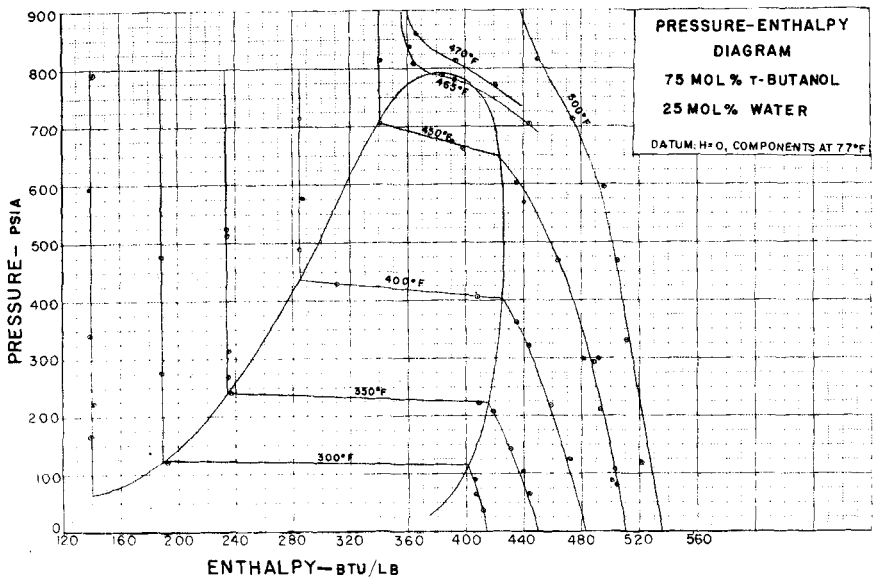

Fig. 3. Pressure-enthalpy diagram for 75% *t*-butanol, 25% water mixture.

plementary enthalpy-temperature and latent heat temperature diagrams for these systems are given by O'Neill.

DISCUSSION

It was found that the methods of McCracken (*6, 7*) and Storvick (*10, 11*) did not accurately predict the effect of pressure on the vapor-phase mixture enthalpies at constant temperature for the normal and *t*-butanol-benzene systems but are adequate in predicting the deviation encountered in the pure alcohols and in dilute solutions of polar-nonpolar mixtures. For the *t*-butanol-water mixture a modification of Storvick's method was found to accurately predict the mixture enthalpies. Since water does not have a homomorph, the values for pressure deviation in enthalpy were obtained directly from the steam tables (*2*) which include the hydrogen bonding effects of the pure water for use in Storvick's equations. The excellent correlation over the complete temperature and pressure range may be due to the fact that the solution was dilute (7.5 wt. % water). A detailed discussion of these results, methods for correlating the pure component data, and methods for predicting the enthalpies of the mixtures from the properties of the pure components is given by O'Neill (*8*).

The calculated heats of association for the *t*-butanol were found to be considerably less than those found for *n*-butanol, especially at the higher temperatures and pressures. The differences in these heats of association indicate that molecular structure does have a pronounced effect on the degree of hydrogen bonding of the alcohols in the vapor phase. It is postulated that molecules which contain highly branched chains, such as *t*-butanol, are incapable of forming large polymolecules owing to the effect of steric hinderance. Since the heat of association is a measure of the degree of hydrogen bonding, it was expected that *n*-butanol would have higher values than the tertiary isomer.

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Time Optimal Control of Nonlinear Systems with Constraints

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The work of Amundson et al. (*1*) has served to hasten the chemical engineer into the application of feedback control theory to chemical systems. The feasibility of a computer as a process controller was demonstrated by Tierney et al. (*12*) and as a process optimizer by Eckman and Lefkowitz (*10*). The recent papers of Kalman et al. (*7*) and Lapidus et al. (*8*) have dealt with the optimum dynamic control of a chemical process or plant using a general purpose digital computer. As shown the concept of dynamic programming may be applied to linearized systems directly to generate the optimum dynamic control strategy or law.

Since chemical systems are usually nonlinear and may not always be approximated by a linearized model, a strategy for generating the optimum dynamic control strategy in the stationary nonlinear case must be developed. While theoretically this can still

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be done by the use of dynamic programming, the computational problems become rather staggering. Thus it is the purpose of this paper to present an alternate general procedure. The development is limited to physical systems which are bounded in the range of their variables, or what has been called *saturated systems.*

An optimum control strategy is one which minimizes the integral or summation of the performance function over all time. Following an argument modified from that presented by Fuller (*3, 4*) it is shown that the optimum control action at any point in time is an instantaneous function of the present state of the process and the input. Although this relationship exists in principle, in a nonlinear case it is not possible to explicitly establish this function to calculate the optimum control action. The approach taken here is to predict, over one sampling period by means of the mathematical process model, the responses for a selected number of control levels. By evaluating the performance function for the predicted values the optimum control action is selected at each sampling period. It is that control action which minimizes the performance function. The search for the desired control action is facilitated by the fact that, in a saturated system, generally the optimum control action is at one of the extreme ends of the range throughout the major part of the transient response. The overall control system with its optimizing scheme will be called the *optimum predictor-controller.*

The superiority of the predictor-controller relative to other controllers is demonstrated quite clearly with the aid of a phase portrait. Moreover with the aid of the phase portraits for the maximum and minimum control action the widest range of possible dynamic action is graphically illustrated, and the feasibility of operating in the various areas of the phase plane can be determined. The phase plane analysis shows that it is impossible to operate dynamically about a nonsteady state point in those regions where the phase trajectories for the extreme control actions are nearly parallel. The degree to which a nonsteady state or an unstable steady state operating point can be reached is also influenced by the relative weights assigned to the deviations in the performance function.

THEORY

The dynamic description of a general process can be represented by a set of n first-order nonlinear ordinary differential equations of the following canonical form:

$$\frac{dx_1}{dt} = \phi_1 (x_1, x_2, \ldots x_n, m_1(t), m_2(t), \ldots m_r(t); t)$$

$$\frac{dx_2}{dt} = \phi_2 (x_1, x_2, \ldots x_n, m_1(t), m_2(t), \ldots m_r(t); t) \quad (1)$$

$$\vdots$$

$$\frac{dx_n}{dt} = \phi_n (x_1, x_2, \ldots x_n, m_1(t), m_2(t), \ldots m_r(t); t)$$

where $x_1, x_2, \ldots x_n$ are the state or dependent variables and $m_1(t), m_2(t), \ldots m_r(t)$ are the input or control variables. Since the state variables can be thought of as coordinates in n dimensional hyperspace, the above set of equations can be represented compactly as a vector differential equation of n components and $n + r + 1$ arguments. This may be written as

$$\frac{d\mathbf{x}(t)}{dt} = \phi [\mathbf{x}(t), \mathbf{m}(t); t] \quad (2)$$

where

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix}, \mathbf{m}(t) = \begin{bmatrix} m_1(t) \\ m_2(t) \\ \cdot \\ \cdot \\ \cdot \\ m_r(t) \end{bmatrix}, \text{ and } \phi = \begin{bmatrix} \phi_1(\mathbf{x}, \mathbf{m}(t), t) \\ \phi_2(\mathbf{x}, \mathbf{m}(t), t) \\ \cdot \\ \cdot \\ \cdot \\ \phi_n(\mathbf{x}, \mathbf{m}(t), t) \end{bmatrix}$$

With the state of the process interpreted as a vector in hyperspace or phase space, each state of the process which is different from another has a unique set of coordinates or components. In a dynamic process the state is changing with time. As a result the state vector describes a locus as a function of time in phase space called a *trajectory.* When a process has reached a steady state, no more changes occur in the state variables with time; consequently the coordinates of the state vector become fixed and the trajectory becomes a fixed point.

