Part II. Feedback Control of a Distributed Parameter Process

A method previously developed is applied to the problem of transient control of a distributed parameter process. Computational difficulties prevalent in most optimization techniques are largely avoided, which suggests applicability to computer control of large transients. The use of such a control to improve the transient performance of a tubular reactor model is examined in detail. Numerical examples are given to demonstrate the criterion for control and the results are discussed.

In a previous paper (*9*) a method was developed for transient control of a wide class of systems, either on-line closed-loop or precalculated open-loop. The result was shown to be a near approximation to rigorous optimization based on an integral objective function or, in view of the arbitrary features of any performance index, it could be viewed as a different, but in a number of instances equivalent, criterion in its own right. In the last analysis, it is the designer's specifications that matter, and these are not necessarily expressible in the form of a simple time integral. Most important, it was shown that a wholly algebraic technique could be successfully applied to the control of a system described by differential equations.

The purpose of this paper is to extend the approach to establish a manageable criterion for the transient control of a distributed parameter system. It is well known that distributed parameter systems may often be satisfactorily approximated by a discrete mathematical model involving a large set of ordinary differential equations. Standard integral optimization techniques (*2, 4, 7, 11, 12*) are applicable in principle, but unusable in fact because of the high dimensionality of the system. The intrinsic computational difficulties have prevented practical application of existing theory (*13*). What is sought in this study is not optimality but rather a means of obtaining suboptimal (but good) control with a minimum of calculations. The discussion which follows addresses itself in particular to the transient control of a tubular reactor.

MODEL OF A TUBULAR REACTOR

Consider a tubular reactor in which the irreversible reaction series $A \rightarrow B \rightarrow C$ is taking place. If the radial gradients can be considered negligible, the independent variables are s, the axial position measured from the inlet, and the time t. The concentrations of A, B, and C are denoted by $X(s, t)$, $Y(s, t)$, and $Z(s, t)$, respectively, and their sum is constant:

$$X(s,t) + Y(s,t) + Z(s,t) = \Psi = \text{constant} \qquad (1)$$

It is assumed that the reactions are exothermic with rates first-order in concentration and following an Arrhenius temperature dependence:

$$\begin{aligned} r^1 = r^1(s,t) &= N_1 \exp\left[-Q_1/T(s,t)\right] X(s,t); \\ &\qquad \text{for } A \rightarrow B \\ r^2 = r^2(s,t) &= N_2 \exp\left[-Q_2/T(s,t)\right] Y(s,t); \\ &\qquad \text{for } B \rightarrow C \end{aligned} \qquad (2)$$

A dynamic model of the reactor can be derived from heat and material balances over a differential slice of the reactor. The equations which result are

$$\begin{aligned} \frac{\partial X}{\partial t} &= D\frac{\partial^2 X}{\partial s^2} - \frac{q}{A}\frac{\partial X}{\partial s} - r^1 \\ \frac{\partial Z}{\partial t} &= D\frac{\partial^2 Z}{\partial s^2} - \frac{q}{A}\frac{\partial Z}{\partial s} + r^2 \\ \frac{\partial T}{\partial t} &= D\frac{\partial^2 T}{\partial s^2} - \frac{q}{A}\frac{\partial T}{\partial s} \\ &\quad - \frac{\Delta H}{\rho C_p} r^1 - \frac{\Delta H}{\rho C_p} r^2 - \frac{UA_w}{A\rho C_p}(T - T_c) \end{aligned} \qquad (3)$$

where, following Liu and Amundson (*8*), the molecular and thermal diffusion coefficients are taken as numerically equal. This is primarily a matter of convenience and individually differing values could be used with no added complications. The last term on the right-hand side of the heat balance allows for external cooling (or heating) of the reactor contents. If the reactor is cooled from the wall, the radial mixing must be sufficient to prevent sizable temperature gradients in the radial direction (*1*). Parameters such as density, heat capacity, etc., are assumed constant. These restrictions may be removed at the expense of further complicating the model. Only two material balances are required, since the concentration of the third component can always be found by Equation (1).

It has been shown (*3*) that the proper boundary conditions for a tubular reactor with axial diffusion are given as

Entrance: $(s = 0^+)$

$$\frac{q}{A} v_{\text{feed}} = \frac{q}{A} v\,(0^+, t) - D\frac{\partial v\,(0^+, t)}{\partial s}; \text{ all } t > 0 \qquad (4)$$

Exit: $(s = L)$

$$\frac{\partial v(L, t)}{\partial s} = 0; \quad \text{all } t > 0 \qquad (5)$$

where v represents the set of four dependent variables X, Y, Z, and T.

To transform the dynamic equations into discrete form, the bed length L is first divided into M equal sections, each of length $\Delta s = L/M$. The temperature and concentrations within each section are approximated as functions of time alone. Again by denoting the set of dependent variables $(X, Y, Z, T,)$ by v, the approximation for the m^{th} section, $m = 1, 2, \ldots, M$, is of the form

$$v_m(t) \approx v(s,t); \text{ for } (m-1)\,\Delta s < s < m\Delta s \qquad (6)$$

The partial derivatives $(\partial v/\partial s)$ and $(\partial^2 v/\partial s^2)$ are approximated by the following finite-difference equations:

$$\begin{aligned} \left[\frac{\partial v(s,t)}{\partial s}\right]_{s=m\Delta s} &\approx \frac{1}{\Delta s}\left[v_m(t) - v_{m-1}(t)\right] \\ \left[\frac{\partial^2 v(s,t)}{\partial s^2}\right]_{s=m\Delta s} &\approx \frac{1}{(\Delta s)^2}\left[v_{m+1}(t) - 2v_m(t) + v_{m-1}(t)\right] \end{aligned} \qquad (7)$$

The relative merits of these, as well as alternative approximations, are discussed in the literature (*6*).

