J value would be appreciably lower than either that obtained by the E function criterion ($J = 1.8469$), or that of Grethlein and Lapidus' results ($J = 1.8527$). As a further test, the control policy from the Lapidus and Grethlein calculations was used as an initial guess and after three iterations no reduction in J was observed (to five significant figures).

DUAL-VARIABLE CONTROL

In the example of the previous sections the heat transfer coefficient U was used as the control variable. This section considers dual-variable control, manipulating U and q simultaneously. The permissible ranges on these variables are set at

$$\begin{aligned} 0 \leqq u_1 \leqq 8.0 \times 10^{-4} &\quad \text{cal./(cc.)(sec.)(°K.)} \\ 0 \leqq u_2 \leqq 20.0 &\quad \text{cc./sec.} \end{aligned}$$

where $u_1 = U$ and $u_2 = q$. The criteria used to determine the optimum values for u_1 and u_2 at any given time are again given by Equations (21) and (22).

The response of the system to this control is shown in Figure 6, in which curve a was obtained by allowing both control variables to switch an unlimited number of times between their limiting values and curve c by switching each control variable to its nominal value as its second switching time is reached. In either case, a significant improvement over single variable control is obtained. If an unlimited number of switches is allowed, $J = 0.5973$ and with two switches per control variable $J = 0.9485$. These values may be compared with the best single variable control J value of 1.8469. It should be emphasized that when two or more control variables are simultaneously used to control the system, the computational benefits of the proposed control scheme become especially prominent.

DISCUSSION

Above all, it should be noted that the primary advantage of using Equation (12) as a criterion for control is its extreme simplicity in comparison with the available alternatives. As has been indicated, the methods which fully account for the effect of the interaction of control decisions on the overall transient behavior require very extensive calculations. The approach of Lapidus and Grethlein retains a modicum of predictive capacity at the expense of having to perform $(3)^p$ integrations of the dynamic equations. On the other hand, the continuous minimization of $\dot{E}$ is at all times based on the instantaneous state of the system and requires no test integrations or iterative matching of boundary conditions. For precalculated control, a single integration is required to simulate the system, that is, to follow the course of the transient, but even this integration is unnecessary if the computer is used on-line.

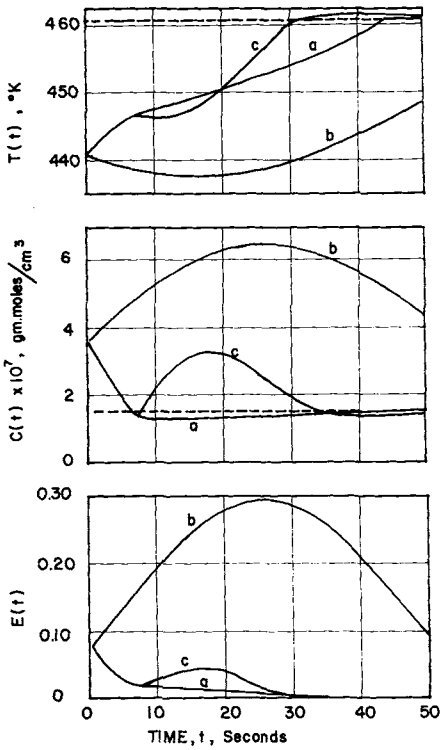

Fig. 6. Transient responses of a stirred-tank reactor. (a) Dual-variable control with unlimited switching. (b) No control. (c) Dual-variable control with limited switching. Broken line represents desired operating level.

A second important advantage of the simpler criterion arises when the system is subject to further disturbances during the course of the transient, disturbances which are initially unspecified. The minimization of J is usually considered an open-loop control problem, and $\mathbf{u}_{opt}$ is precalculated for the entire transient period based on an assumed knowledge of the system, its initial state, and all subsequent inputs. If unforeseen disturbances arise, adopting the precalculated $\mathbf{u}_{opt}$ as a control policy may in fact turn out to be a very poor choice of control. On the other hand, such disturbances may be counteracted by incorporating the criterion of Equation (12) into a feedback computer control system such as shown in Figure 7. For impulse disturbances the control action continues to decrease E as fast as possible, although the state of the system abruptly changes at the time of the disturbance. For other types of disturbances, the rigorous minimization of E is resumed whenever the disturbing influence ceases, that is, when the system is once again autonomous.