The present study is concerned only with processes which have dynamic characteristics independent of time, that is are stationary. Systems with dynamic characteristics changing slowly compared with process time constants can be considered stationary over finite time intervals. For a stationary process Equation (2) can be written as

$$\frac{d\mathbf{x}(t)}{dt} = \phi [\mathbf{x}(t), \mathbf{m}(t)] \quad (3)$$

where time occurs only implicitly by way of the input vector.

In principle the transient behavior (dynamic response) is obtained by solving the differential equations describing the process with the proper initial conditions and input functions. The set of equations represented by Equation (3) have a unique solution provided that the various ϕ_i's in the vector ϕ are continuous and have first partial derivatives with respect to $x_1, x_2, \ldots x_n$. As a result a future state of the process at any time t can be evaluated if some initial state $\mathbf{x}(t_o)$ is given in addition to the input vector $\mathbf{m}(\lambda)$ for all time from $t_o \leq \lambda \leq t$ (*6*).

The existence of a solution does not imply that it is necessarily an analytic solution. In most nonlinear cases only a numerical solution is possible. From what has been pointed out above any solution of Equation (3) is dependent on the indicated arguments and can be implicitly represented as

$$\mathbf{x}(t) = \Phi [\mathbf{x}(t_o), \mathbf{m}(\lambda); (t - t_o)] \quad \text{for all } t_o \leq \lambda \leq t \quad (4)$$

A property of the solution is that the integration can be terminated at any arbitrary time and then continued with the terminated state of the first integration being the initial state for the second integration.

While it is possible to obtain an analytical solution for a set of linear differential equations, the same cannot be said for nonlinear equations. Thus linear control theory is highly advanced because of many techniques for obtaining and manipulating analytical solutions. The integrated equations give the transient response; the stability of the process can be determined from the roots of the characteristic equation; the dynamic characteristics are universely described in terms of the transfer function, and so on. Moreover the development of techniques for the optimization of the process performance, such as dynamic programming, depend on the ability to differentiate the integrated process equations (*7*). The control theory for nonlinear processes is less concise and compact but rather indicates certain guide lines and principles of attack. The approach is numerical rather than analytical, and the theory is used to establish the soundness of the computations.

Since a computer can only operate on digits which represent the state of a process at a discrete point in time, any control system utilizing a digital computer will necessarily be a sampled-data system. From the point of view of

the controller a process is represented as a sequence of numbers spaced in time. Similarly the control action is a sequence of numbers. It is convenient to make the time interval between sampling points equal to T so that real time can be represented at the sampling points by

$$t = T, 2T, 3T, \ldots kT \ldots$$

Although the input and state vectors of the process vary continuously with time, their specific value at the sampling point $t = kT$ is represented by $\mathbf{m}(kT)$ and $\mathbf{x}(kT)$ or more simply by $\mathbf{m}(k)$ and $\mathbf{x}(k)$.

A very useful advantage of using the state concept is that it can be applied directly to sampled-data systems. If the sampling period is taken small enough so that the input $\mathbf{m}(t)$ for $kT \leq t \leq (k+1)T$ can be considered essentially constant and equal to $\mathbf{m}(k)$ for the entire period, the dynamic equation for the process will become

$$\frac{d\mathbf{x}}{dt} = \phi\,[\mathbf{x}, \mathbf{m}(k)] \qquad \text{for } kT \leq t \leq (k+1)T \quad (5)$$

With a constant input the above equation can be integrated over one sampling period. Thus the dynamic behavior of the process may be expressed in the form

$$\mathbf{x}(k+1) = \Phi\,[\mathbf{x}(k), \mathbf{m}(k), T] \quad (6)$$

With a knowledge of the state of the process and the input vector at any time $t = kT$, this equation gives the state of the process at the next sampling point.

DYNAMIC OPTIMIZATION

Performance Criteria

Before it is possible to single out a particular controller as being optimum in relation to all other controllers, it is necessary to define quantitatively some measure of merit by which the performance of the system is evaluated. The simplest type of measure of performance is some function of the difference between the actual output of a process at a given time and that desired for the dynamic system. A convenient measure may be defined as

$$P(t) = a_1\,[x_1(t) - x_1^d]^2 + a_2\,[x_2(t) - x_2^d]^2 + \ldots \quad (7)$$

While other possibilities suggest themselves as suitable performance functions, the above choice is perhaps the simplest meaningful one which is easily manipulated. In order to evaluate the overall dynamic response of a system, the measure has to be extended over the time domain. When one assumes that the control vectors are changed only at the sampling point, Equation (7) is summed over all time

$$J(N) = \sum_{k=1}^{N} P(kT)T \qquad N \to \infty \quad (8)$$

where N is taken sufficiently large to cover the entire transient period. Thus the optimum dynamic response is obtained when a discrete set of control inputs $\mathbf{m}(k)$ are found such that

$$J^\circ(N) = \min_{\mathbf{m}(k)} \sum_{k=1}^{N} P(kT)T \qquad N \to \infty \quad (9)$$

Dynamic Optimization of Discrete Nonlinear Systems

Following the development of Fuller (3, 4), with proper modification for a discrete control system with independent inputs, one can show how an optimum control strategy can be selected at each sampling period for a general nonlinear process. The problem will consider the control system shown in Figure 1, where $c(t)$ is the control variable and $\mathbf{m}(t)$ is the state of independent input functions. Note that this is a slight revision of the author's previous nomenclature. The input vector is considered quite general in that its components can represent several inputs and their derivatives in phase space. $\mathbf{m}(t)$ is independent in the sense of being uncontrolled by $c(t)$. The only restriction on the components of $\mathbf{m}(t)$ is that they must be deterministic functions of time, that is not stochastic. For ease in the discussion the control action is restricted to a single variable.