Substitution of the approximate Equations (6) and (7) into Equation (3) yields the following set of $3(M - 1)$ ordinary differential equations:

$$\begin{aligned} \dot{X}_m(t) &= \alpha_1 X_m(t) + \alpha_2 X_{m-1}(t) + \alpha_3 X_{m+1}(t) - r_m^1(t) \\ \dot{Z}_m(t) &= \alpha_1 Z_m(t) + \alpha_2 Z_{m-1}(t) + \alpha_3 Z_{m+1}(t) + r_m^2(t) \\ \dot{T}_m(t) &= \alpha_1 T_m(t) + \alpha_2 T_{m-1}(t) + \alpha_3 T_{m+1}(t) \end{aligned} \qquad (8)$$

$$+ \alpha_4 r_m^1(t) + \alpha_5 r_m^2(t) + \alpha_6[T_m(t) - T_c]$$

$$\text{for} \quad m = 1, 2, \ldots, (M-1)$$

where the α_i are combinations of system parameters and computational constants. Similarly, the boundary conditions [Equations (4) and (5)] may be approximated by discrete equations:

$$\mathbf{v}_o(t) = \frac{DA}{q\Delta s + DA} \mathbf{v}_1(t) + \frac{DA}{q\Delta s + DA} \mathbf{v}_{\text{feed}}; \quad \text{Entrance } (s = 0^+) \qquad (9)$$

$$\mathbf{v}_M(t) = \mathbf{v}_{M-1}(t); \quad \text{Exit } (s = L) \qquad (10)$$

where $\mathbf{v}_o(t)$ represents the conditions just inside the reactor entrance, that is, at $s = 0^+$, and $\mathbf{v}_M$ represents the exit conditions.

If solutions are to be obtained by digital computation, the continuous time variable must also be replaced by a discrete approximation:

$$\mathbf{v}_m(k\Delta t) = \mathbf{v}_m(t); \quad k\Delta t \leqq t < (k+1)\Delta t, \quad m = 0, 1, \ldots M \qquad (11)$$

By substituting from Equation (8) for $\dot{\mathbf{v}}_m(k\Delta t)$, the state of the system at $t = (k+1)\Delta t$ may be found from a known state at $t = k\Delta t$ by the approximate relation

$$\mathbf{v}_m[(k+1)\Delta t] = \mathbf{v}_m(k\Delta t) + \Delta t \; \dot{\mathbf{v}}_m(k\Delta t); \quad m = 1, 2, \ldots, (m-1) \qquad (12)$$

The time derivatives at the entrance ($m = 0$) and at the exit ($m = M$) are not given by Equation (8). However, once the values of $\mathbf{v}_m[(k+1)\Delta t]$ for $m = 1, 2, \ldots, (M-1)$ have been established, the boundary conditions require that

$$\mathbf{v}_o[(k+1)\Delta t] = \frac{DA}{q\Delta s + DA} \mathbf{v}_1[(k+1)\Delta t] + \frac{q\Delta s}{q\Delta s + DA} \mathbf{v}_{\text{feed}} \qquad (13)$$

$$\mathbf{v}_M[(k+1)\Delta t] = \mathbf{v}_{M-1}[(k+1)\Delta t]$$

By starting from a given initial state, $\mathbf{v}_m(0)$, $m = 0, 1, \ldots, M$, the discrete equations are used to advance the solution in stepwise fashion from one time interval to the next.

THE CONTROL FUNCTION

By following the development already referred to, the system performance is based on a scalar quadratic E function, which serves as an instantaneous measure of the deviation of the system from its desired state.

$$E(t) = \sum_{m=1}^{m-1} a_m^y [Y_m(t) - Y_m^d]^2 + a_m^z[Z_m(t) - Z_m^d]^2 + a_m^T[T_m(t) - T_m^d]^2 \qquad (14)$$

Included in this function are weighted terms which correspond to the squared deviations of temperature and concentration at the exit of each discrete reactor section except the last. The conditions at the entrance ($m = 0$) and at the exit ($m = M$) are not explicitly taken into account. They are fixed at all times, however, by the boundary conditions. It is also unnecessary to include all three components of concentration (X_m, Y_m and Z_m) in the E function, since in this case only two components may be independently controlled.

The criterion for control is the continuous minimization of $\dot{E}(t)$, that is, at intervals of Δt in discrete time. A discussion of the physical interpretation of this criterion is given in references *9* and *10*. Formal differentiation of $E(t)$ with respect to time yields the expression

$$\dot{E}(t) = 2\sum_{m=1}^{m-1} a_m^y[Y_m(t) - Y_m^d] \dot{Y}_m(t) + a_m^z[Z_m(t) - Z_m^d]\dot{Z}_m(t) + a_m^T[T_m(t) - T_m^d]\dot{T}_m(t) \qquad (15)$$

which leads to the sought-for control policy when combined with the state equations rearranged in a form that is linear in the control variables. If among the possible choices the heat transfer coefficient U and the flow rate q are taken as the control variables $u_1(t)$ and $u_2(t)$, respectively, the state equations become

$$\begin{aligned} \dot{X}_m(t) &= u_2 \; f^x_{m,2} + g_m^x \\ \dot{Z}_m(t) &= u_2 \; f^z_{m,2} + g_m^z \\ \dot{T}_m(t) &= u_1 \; f^T_{m,1} + u_2 \\ & f^T_{m,2} + g_m^T; \; m = 1, 2, \ldots, (M-1) \end{aligned} \qquad (16)$$

and $\dot{E}$ may be expressed in the form

$$\dot{E}(t) = b_1(t) \; u_1(t) + b_2(t) \; u_2(t) + \Phi(t) \qquad (17)$$

where

$$b_1 = 2\sum_{m=1}^{M-1} a_m^T \; f^T_{m,1} \; (T_m - T_m^d)$$

$$b_2 = 2\sum_{m=1}^{M-1} [a_m^y \; f^y_{m,2}(Y_m - Y_m^d) + a_m^z \; f^z_{m,2}(Z_m - Z_m^d) + a_m^T \; f^T_{m,2}(T_m - T_m^d)] \qquad (18)$$

$$\Phi = 2\sum_{m=1}^{M-1} [a_m^y \; g_m^y \; (Y_m - Y_m^d) + a_m^z \; g_m^z \; (Z_m - Z_m^d) + a_m^T \; g_m^T \; (T_m - T_m^d)]$$