The use and effectiveness of the E function approach to transient control has been demonstrated; in order to be

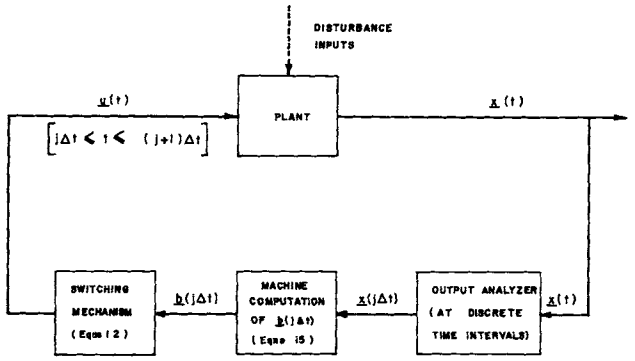

Fig. 7. Schematic representation of on-line computer application of *E* function control scheme.

of general usefulness, however, the control scheme should be expected to perform satisfactorily its task for all initial states which may be encountered in practice. The scheme has been tested for other initial states, different choices of control variables, and for another set of parameters (*10*). The results indicate that this control criterion can provide a computationally simple means of obtaining effective transient control over a rather complicated nonlinear process, but as in any optimization, the result should be checked against the designer's specifications (as regards stability, for example).

Last, it may be noted that the method is well suited to handling a large number of state variables and/or control variables. This aspect of the *E* function control scheme will be further developed in a companion paper which treats the transient control of a distributed parameter system.

ACKNOWLEDGMENT

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NOTATION

$\mathbf{A}$ = symmetric matrix of constants in quadratic forms
A_r = heat transfer area for stirred-tank reactor
a_i = weighting factor for x_i in E function
b_j = an algebraic summation defined by Equation (15)
C_p = specific heat
c = concentration of reacting species
E = scalar function defined by Equation (8)
ΔH = heat of reaction
J = integral performance index defined by Equation (16)
N = frequency factor
Q = activation energy divided by the gas constant
q = volumetric flow rate
r = rate of reaction per unit volume
T = temperature
t = time
Δt = time increment used in numerical integration
U = overall heat transfer coefficient
u = control variable
$\mathbf{u}$ = vector of control variables $u_1, u_2, \ldots, u_p$
V = reactor volume
x = dependent variable of process
$\mathbf{x}$ = vector of dependent variables $x_1, x_2, \ldots, x_n$
$\mathbf{y}$ = deviation vector defined by Equation (7)
ρ = density

Subscripts

o = feed condition
ss = steady state value
c = coolant condition
max = maximum permissible value
min = minimum permissible value
opt = optimum

Superscripts

o = initial condition at $t = 0$
d = desired level of operation
T = the transpose of a matrix

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APPENDIX

The overall control policy and simulated system response may be obtained by digital computation. For this purpose the transient period is broken into time increments Δt and the state of the system at $t = k\Delta t$ is represented by $\mathbf{x}(k\Delta t)$ for $k = 0, 1, \ldots, K$ where $K\Delta t = t_f$. The computational scheme takes on the following form:

1. From the known desired state and the present state of the system (initially, $k = 0$, and the "present" state is the given initial state), calculate the numerical values of b_j, $j = 1, 2, \ldots, p$ by Equation (15).

2. Set the p control variables $u_1, u_2, \ldots, u_p$ by the control criterion of Equation (12) over the time interval $k\Delta t \leqq t < (k+1)\Delta t$. If desired, after a fixed number of switches, set $u_j = (u_j)_{ss}$ rather than $(u_j)_{\min}$ or $(u_j)_{\max}$.

3. From Equation (6) and the value for each u_j determined in step 2, the state of the system at $t = (k+1)\Delta t$ is obtained by the approximate relation

$$\mathbf{x}[(k+1)\Delta t] = \mathbf{x}(k\Delta t) + \Delta t\, \dot{\mathbf{x}}(k\Delta t)$$

4. Let k equal $k + 1$, thus moving one Δt increment forward in real time. If $k < K$, return to step 1; otherwise the transient calculations are completed.

By using a simple Euler method to obtain an approximate integration of the system equations, as in step 3 above, the size of the increment Δt must be carefully chosen, that is, made small enough to insure a valid solution. The proper size for Δt may be determined by halving repeatedly Δt until the results are no longer significantly affected by a further reduction in the Δt size. Although the Euler method was sufficient for the applications considered in this paper, other numerical integration schemes are available and may be more suitable in certain circumstances. These numerical considerations are discussed in detail in reference 8*b*.

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