The dynamics of the process are thus expressed by equations of the form

$$\frac{dx_i}{dt} = \phi_i\,[x_1, x_2, \ldots x_n; m_1, m_2, \ldots m_{r-1}; c(t)] \qquad i = 1, 2, \ldots n \quad (10)$$

and the independent inputs are expressed by

$$\frac{dm_j}{dt} = \gamma_j\,[m_1, m_2, \ldots m_{r-1}] \qquad j = 1, 2, \ldots r-1 \quad (11)$$

If a discrete control system is considered with a sampling period which is small compared with the changes in the input, Equations (10) and (11) can be integrated over a sampling interval T taking $m_1, m_2, \ldots$ as constant throughout the interval; that is at any sampling point k the integration gives

$$x_i(k+1) = \Phi_i\,[\mathbf{x}(k), \mathbf{m}(k), c(k), T] \qquad i = 1, 2, \ldots n$$
$$m_j(k+1) = \Gamma_j[\mathbf{m}(k), T] \qquad j = 1, 2, \ldots r-1 \quad (12)$$

Furthermore the performance criterion is defined as

$$J(N) = \sum_{k=1}^{N} P(k)T$$

where $P(k)$ is a general function of the desired output $\mathbf{x}^d$ and the actual state of the system $\mathbf{x}(k)$, that is

$$P(k) = P[x_1^d, x_2^d, x_3^d, \ldots x_m^d; x_1(k), x_2(k), \ldots x_n(k)] \qquad \text{where } m \leq n \quad (13)$$

Since $m \leq n$, not all of the state variables need be an output of interest.

With the use of Equation (12), $P(k)$ can be transformed into another function:

$$P(k) = P[x_1^d, x_2^d, \ldots x_m^d; x_1(k-1), \ldots x_n(k-1); m_1(k-1), \ldots m_{r-1}(k-1), c(k-1)] \quad (14)$$

Thus the value of the performance function at the kth sampling period depends on the state of the process, the state of the input, and the control action at the previous sampling period $k-1$. Again, the states of the process and input at $k-1$ can be related to their states and control action at $k-2$ by means of Equations (12). If one follows this sequence all the way back to the initial state, $P(k)$ can be transformed into still another function with new arguments:

$$P(k) = P_k[x_1^d, \ldots x_m^d; x_1(0), \ldots x_n(0); m_1(0), \ldots m_{r-1}(0), c(\lambda)] \quad (15)$$

and

$$J(N) = \sum_{k=1}^{N} P_k[\mathbf{x}^d, \mathbf{x}(0), \mathbf{m}(0), c(\lambda)]T \qquad 1 \leq \lambda \leq k \text{ as } N \to \infty \quad (16)$$

Thus the performance criterion J becomes an infinite sum of performance functions. At each sampling period k the value of P_k is dependent not only on the desired state but also on the initial states of the process and input and on every control action prior to k.

A word is perhaps in order about the interpretations of the summation indicated in the evaluation of J. If the system is stable, the dynamic response will ultimately come to an equilibrium or steady state at $k = N_e$. Since the performance criterion is used to quantitatively evaluate the dynamic response of a process to a control action, it can still be used for this purpose by summing only those terms which occur during the transient period; that is $1 \leq k \leq N_e$. Thus two different con-

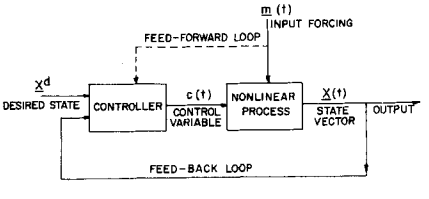

Fig. 1. Nonlinear control system considered for optimization.

trol schemes can be evaluated by comparing the summation over the transient period.

For a given situation the desired state $\mathbf{x}^d$ and the initial states $\mathbf{x}(0)$ and $\mathbf{m}(0)$ are fixed; thus the value of J depends on all the choices of $c(\lambda)$ from the initial time to the time where the system has reached equilibrium. Conceptually the optimum choice of the $c(\lambda)$'s will be that sequence which minimizes the performance criterion, namely

$$\underset{c(\lambda)}{\text{Min}}\ J(N_e) = \sum_{k=1}^{N_e} P_k[\mathbf{x}^d, \mathbf{x}(0), \mathbf{m}(0), c_{\text{opt}}(\lambda)]T \quad 1 \leq \lambda \leq k \quad (17)$$

For some other desired states and/or some other initial conditions some other sequences of $c(\lambda)$'s will be optimum. It is clear that c_{opt} depends on some type of function, the actual form of which at present is unknown, of the following arguments:

$$c_{\text{opt}}(\lambda) = c[\mathbf{x}^d, \mathbf{x}(0), \mathbf{m}(0), \lambda] \quad (18)$$

The authors want to modify the above relationship so that the optimum control action at any sampling period is an instantaneous function of the states of the process and the inputs. Suppose that the optimum control action as defined by Equation (18) is applied to a process from the initial time to some arbitrary period n. Then clearly the performance criterion can be written as

$$\underset{c(\lambda)}{\text{Min}}\ J(N_e) = \sum_{k=1}^{n} P_k[\mathbf{x}^d, \mathbf{x}(0), \mathbf{m}(0), c_{\text{opt}}(\lambda)]T + \underset{c(\lambda)}{\text{Min}} \sum_{k=n+1}^{N_e} P_k[\mathbf{x}^d, \mathbf{x}(n), \mathbf{m}(n), c(\lambda)]T \quad (19)$$

Since the first summation is completely determined, the optimization depends on the choice of the control action in the second summation; that is the continuation of an optimal policy is still optimum [the principle of optimality (2)]. Thus in terms of the second summation Equation (18) becomes

$$c_{\text{opt}}(\lambda) = c[\mathbf{x}^d, \mathbf{x}(n), \mathbf{m}(n), \lambda - n] \quad \text{for } \lambda \geq n \quad (20)$$

If $\lambda = n$

$$c_{\text{opt}}(n) = c[\mathbf{x}^d, \mathbf{x}(n), \mathbf{m}(n), 0]$$

But n was chosen arbitrarily, and so the specific index n can be dropped. Thus for any k

$$c_{\text{opt}}(k) = c[\mathbf{x}^d, \mathbf{x}(k), \mathbf{m}(k)] \quad (21)$$

which shows that the optimum control action at any period k is an instantaneous function of the states of the process, the input, and the desired state.

In the nonlinear case the determination of the exact nature of Equation (21) is difficult to ascertain. However by restricting one's attention to systems

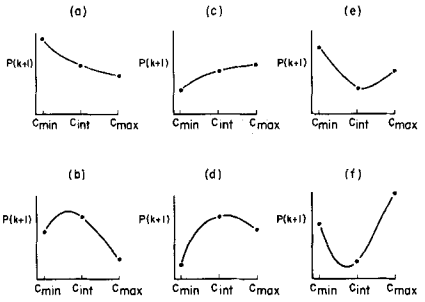

Fig. 2. Possible configurations for predicted performance function.

with bounded inputs and control action (which is a characteristic of all real systems), the saving grace of saturation comes to one's aid. When the control action is limited by saturation, that is $\alpha \leq c(k) \leq \beta$, then Silva (*11*), La Salle (9), and others have shown that the optimum control action is on the boundaries of its limits (except perhaps for a small period of time near the end of the transient). As a result the control action is a discontinuous function of time consisting of alternating step changes between the maximum and minimum level. This is known as a *relay control system* or *bang-bang control system*. In the tail end of the transient, where the actual output is very close to the desired state output, the additional summation of terms (which are small in comparison with earlier terms) to an already large accumulation of terms only affects the overall evaluation of the performance criterion slightly. In fact if the control action during this end regime is not exactly optimum, the performance is still, for practical purposes, close enough to optimum to be superior to any other response.