If now the control variables are constrained by $(u_1)_{\min} \leqq u_1(t) \leqq (u_1)_{\max}$, and $(u_2)_{\min} \leqq u_2(t) \leqq (u_2)_{\max}$, the requirements for a minimum $\dot{E}$ correspond to the following criteria for control:

$$\left.\begin{aligned} u_j &= (u_j)_{\max} \text{ whenever } b_j < 0 \\ u_j &= (u_j)_{\min} \text{ whenever } b_j > 0 \end{aligned}\right\} ; \; j = 1, 2 \qquad (19)$$

For each u_j a switchover from one extreme to the other occurs when the corresponding $b_j = 0$. With this criterion the control settings at any given time will be those required to obtain the fastest possible reduction in the value of E at that moment. The numerical value of the E function is zero only when the process is at the desired state.

THE CONTROL OF START-UP

The foregoing development may be illustrated by specific examples of possible applications. For start-up it is assumed that the reactor contents are initially cold and unreacted. To be specific, the initial state of the process is given as

$X_m^o = 0.30$ lb.-mole/cu.ft.
$Y_m^o = Z_m^o = 0.00$ lb.-mole/cu.ft.; for $m = 0, 1, \ldots, M$
$T_m^o = 560$°R.

Under steady state operating conditions, the control variables have nominal or steady state values: $(u_1)_{ss} = U_{ss} = 0.6$ B.t.u./(min.)(sq.ft.)(°F.), $(u_2)_{ss} = q_{ss} = 4.0$ cu. ft./min. By using these values, the temperature and concentration profiles which result from a steady state solution of the discrete equations are shown in Figure 1. These profiles are taken as the desired state of the system. In particular, the desired exit conditions are given by $X_m^d =$

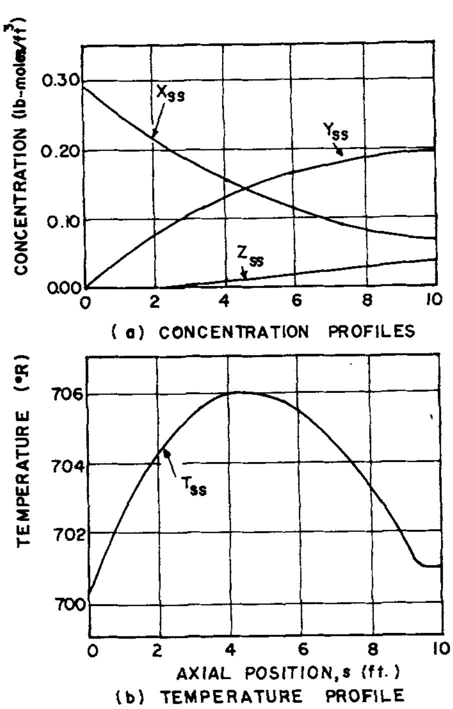


Fig. 1. Steady state profiles for the tubular reactor.

0.06743 lb.-mole/cu.ft., $Y_M{}^d$ = 0.19550 lb.-mole/cu.ft., $Z_m{}^d$ = 0.03707 lb.-mole/cu.ft., and $T_m{}^d$ = 700.95°R. Taking the mathematical model already developed as an adequate description of the dynamic behavior of the process, one can choose the following hypothetical set of system parameters as a basis for numerical study:

A = 2 sq.ft.
L = 10 ft.
A_w = 5 sq.ft./ft.
ρ = 50 lb./cu.ft.
C_p = 0.70 B.t.u./(lb.)(°F.)
D = 0.2 sq.ft./min.
T_c = 530°R.
T_{feed} = 700°R.
M = 20
Δt = 0.05 min.

ΔH_1 = − 5,000 B.t.u./lb.-mole
ΔH_2 = − 3,000 B.t.u./lb.-mole
N_1 = 8.35 × 10⁶ min.⁻¹
N_2 = 4.225 × 10⁸ min.⁻¹
Q_1 = 12,000°R.
Q_2 = 16,000°R.
Ψ = 0.30 lb.-mole/cu.ft.
X_{feed} = 0.30 lb.-mole/cu.ft.
Y_{feed} = 0.00 lb.-mole/cu.ft.
Z_{feed} = 0.00 lb.-mole/cu.ft.

For the system studied, $M = 20$ represents about the minimum number of divisions for a reasonably accurate discrete approximation (comparisons were run also at $M = 10$ and $M = 40$).

According to the general form of Equation (14), it is possible to include terms in the E function which measure the deviation from the desired state at every section m where $m = 0, 1, \ldots, (M-1)$, but it might legitimately be asked whether all possible terms need to be included in the summation. It would not do to consider only conditions at the reactor exit, for such a choice would neglect interactions between the stages in space. The E function must reflect in some way the state of the entire process and should therefore include at least some terms which represent the conditions at various points within the reactor.