In this study the functional relationship between the optimum control action and the phase coordinates of the process and input need not be, and cannot be, elucidated. Since a computer will be used for the controller, it is only necessary to have a computational scheme for generating the control action. The existence of the theoretical relationship given by Equation (21) and the knowledge that in most cases the optimum control action is a relay type form the valid basis for such a computational scheme. Equation (21) establishes in principle that the optimum control action can be determined from the present state of the process, the present state of the input, and the desired state. The knowledge that the optimum control action most often is a relay type reduces the search for the optimum control action to essentially two values.

Suppose for the sake of argument that the optimum control action for a given situation is one maximum period, one minimum period, and an end regime where the control action is not saturated. Then the overall performance criterion can be written as

$$J(N_e) = \sum_{k=1}^{n_1} P_k[\mathbf{x}^d, \mathbf{x}(0), \mathbf{m}(0), c_{\max}]T + \sum_{k=n_1+1}^{n_2} P_k[\mathbf{x}^d, \mathbf{x}(n_1), \mathbf{m}(n_1), c_{\min}]T + \sum_{k=n_2+1}^{N_e} P_k[\mathbf{x}^d, \mathbf{x}(n_2), \mathbf{m}(n_2), c_{\text{end}}]T \quad (22)$$

At the proper time the optimum controller switches from $c_{\max}$ to $c_{\min}$ and from $c_{\min}$ to c_{end}.

The optimum control action at any given sampling period is generated by the following computation scheme. Since the present state of the process $\mathbf{x}(k)$ is known as a result of a feedback measurement and the state of the input $\mathbf{m}(k)$ is known as a result of a feedforward measurement, the state of the process at the next sampling period $\mathbf{x}(k+1)$ can be calculated from Equation (12) for any number of control actions. Specifically the state of the process is calculated for the maximum control action $c_{\max}$, the minimum control action $c_{\min}$, and some intermediate control action c_{int}; thus

$$\begin{aligned} \mathbf{x}^1(k+1) &= \Phi[\mathbf{x}(k), \mathbf{m}(k), c_{\max}, T] \\ \mathbf{x}^2(k+1) &= \Phi[\mathbf{x}(k), \mathbf{m}(k), c_{\min}, T] \\ \mathbf{x}^3(k+1) &= \Phi[\mathbf{x}(k), \mathbf{m}(k), c_{\text{int}}, T] \end{aligned} \quad (23)$$

where the superscript numbers are used to distinguish the predicted states. The responses to the various control actions are evaluated with the aid of the performance function for the $(k+1)$ period, namely

$$\begin{aligned} P^1(k+1) &= P[\mathbf{x}^d, \mathbf{x}^1(k+1)] \\ P^2(k+1) &= P[\mathbf{x}^d, \mathbf{x}^2(k+1)] \\ P^3(k+1) &= P[\mathbf{x}^d, \mathbf{x}^3(k+1)] \end{aligned} \quad (24)$$

The possible configurations for the predicted performance function and the control action are shown in Figure 2. The computer routine selects the optimum control action at $t = kT$ on the basis of a predicted minimum performance function at $t = (k+1)T$. This type of control system will be called an *optimum predictor-controller*. For configuration (a) or (b), $c_{\max}$ is selected as the optimum control action. For configuration (c) or (d), $c_{\min}$ is selected as the optimum control action. The need to predict the performance for some intermediate control action becomes clear when the optimum is not one of the extreme values. When configuration (e) or (f) occurs, the computer fits a second-order curve through the three points already calculated and finds the minimum in the

TABLE 1. VALUES FOR INPUTS AND PARAMETERS FOR CSTR SYSTEM

m independent inputs		Parameters	
F_{10}	= 10.0 cc./sec.	V	= 1,000 cc.
T_{10}	= 350°K.	k_o	= 7.86×10^{12} sec.$^{-1}$
T_{co}	= 340°K.	E_a	= 28,000 cal./mole
X_{10}	= 0.0065 mole/liter	ΔH_R	= 27,000 cal./mole
		ρ	= 1.0 g./cc.
		σ	= 1.0 cal./mole °K.
		U	= 10.0 cal./sec. °K.
		K	= 0.20

curve. The corresponding value of c becomes the optimum control action for that period.

It is important to realize that the above computation scheme selects the optimum control action on the basis of a predicted performance for one sampling period. When the system comes to $t = (k + 1)T$, the entire procedure is repeated to select the optimum control for this new period. Since this routine is a piece-by-piece optimization procedure, it does not necessarily follow that the overall performance criterion has been optimized over the entire time of the transient. However in a bounded system, where the optimum control action is a relay type, the piece-by-piece optimization gives a dynamic response which is optimum from the overall point of view.

NUMERICAL EXAMPLE

To demonstrate the performance of the predictor-controller the well-known model of a continuous stirred tank reactor (CSTR) with a first-order exothermic reaction developed by Amundson et al. (*1*) and used recently by Kalman et al. (*7*) is chosen. It should be emphasized that this is only one system to which the predictor-controller has been applied; other systems including one real process have also been studied (*5*).

The material and heat balance for the CSTR can be written as

$$\frac{dX_1}{dt} = \frac{F_{10}}{V} X_{10} - \frac{F}{V} X_1 - kX_1 \quad (25)$$

$$\frac{dT_1}{dt} = \frac{F_{10}}{V} T_{10} - \frac{F}{V} T_1 - kX_1 \frac{\Delta H_R}{\rho\sigma} - \frac{UKF_{20}}{V\rho\sigma(1 + KF_{20})} (T_1 - T_{co}) \quad (26)$$

Equations (25) and (26) form a set of simultaneous nonlinear differential equations which describe the dynamic behavior of the reactor in terms of the input variables F_{10}, F_{20}, T_{10}, T_{co}, and X_{10}, the state variables X_1 and T_1, and the parameters V, k_o, E_a, ρ, ΔH_R, σ, and U. The input variable used to control the process will be the cooling water flow rate F_{20}; the other inputs will be independent and included in $\mathbf{m}(t)$. Thus the above equations may be expressed simply as

$$\frac{dX_1}{dt} = \varphi_1 [X_1, T_1, \mathbf{m}(t), F_{20}(t)]$$

$$\frac{dT_1}{dt} = \varphi_2 [X_1, T_1, \mathbf{m}(t), F_{20}(t)]$$

For the given set of parameters and constant input conditions [$\mathbf{m}(t) = \mathbf{m}$] in Table 1 the steady state solution of Equations (25) and (26) leads to the familiar operating characteristics shown in Figure 3. At the point or points of intersection the heat generated is just equal to the heat removed, establishing a steady condition. As the cooling water rate is increased, the upper steady state temperature decreases as a result of the additional heat removal. Eventually if the heat removal becomes too large, the reactor has only one steady state point, at the low temperature.

Before control of this process is attempted, the dynamic open loop characteristics can be studied by considering the response to step changes in the input. Suppose the process is initially at some steady state level [$X_1(t_o)$, $T_1(t_o)$], and at time t_o the input variable undergoes a step change. The state of the process now moves from this initial condition to some new steady state, in accordance with the simultaneous solutions of Equations (25) and (26).

For a second-order system the dynamic behavior of a process can be represented very conveniently as the trajectory of the state variables in a phase space of two dimensions or what is called a *phase plane* (*3*). The coordinates chosen for the phase plane are the variables of interest—temperature and concentration. Since the solution of Equations (25) and (26) is unique for a given initial state at t_o and the nature of the inputs for all time $t > t_o$, there is correspondingly a unique trajectory. By considering the whole family of solutions to Equations (25) and (26) for a cooling water flow rate of $F_{20} = 5.0$ and for the other inputs and parameters given in Table 1, a complete phase portrait of trajectories is developed as shown in Figure 4. Recall from Figure 3 that there are three steady state temperatures for $F_{20} = 5.0$, and all trajectories terminate on one of these three steady state points marked *A*, *B*, or *C*. The unstable nature of the middle steady state is clearly shown because trajectories diverge from it, rather than to it.

Although Figure 4 was derived from considering one initial state and then following the solution along a trajectory until it terminated on some steady state point, the phase portrait can also have another interpretation. Suppose the system is operating at the upper steady state point *A*, and, suddenly, an input disturbance of short duration lowers the reactor temperature to point *D*. The phase portrait now shows how the system restores itself under its own power (that is under the influence of the same inputs and control action that prevailed before the disturbance occurred). Although the trajectory may be rather indirect, it eventually returns to *A*. If the disturbance has displaced the system to point *E*, then the reactor can not restore itself to its original operating point, but in fact, will die out so to speak to the low temperature level at point *C*.

The role to be played by the controller becomes clear; in the case where the process is stable, it will attempt to restore the process more directly; in the case where the process is unstable, it will attempt to restore the process if at all possible. By changing the control variable the effective forcing of the process is changed which modifies the dynamic characteristics of the process. In terms of the phase portrait the controller gives the process alternate trajectories to follow at any state. Without a change in control action the system is locked in a set course.

If the control action is limited by physical considerations to a range between $0 \leq F_{20} \leq 20.0$, the greatest modification in the dynamic behavior of the process that is possible can be seen by comparing the phase portraits for these two extreme values with that for $F_{20} = 5.0$. In Figure 5 is shown the phase portrait of the solutions to Equations (25) and (26) for $F_{20} = 0$ with the points *A'*, *B'*, and *C'* as terminals for all trajectories. For the sake of comparison the points *A*, *B*, and *C* are shown to indicate how the steady state points relocate in going from $F_{20} = 5.0$ to $F_{20} = 0$. With $F_{20} = 0$ one would expect the reactor to operate in general at a high temperature.

Another phase portrait can be determined for $F_{20} = 20.0$ as shown in

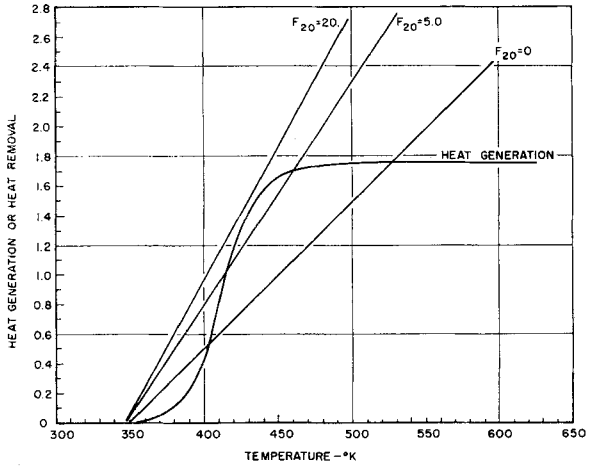

Fig. 3. Steady state operating levels for CSTR for various cooling water flow rates.

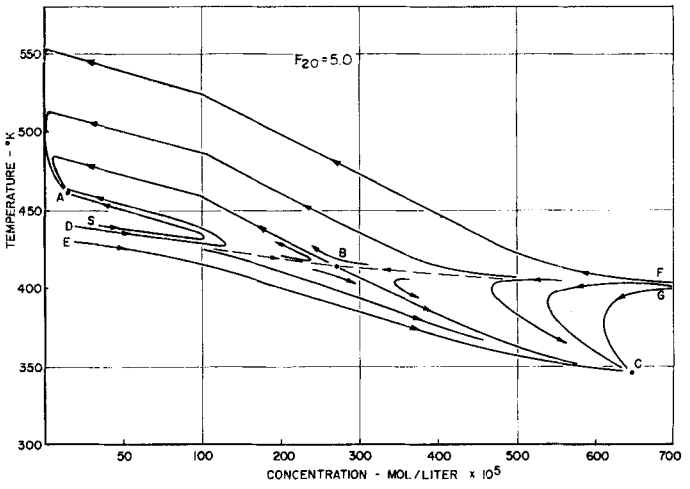

Fig. 4. Complete phase plane portrait of trajectories.

Figure 6. As was pointed out (Figure 3), there is only one steady state point for $F_{20} = 20.0$; consequently all the trajectories eventually terminate at one and only one steady state marked C''. On the assumption that the equipment can withstand the high temperature and the reactant and product are stable, all the trajectories that run up to the high temperature region make a sharp turn when the reactant is depleted and return to point C''. Again points A and B are shown to indicate where the steady state would be if $F_{20} = 5.0$.

Only when the system is under variable forcing can there be more than one trajectory passing through a nonsteady state point. In fact by superimposing Figures 5 and 6 there are now two trajectories passing through each point in the phase plane. Each time the control action switches from $F_{20} = 20.0$ to $F_{20} = 0$, or vice versa, the system switches from one set of trajectories to the other. In Figure 7 there is shown a magnified region of the phase plane with two sets of trajectories; one set of lines are the loci followed by the system if the control action is $F_{20} = 20.0$, while the other set of lines are the loci followed by the system if the control action is $F_{20} = 0$. Suppose for example the process is moving along the trajectory marked BC with $F_{20} = 20.0$. When it reaches point C the controller decides to make $F_{20} = 0$; now the process will follow along the trajectory marked CF until it decides to change again. If the controller had decided to keep $F_{20} = 20.0$, the process would have continued along trajectory BCD.