TABLE 1. NUMERICAL VALUES USED IN THE E FUNCTION OF EQUATION (20)

The desired state of the process

m	$Y^d{}_m$, lb.-moles/cu. ft.	$Z^d{}_m$, lb.-moles/cu. ft.	$T^d{}_m$, °R.
1	0.024876	0.000457	701.45
7	0.12092	0.008152	705.45
13	0.17284	0.022160	705.04
19	0.19550	0.037077	700.95

Weighting factors, m = 1, 7, 13, 19

$a^y{}_m$	$a^z{}_m$	$a^T{}_m$
100	10,000	0.001

In accordance with this observation, the following E function is selected:

$$E(t) = \sum_{\substack{m=1,7,\\13,19}} \{a_m{}^y\,[Y_m(t) - Y_m{}^d]^2 + a_m{}^z\,[Z_m(t) - Z_m{}^d]^2 + a_m{}^T\,[T_m(t) - T_m{}^d]^2\} \quad (20)$$

The desired state of the process at m = 1, 7, 13, 19 is obtained from the solution of the steady state equations in discrete form, and the weighting factors are chosen to make the terms of Equation (20) roughly equivalent in importance. The numerical values used are given in Table 1.

By simulating the start-up transient response which results in each case, three types of control will be examined and compared with the uncontrolled start-up response. The uncontrolled response corresponds to a solution in which the control variables $u_1(t)$ and $u_2(t)$ are maintained at their nominal values throughout the transient period. For the first type of control, it is assumed that $u_1(t)$, the heat transfer coefficient U, is the only means of control. The restrictions imposed are

$$0 \leqq u_1(t) \leqq 1.0 \text{ B.t.u./(min.)(sq. ft.)(°F.) and}$$
$$u_2(t) = (u_2)_{ss} = 4.0 \text{ cu. ft./min.}$$

The situation is then reversed and the flow rate $u_2(t)$ is taken as the sole means of control. For this case the constraints on the control variables are given as: $u_1(t) = (u_1)_{ss} = 0.6$ B.t.u./(min.)(sq. ft.)(°F.) and $2 \leqq u_2(t) \leqq 8$ cu. ft./min. Finally, the effect of a two-variable control is considered by simultaneously letting $0 \leqq u_1(t) \leqq 1.0$ B.t.u./(min.)(sq. ft.)(°F.) and $2 \leqq u_2(t) \leqq 8$ cu. ft./min.

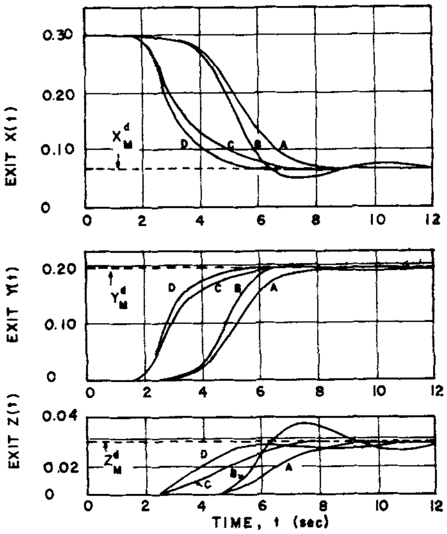


Fig. 2. Comparison of start-up responses for a tubular reactor (concentration responses). A: No control. B: Control by U. C: Control by q. D: Dual-variable control (U and q).

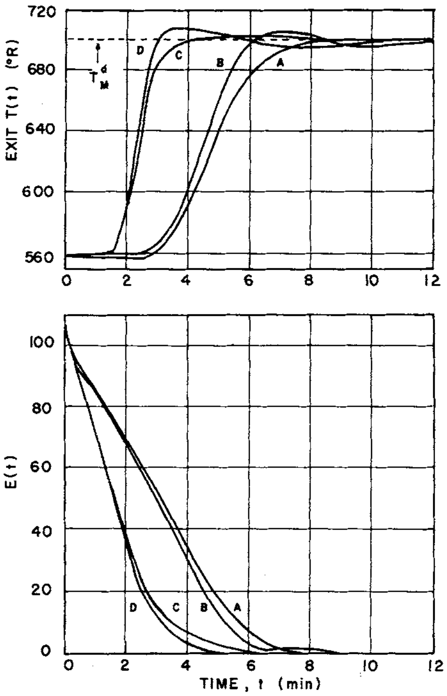


Fig. 3. Comparison of start-up responses for a tubular reactor [temperature and $E(t)$ responses]. *A*: No control. *B*: Control by *U*. *C*: Control by *q*. *D*: Dual-variable control (*U* and *q*).

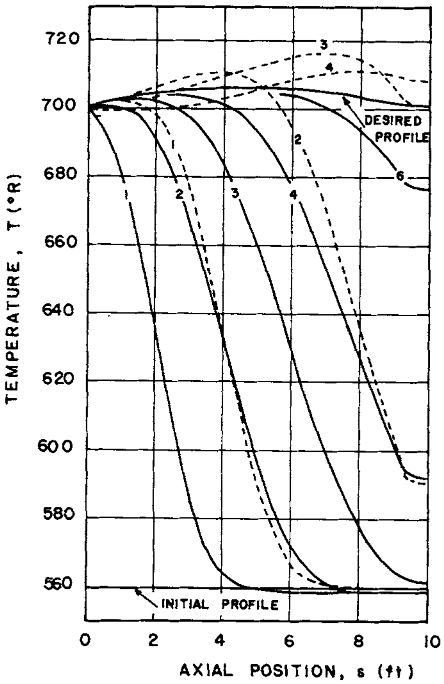
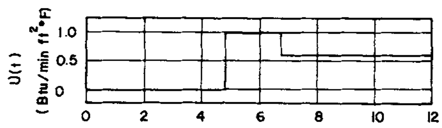


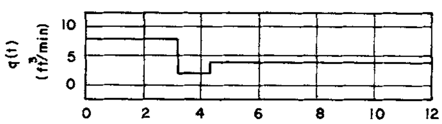
Fig. 5. Instantaneous temperature profiles for tubular reactor start-up response. Plotted with time in minutes as a parameter. Solid line represents no control; broken line represents dual-variable control.