In order to give an idea of how fast the state of the process is changing while following a particular locus, the time (in seconds) is marked along the trajectories. Thus by designating the top of Figure 7 as north, it is apparent that the state of the process changes most rapidly when heading along a trajectory in the northwest direction. Moreover as the trajectories heading northwest lie further north, the rate of change of the state of the process increases. In general, for the trajectories heading southeast to the lower temperature region, the state of the process changes least rapidly. In other words the system can heat up quickly by a rapid consumption of the reactant, but it is slower in cooling down.

It should be realized by examining Figures 5 and 6 or 7 that the controller has the greatest flexibility in the regions of the phase plane where the trajectories for the maximum and minimum control action are most divergent. In the upper right half of Figure 7 for example the trajectories are nearly parallel for the two extreme values of the control variable. Moreover any value of the control action between zero and twenty will necessarily have a trajectory in the same direction. Consequently no matter what cooling water flow rate the controller may decide to use, the response of the process in this region will have to be along the given direction until the process comes into an area of intersecting trajectories. On the other hand, in the lower half and in the extreme left side of Figure 7, the trajectories for the maximum and minimum control action are either completely opposite in direction or at least more divergent than before. As a result every value of the control action between zero and twenty will have a trajectory whose direction at any point will fall between the directions of the two extreme trajectories passing through the same point. Consequently the direction of the response of the process in these regions is directly affected by the value of the control variable.

The utility of Figures 5 and 6 or 7 becomes apparent when one realizes that an optimum relay controller will call for maximum and/or minimum control action throughout a transient with the exception of the end regime. Thus they form a complete map of all the trajectories the process can follow while under the influence of the controller.

The problem for the controller will be to restore the process to the desired state (or to approach the desired state as close as possible) after undergoing an input disturbance of arbitrary size. The control action will be selected so that the dynamic response minimizes the performance criterion. In the present example, where both concentration and temperature are to be controlled, a suitable overall performance criterion would be that defined by

$$J(N) = \sum_{k=1}^{N} P(k)T$$

with

$$P(k) = a_1 [X_1^d - X_1(k)]^2 + a_2 [T_1^d - T_1(k)]^2 \quad (27)$$

Since the concentration and temperature are numbers of different orders of magnitude, the weighing factors a_1 and a_2 will be chosen to scale the squared concentration and temperature deviations in such a way that they become numbers of the same order of magnitude.

The choice of the desired state is subjective and will depend on the purpose for which the process is operated. Therefore for the sake of generality the authors will investigate the performance of the control system for a variety of desired states, namely when the desired state corresponds to a stable steady point, a nonsteady state point, and an unstable steady state point.

The first example will consider the problem of restoring the process to the

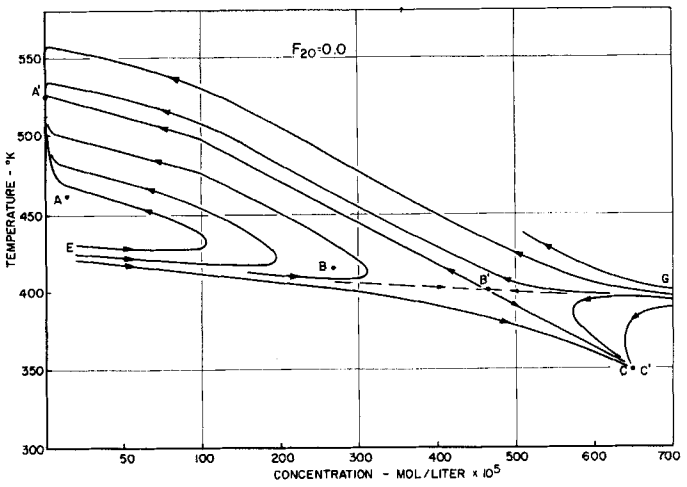

Fig. 5. Phase portrait of CSTR system for $F_{20} = 0$, minimum control action.

upper stable steady state point in Figure 4, point A. The coordinates are

$$X_1^a = 15.31 \times 10^{-5} \text{ m./liter}$$
$$T_1^a = 460.91°\text{K}.$$

Suppose initially the process is at a state corresponding to point S; that is

$$X_1(0) = 35.31 \times 10^{-5} \text{ m./liter}$$
$$T_1(0) = 440.91°\text{K}.$$

Although this disturbance may appear small, it is beyond the region where a linear approximation about point A is meaningful. Clearly, if one would wait long enough, the process will restore itself; in Figure 4 following the trajectory from S to A requires about 120 sec. It is the purpose of the controller to move the state of the process to point A in the optimum fashion.

A close examination of the phase plane in Figure 7 should give one a good feel for what a control system has to do in order to restore the state of the process to point A as directly as possible. Since the state of the system at point S is too low in temperature and too high in concentration, one would expect that the temperature would rise fastest and the reactant consumed quickest by not removing any heat with the cooling water. As Figure 7 shows quite clearly, the trajectory for $F_{20} = 0$ seems to be the most direct route from the region of the initial state and toward the region of the desired state, while the trajectories for $F_{20} = 20.0$ in the region of the initial state carry the system even further from the desired region. In fact it seems reasonable to say that any control action calling for F_{20} to be greater than zero during the early transient period would result in a less direct route toward the desired region. Granted that initially the most direct route from the initial state toward the desired region is along trajectory SCF, it is also obvious from Figure 7 that, when the state of the process approaches the neighborhood of point A, the control action must change to some other value(s), or the state of the process will move past the desired state into the very high temperature region.

In order to see precisely how these qualitative ideas concerning the nature of the process are indeed incorporated into the selection of the control action, the authors will illustrate in some detail how the optimum predictor-controller works. With the aid of a digital computer the optimum control action is generated as follows. Starting with the initial state, the computer has to decide on what control action it will use during the first sampling period (which will be taken as ½ sec.). By using the model it predicts where the state of the process will be at the next sampling point for the maximum, an intermediate, and the minimum control action. The integration of Equations (25) and (26) over a time interval of ½ sec. for the inputs and parameter given in Table 1 gives the predicted states shown in the first part of Figure 8, where the superscripts refer to the predicted state. By evaluating the performance function for these three predicted states, namely

$$P^1(1) = 10^6 (15.31 \times 10^{-5} - 36.51 \times 10^{-5})^2 + 10^{-4} (460.91 - 440.96)^2$$
$$= 847.4425 \times 10^{-4} \quad \text{for } F_{20} = 0.0$$
$$P^2(1) = 10^6 (15.31 \times 10^{-5} - 36.96 \times 10^{-5})^2 + 10^{-4} (460.91 - 440.66)^2$$
$$= 878.78 \times 10^{-4} \quad \text{for } F_{20} = 5.0$$
$$P^3(1) = 10^6 (15.31 \times 10^{-5} - 36.45 \times 10^{-5})^2 + 10^{-4} (460.91 - 440.60)^2$$
$$= 859.39 \times 10^{-4} \quad \text{for } F_{20} = 20.0$$

the computer selects $F_{20} = 0$ as the initial control action to be applied to the system since it gives the minimum performance function. Note that the weights in the performance function were taken as $a_1 = 10^6$ and $a_2 = 10^{-4}$ so that deviations in concentration and temperature are expressed in numbers of the same order of magnitude. With the initial control action set at $F_{20} = 0$, the initial state of the process moves along the trajectory marked SCF in Figure 7. When the first sampling period is over, the state of the process is

$$X_1(1) = 36.51 \times 10^{-5} \text{ m./liter}$$
$$T_1(1) = 440.96°\text{K}.$$

For each sampling period the calculations are repeated, and the response of the system is shown in Figure 9. In fact $F_{20} = 0$ is the optimum