In each case the controller acts at increments of $\Delta t = 0.05$ min. to select the particular control settings for u_1 and/or u_2 which satisfy the criteria of Equation (19).

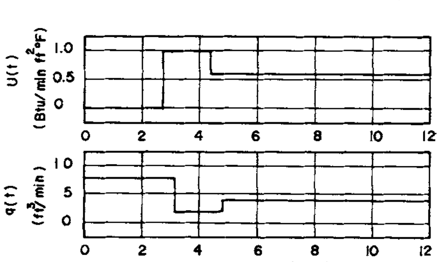
The results so obtained are partially shown in Figures 2, 3, and 4 as: a comparison of the transient responses at the reactor exit, the responses in terms of E as a function of time, and the control policies selected by the controller for each of the three controlled responses. For no control and for dual-varible control, Figures 5 and 6 show the resulting temperature and concentration profiles within the reactor as the transient progresses. The desired steady state profiles are ultimately obtained in each case.



(a) SINGLE VARIABLE CONTROL BY U.



(b) SINGLE VARIABLE CONTROL BY q.



(c) DUAL VARIABLE CONTROL BY U AND q.

Fig. 4. Control policies which correspond to the response curves of Figures 2 and 3. Obtained by the control criterion of Equation (19).

One measure of overall effectiveness for a particular control policy is J, the resulting area under the $E(t)$ vs. t curve. Corresponding to the $E(t)$ curves of Figure 3, the values of J (for $t_f = 15$ min.) are found to be

$J_A = 315.19$ (no control)
$J_B = 296.48$ (control by U)
$J_C = 180.82$ (control by q)
$J_D = 168.28$ (dual-variable control: by U and q)

Comparison of these values shows that a substantially improved start-up response is obtained either with dual-variable control or with the flow rate q as the only control variable. The temperature-concentration curves show perhaps more directly the effect of controlling the system according to the E function criterion.

RECOVERY AFTER DISTURBANCE

Suppose that while operating at steady state (as in Figure 1), the tubular reactor suffers a large temperature disturbance, perhaps due to a temporary failure of the cooling system. Upon cessation of the disturbance, the temperature throughout the reactor may be considerably above that of the steady state profile. For simplicity, assume that at this moment the steady state concentration profiles are unchanged, but that the temperature at all points within the reactor is 740°R. For the control problem, these conditions correspond to the initial state of the process

$$\begin{aligned} X_m^o &= X_m^d \\ Y_m^o &= Y_m^d \\ Z_m^o &= Z_m^d \qquad ; m = 0, 1, \ldots, 20 \\ T_m^o &= 740°\text{R}. \end{aligned}$$

where the X_m^d, Y_m^d, and Z_m^d values correspond to the steady state concentration profiles of Figure 1.

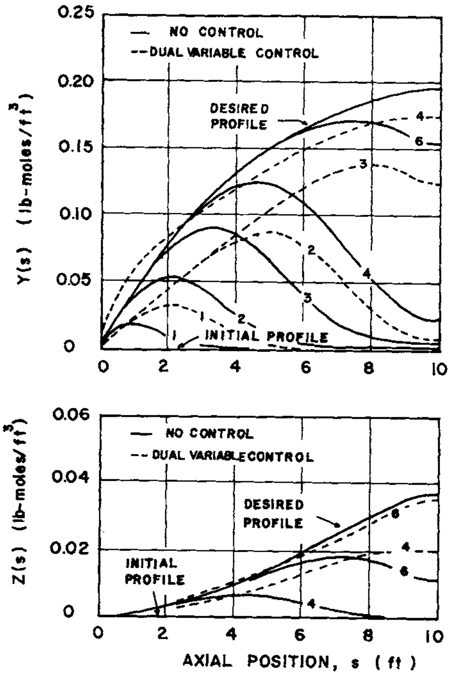


Fig. 6. Instantaneous concentration profiles (Y and Z) for tubular reactor start-up plotted with time in minutes as a parameter.

By regarding the second reaction in the series $A \rightarrow B \rightarrow C$ as an undesirable side reaction, it is important to prevent the exit concentration of C, that is, Z_M, from becoming too large. With an initially high temperature, some increase in Z_M is inevitable, since both reactions are irreversible, exothermic, and strongly temperature dependent. In this situation, an on-line computer controller may be a worthwhile means of promoting a rapid recovery of the desired operating state.

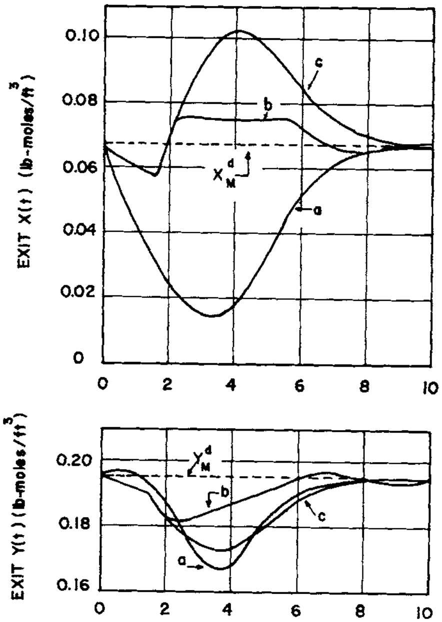


Fig. 7. Exit responses to temperature disturbances. (a). Uncontrolled response. (b) Dual-variable control (unlimited switching). (c) Dual-variable control (limited switching).