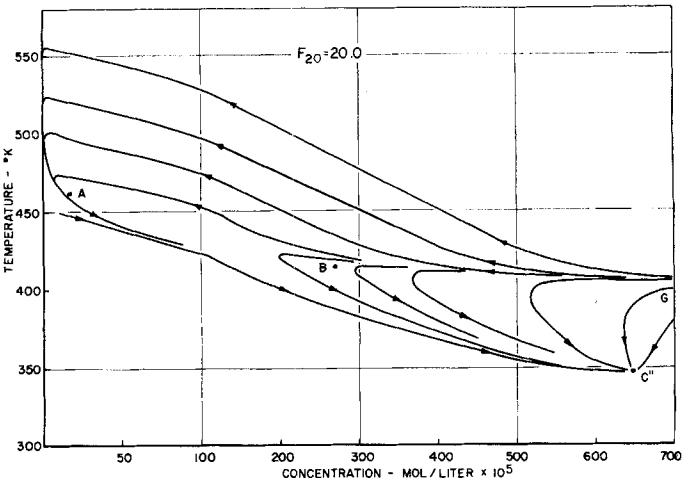

Fig. 6. Phase portrait of CSTR system for $F_{20} = 20.0$, maximum control action.

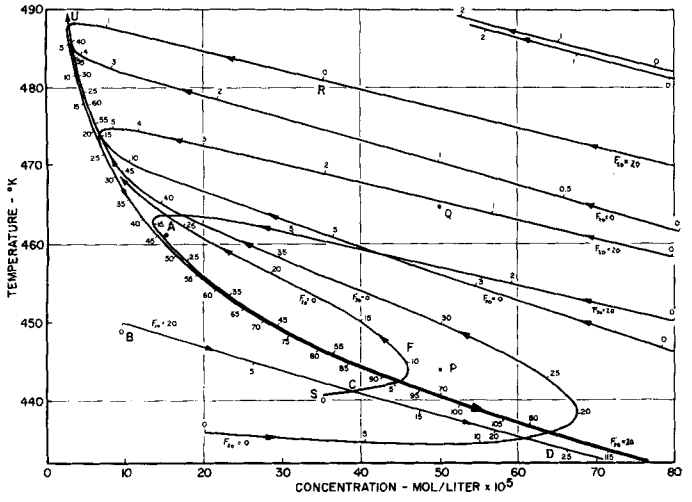

Fig. 7. Enlarged phase portrait about upper steady state point.

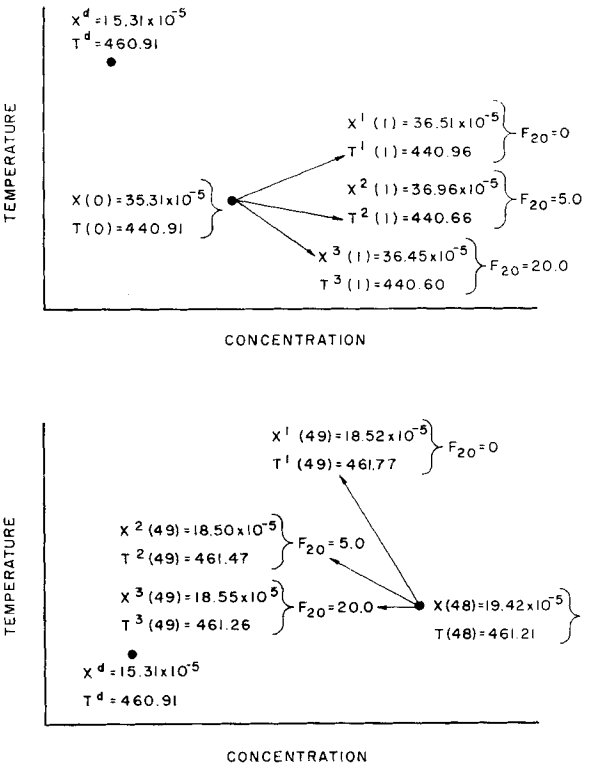

Fig. 8. Predicted states of operation.

control action for the first forty-eight sampling periods (24 sec. real time). At $k = 48$ the state of the process is at point G with

$$X_1(48) = 19.42 \times 10^{-5} \text{ m./liter}$$
$$T_1(48) = 461.21°\text{K}.$$

In order to generate the control action for this sampling period the computer predicts the values shown in the second part of Figure 8 and selects $F_{20} = 20.0$ as the optimal control action.

As shown in Figure 9, the trajectory of the system now switches at point G from the locus it had been following for $F_{20} = 0$ to a new locus for $F_{20} = 20.0$. The controller continues to select $F_{20} = 20.0$ as the optimum control action for the next six sampling periods until $k = 54$ (27 sec. real time). At this point the state of the system has advanced to

$$X_1(54) = 16.27 \times 10^{-5} \text{ m./liter}$$
$$T_1(54) = 460.95°\text{K}.$$

In selecting the control action for this sampling period the computer generates a configuration, where the minimum performance function does not result from a control action at an extreme value. This is the first indication that the system has reached the end regime. By fitting a second-order curve to the three points it determines the minimum at $F_{20} = 13.35$. During the end regime the computer continues to select the control action at each sampling period. As seen in Figure 9, the system no longer follows a given trajectory but wavers its way to the desired state at point A. A simple proportional control action could have been used in the end regime just as well. As was pointed out previously, the contribution of the end regime to the transient response is very small. For example the overall performance criterion at $k = 54$, where the end regime starts, has a value of

$$J(54) = \sum_{k=1}^{54} P(k)T = 1.85266$$

By the time the state of the system has advanced ten more sampling periods to

$$X_1(64) = 15.36 \times 10^{-5} \text{ m./liter}$$
$$T_1(64) = 460.95°\text{K}.$$

the performance criterion is practically the same; namely

$$J(64) = \sum_{k=1}^{64} P(k)T = 1.85276$$

The computer has selected a control action which has moved the system from its initial state at point S to practically on top of the desired state in 32 sec. in the most direct route physically possible. The natural response without control is 120 sec.