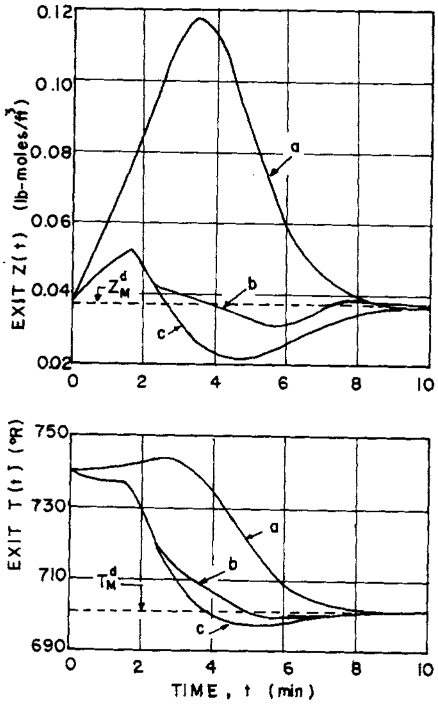


Fig. 8. Exit responses to temperature disturbance. (a) Uncontrolled response. (b) Dual-variable control (unlimited switching). (c) Dual-variable control (limited switching).

To observe the effectiveness of the control scheme, let the E function again be given by Equation (20) and the parameter values of Table 1. The results of the simulated reactor response with a dual-variable control policy determined by the criteria of Equation (19) are partially shown in Figures 7 through 11. A time increment of $\Delta t = 0.025$ min. was used in the numerical integration of the system equations. For comparison, responses are shown which correspond to the following cases:

1. Uncontrolled response: The control settings are fixed throughout the transient at their nominal values.
2. Dual-variable control: Decisions for each control variable (U and q) are made at intervals of $\Delta t = 0.025$ min. with Equation (19) as a criterion.
3. Dual-variable control (limited switching): Same as case 2, except that by limiting the control action to a maximum of two switches per control variable (the second switch being to the nominal control setting), the chattering effect is eliminated.

In Figure 9 the E vs. t curves illustrate the overall effectiveness of the control scheme. The corresponding values of J are, for a 10-min. duration:

1. Uncontrolled response: $J = 251.47$
2. Dual-variable control (unlimited switching): $J = 13.54$
3. Dual-variable control (limited switching): $J = 20.47$

By using dual-variable control, the E function control scheme effectively reduces the J value by more than an order of magnitude. Limiting the controller to two switches per control variable results in almost as great a reduction in J as does allowing the controller an unlimited number of switches.

The transient responses at the reactor exit are plotted in Figures 7 and 8. The controlled response curves exhibit a greater improvement in the transient responses for $T_M(t)$ and $Z_M(t)$ than for $X_M(t)$ and $Y_M(t)$. By weighting T and Z deviations more heavily, the controller has in effect been directed to concentrate its efforts upon these variables; however, each control is based on a summation of terms, taking into account the reactor condi-

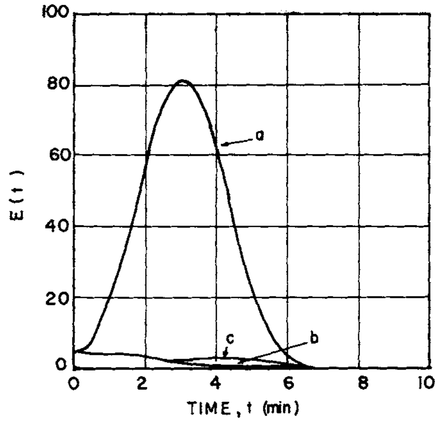


Fig. 9. The E function vs. time for temperature disturbance transient response. (a) Uncontrolled response. (b) Dual-variable control (unlimited switching). (c) Dual-variable control (limited switching).

tions at several points within the reactor in addition to the exit conditions. In Figures 10 and 11 the temperature and concentration profiles are shown for several values of time during the transient. These results compare the uncontrolled response to that from dual-variable control with unlimited switching. If the deviation from the desired profiles is largest at some interior point of the reactor, the corresponding terms in the E function become large. Furthermore, the signs of the criterion functions b_1 and b_2 [see Equation (18)] are determined by an algebraic summation of terms that are proportional to the magnitudes of the deviations at each discrete section. In minimizing E, the controller will thus inherently give the most attention to reducing the largest deviations, wherever they may occur.

DISCUSSION

Many aspects of the E function transient control scheme have been developed and demonstrated in the previous sections. There remain, however, some features of the method which merit further discussion: applications involving a large number of control variables, state variable constraints, and on-line computer controller applications.

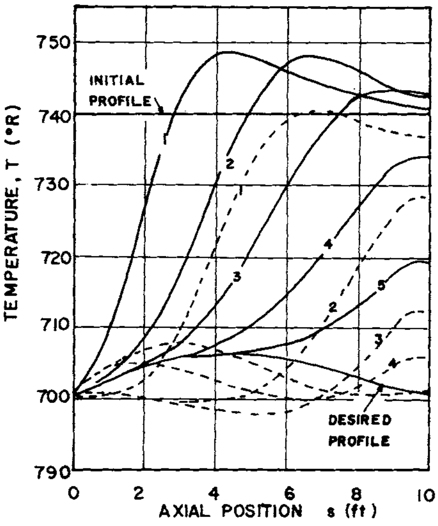


Fig. 10. Instantaneous temperature profiles for transient response to disturbance with time in minutes as a parameter. Controlled case corresponds to unlimited switching. Solid line represents no control; broken line represents dual-variable control.

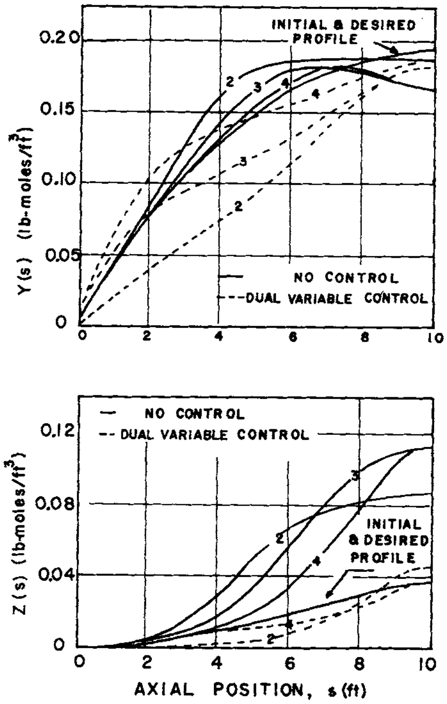


Fig. 11. Instantaneous concentration profiles (Y and Z) for transient response to disturbance with time in minutes as a parameter. Controlled case corresponds to unlimited switching.

Multivariable Control

As set up for the example systems, the control scheme is capable of determining simultaneously the control policies $u_1(t)$ and $u_2(t)$ which are optimal in the sense of minimizing $\dot{E}(t)$ at each discrete time interval. When physically possible and economically justified, additional control variables could be incorporated into the control scheme to improve further the performance of the process, without introducing disproportionate complication.

To illustrate this point, suppose that it were desirable to vary the heat transfer coefficient with axial position as well as with time, that is, $U = U(s, t)$. If U is related to the coolant flow, this would presumably require independent cooling of the reactor by sections. By letting $U_i = U_i(t)$ represent the value of U in the i^{th} cooling section, Equation (8) may again be taken as a dynamic description of the process if α_6 is redefined as

$$\alpha_6 = \frac{-A_w}{A\rho C_p} U_m(t) \qquad (21)$$

Figure 12 schematically illustrates such a discrete reactor model. If the flow rate q is also considered a control vari-

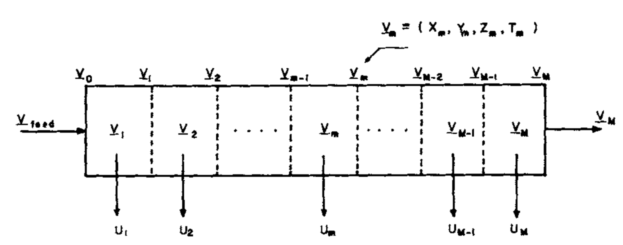


Fig. 12. Schematic representation of independent cooling of each of the M reactor sections of the discrete tubular reactor model.

able, the criterion for control involves the simultaneous manipulation of M control variables:

$$u_m(t) = U_m(t) \ ; \ m = 1, 2, \ldots, (M-1) \qquad (22)$$
$$u_M(t) = q$$

subject to the constraints

$$(u_m)_{\min} \leqq u_m(t) \leqq (u_m)_{\max} \ ; \ m = 1, 2, \ldots, M \ ; \quad \text{all } t \geqq 0 \qquad (23)$$

A simple rearrangement of terms transforms the system equations into a form that differs only in subscripting from Equation (16) which is based on a uniform value of U for the entire length of the reactor. Similarly, the relations for E and the criterion b change in some details (*10*), but the total number of arithmetic operations necessary to determine $b_1, \ldots, b_m$ for M variable control is identical with the number required to establish b_1 and b_2 for dual-variable control. Each added control variable calls for one additional algebraic summation. In contrast, the computations required to minimize an integral performance index of the usual form (with respect to twenty simultaneous variables) would be literally prohibitive.

State Variable Constraints

Sometimes it is particularly important that certain dependent variables of the process should not be allowed to exceed predefined limits. The E function control scheme is adaptable to this purpose in either of two ways. One method includes terms in $E(t)$ especially devised to inhibit constraint violations; used effectively in other optimization procedures, such terms are known as penalty functions (*11*). For example, in order to control the tubular reactor subject to the temperature constraints

$$T_{\min} \leqq T_m(t) \leqq T_{\max} \quad m = 1, 2, \ldots, M; \quad \text{all } t \geqq 0 \qquad (24)$$

the E function could be replaced by an augmented function $E'(t)$ such that

$$E'(t) = E(t) + \sum_{m=1}^{M-1} \{\nu[T_m(t)/T_{\max}]^{\sigma} + \nu[T_{\min}/T_m(t)]^{\sigma}\} \qquad (25)$$

where ν and σ are arbitrarily chosen large constants. As long as the temperature constraints are not violated, the additional terms are very small and do not affect the control decisions, that is, $E'(t) = E(t)$. If, however, the temperature at any point in the reactor approaches the upper or lower bound, the corresponding penalty function becomes the predominate term in $E'(t)$. Accordingly, the control action required to minimize $E'(t)$ would coincide with the action necessary to prevent a constraint violation.

An alternative means of incorporating state variable constaints into the E function control scheme is to use a set of such functions, each valid in a particular region of the state variable space. Any number of E functions could be individually tailored to handle additional state variable constraints without significantly increasing the computational load. The task of the controller would be to select the appropriate E function (from a knowledge of the instantaneous state of the system), and to determine the control settings which minimize the corresponding $\dot{E}$.

On-Line Control

The method presented here can be used for on-line (closed-loop) or precalculated (open-loop) control. The advantages of the former are well known (*5*): the accuracy of the model is not as critical, and the feedback information, in effect, acts to up-date or correct the approximate model thus avoiding cumulative errors. By the same token, on-line control is capable of counteracting the effect of disturbances not explicitly considered in the prior calculations. With regard to chemical processes, typically described by approximate models, the advantages of on-line control are perhaps especially significant.

In the form presented, the control scheme assumes an instantaneous knowledge of the system state. In practice this assumption is reasonable only if the data acquisition and computation time are small relative to the time constants of the plant. By digital computation, the required on-line algebraic operations can be completed in a fraction of a second, in direct contrast to the rigorous integral optimization methods. The effectiveness of control depends also upon how rapidly the control variables can be switched from one extreme to the other. A means of modifying the control scheme to compensate at least partially for a slow switch is discussed elsewhere (*10*), but it is of course preferable to design switching mechanisms with negligible inertia relative to the system parameters.

ACKNOWLEDGMENT

This research was supported by a grant from the National Science Foundation.

NOTATION

A = chemical species in the reaction series $A \rightarrow B \rightarrow C$; cross-sectional area of tubular reactor
A_w = wall area per unit length for tubular reactor
a_i = weighting factor for x_i in E function
b_j = algebraic summation defined by Equation (17)
C_p = specific heat
D = diffusivity, either mass or thermal
E = positive definite scalar function defined by Equation (14)
$f^T{}_{m,1} = (A_w/A\rho C_p)\ [T_c - T_m(t)]$
$f^T{}_{m,2} = (1/A\Delta s)\ [T_{m-1}(t) - T_m(t)]$
$f^x{}_{m,2} = (1/A\Delta s)\ [X_{m-1}(t) - X_m(t)]$
$f^z{}_{m,2} = (1/A\Delta s)\ [Z_{m-1}(t) - Z_m(t)]$
$f^y{}_{m,2} = -\ [f^x{}_{m,2} + f^z{}_{m,2}]$
$g^y{}_m = -\ [g^x{}_m + g^z{}_m]$
$g^T{}_m = [D/(\Delta s)^2][T_{m+1}(t) - 2\,T_m(t) + T_{m-1}(t)] - (\Delta H_1/\rho C_p)\ r_m{}^1(t) + (\Delta H_2/\rho C_p)\ r_m{}^2(t)$
$g^x{}_m = [D/(\Delta s)^2][X_{m+1}(t) - 2\,X_m(t) + X_{m-1}(t)] - r_m{}^1(t)$
$g^z{}_m = [D/(\Delta s)^2][Z_{m+1}(t) - 2\,Z_m(t) + Z_{m-1}(t)] + r_m{}^2(t)$
ΔH = heat of reaction
J = integral performance index
L = length of tubular reactor
M = total number of discrete sections for obtaining a discrete approximation to the tubular reactor model
N = frequency factor
Q = activation energy divided by the gas constant
q = volumetric flow rate
r = rate of reaction per unit volume
s = axial position measured from tubular reactor inlet
Δs = L/M
T = temperature
t = time
Δt = time increment used in numerical integration
U = overall heat transfer coefficient
u = control variable
$\mathbf{v}$ = vector representing X, Y, Z, and T
X = concentration of A in reaction series $A \rightarrow B \rightarrow C$
Y = concentration of B in reaction series $A \rightarrow B \rightarrow C$
Z = concentration of C in reaction series $A \rightarrow B \rightarrow C$

Greek Letters

$$\alpha_1 = -2\left[\frac{D}{(\Delta s)^2} + \frac{1}{A\Delta s}\,q\right]$$

α_2 = $(D/(\Delta s)^2) + (1/A\Delta s)\, q$
α_3 = $(D/(\Delta s)^2)$
α_4 = $(-\Delta H_1/\rho C_p)$
α_5 = $(-\Delta H_2/\rho C_p)$
α_6 = $(-UA_w/A\rho C_p)$
ρ = density
Ψ = constant total concentration = $X + Y + Z$

Subscripts

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

Superscripts

o = initial condition at $t = 0$
d = desired level of operation
x, y, z, T = associate functions or constants with X, Y, Z, and T, respectively

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Manuscript received November 8, 1965; revision received March 8, 1966; paper accepted March 9, 1966.

Generalized Couette Flow of an Ellis Fluid

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The motion of an ordinary Newtonian fluid in a channel caused by a pressure gradient alone, or caused by the motion of one of the walls, can be obtained separately; and the problem of generalized Couette flow (the motion due to both causes simultaneously) can be obtained by superposition. For an Ellis fluid, because of the nonlinearity of the viscosity-stress law, the principle of superposition is not applicable. This paper is devoted to the solution of this problem of generalized Couette flow of an Ellis fluid in parallel flat plate and circular annular channels.

Ellis fluid has been characterized by Matsuhisa and Bird (*1*) to be one for which the coefficient of viscosity η is not a constant but varies with the stress in accordance with the law

$$\frac{1}{\eta} = \frac{1}{\eta_o}\left[1 + \left|\frac{\tau}{\tau_{1/2}}\right|^{\alpha-1}\right] \tag{1}$$

where

$$\tau = \frac{1}{2}\sqrt{\sum_i \sum_j \tau_{ij}^2} \tag{2}$$

Equation (1) contains three constants η_o, α, and $\tau_{1/2}$ which must be determined experimentally for each fluid. The constant η_o can be interpreted as the viscosity at zero stress. The numerical constant α has been found for most fluids to have a value between 1 and 2. When $\alpha = 1$, Equation (1) shows that η is constant (equal to ½ η_o). We can, thus, look upon the ordinary Newtonian fluid to be a special case of the Ellis fluid for $\alpha = 1$. The case η = ½ η_o can also be looked upon as pertaining to a physical situation for which the stress τ remains constant always (equal to $\tau_{1/2}$).

Matsuhisa and Bird have obtained a few simple solutions of the fluid motion governed by the viscosity law (*1*). These solutions made use of the fact of dynamic symmetry, which simplified the analysis. When one considers a one-dimensional flow problem, the inertia terms in the momentum equation may either drop out or become linearized because of the geometry of the problem, but the final equation for the Ellis fluid still remains nonlinear. Such independent causes as the motion of one of the channel walls while the other is held stationary or the presence of a nonzero pressure gradient produce motions which for the ordinary Newtonian fluid may be superposed. For the Ellis fluid, because of the nonlinear vis-