Also shown in Figure 9 is the response of the process from an initial state at point R where

$$X_1(0) = 35.31 \times 10^{-5} \text{ m./liter}$$
$$T_1(0) = 480.91°\text{K}.$$

The uncontrolled response requires more than 174 sec. for the system to return to point A. The computer selects $F_{20} = 20.0$ as the optimum control action for ninety sampling periods (45 sec. real time). As a result the system follows along trajectory RUV for the major part of the transient. At $k = 90$ the system has reached the end regime with the application of only the maximum control action, where

$$X_1(90) = 14.41 \times 10^{-5} \text{ m./liter}$$
$$T_1(90) = 460.81°\text{K}.$$

This is in contrast to the previous example where the optimum control action called for both extreme values. In the end regime the system again wavers its way to the desired state at point A. At $k = 100$ (50 sec. real time) the system has reached

$$X_1(100) = 15.18 \times 10^{-5} \text{ m./liter}$$
$$T_1(100) = 460.89°\text{K}.$$

Since the initial point R is in the region of parallel trajectories, the system has to move to point U before the controller can really return the state to the desired level. The important point here is that the computer can generate meaningful control action equally well when the state of the system is in an area of widely diverging trajectories or in an area of parallel trajectories, as long as the desired state is a stable steady state.

Suppose one wants to operate the process at some desired state which is not a steady state point. It follows that the process can not stay fixed on a nonsteady state point, but at most it can hope to stay near the desired point by means of some kind of dynamic operation, such as cycling. The possibility of operating about or near a nonsteady state point depends ultimately on where in the phase plane the point is located. For an example in Figure 7 point P is in the region of the phase plane where the trajectories for various

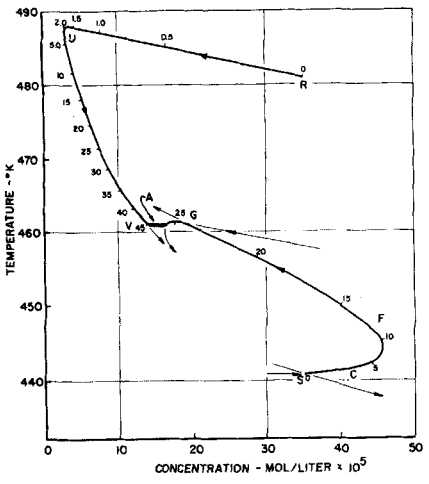

Fig. 9. Optimum response to initial displacement with desired state corresponding to a steady state point.

control actions are divergent. As a result it is possible for the controller to ride the system around the neighborhood of point P for any length of time. On the other hand point Q is in a region where the trajectories for all control actions are essentially parallel. As a result it is impossible for the controller to keep the system near point Q for even a short length of time.

In order to see how successful the optimum controller is in moving the process from an arbitrary initial point to the desired point P or Q, refer to Figure 10. For the first case consider the desired state at point P with

$$X_1^d = 50.00 \times 10^{-5} \text{ m./liter}$$
$$T_1^d = 445.00°\text{K.}$$

and the initial state at point S. Trajectory SFL is the path selected by the optimum predictor-controller when the performance function is defined as

$$P(k) = a_1 [X_1^d - X_1(k)]^2 + a_2 [T_1^d - T_1(k)]^2$$

During the first 9.5 sec. the system comes to point F on a trajectory for $F_{20} = 0$. From point F the system slowly moves to point L with frequent changes in the control action which eventually approach $F_{20} = 10.0$. By 27.0 sec. the state seems to approach a steady state at point L with

$$X_1 = 45.10 \times 10^{-5} \text{ m./liter}$$
$$T_1 = 444.51°\text{K.}$$

Thus instead of approaching point P the controller directs the system to the nearest steady state point. It is pointed out that this is not a characteristic of the control scheme but merely a coincidence in that point L happens to be a steady state point for $F_{20} = 10.0$.

Although the temperature of point L is very close to the desired temperature, the concentration is off by about 10%. This indicates that the weights used in the performance function did not penalize concentration deviations with the same severity as temperature deviation. Consequently by reducing the weight of the temperature deviation to $a_2 = 10^{-5}$ and keeping $a_1 = 10^8$, the controller selects trajectory STNM which initially moves the system even further away from the desired temperature but brings it to another trajectory, which eventually is able to move the system closer to the desired state than before. The process first moves to point T with $F_{20} = 20.0$, then to point N with $F_{20} = 0$. Within 20 sec. the state is about point M where the coordinates oscillate within the ranges indicated below:

$$48.208 \times 10^{-5} \leq X_1 \leq 48.209 \times 10^{-5}$$
$$443.49 \leq T_1 \leq 443.50$$

Although the fluctuation in the state of the process is very small and can be considered constant for practical purposes, it is important to realize that the state about point M is a dynamic state which is maintained as a result of the control action.

For the second case consider point Q as the desired state with

$$X_1^d = 50.00 \times 10^{-5} \text{ m./liter}$$
$$T_1^d = 465.00°\text{K.}$$

and the initial state again at point S. Trajectory $SFKGH$ is selected by the controller if $a_1 = 10^8$ and $a_2 = 10^{-4}$. The process moves up to point G along the trajectory for $F_{20} = 0$, then it switches over to a trajectory for $F_{20} = 20.0$ for three sampling periods, and finally it approaches a region about point H after 40 sec. where the fluctuations of the coordinates are within the range indicated below:

$$13.90 \times 10^{-5} \leq X_1 \leq 13.96 \times 10^{-5}$$
$$462.24 \leq T_1 \leq 462.56$$

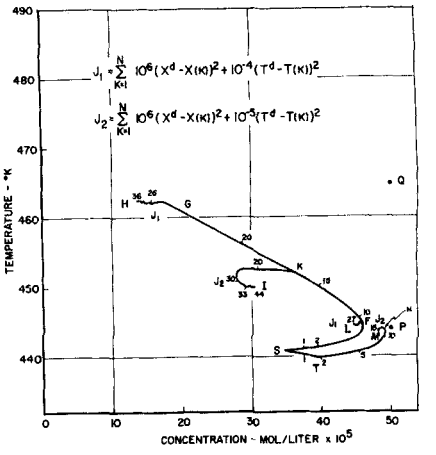

Fig. 10. The effect of the choice of weights on optimum response to an initial displacement with the desired state corresponding to a nonsteady state point.

Again the dynamic state is achieved where the temperature coordinate is within 3 deg. of the desired level but the concentration is far too low.

If the weight for the temperature deviation is reduced to $a_2 = 10^{-5}$ while $a_1 = 10^8$, the controller selects trajectory $SFKI$. This trajectory is identical with the previous one until point K is reached; then it switches to a trajectory for $F_{20} = 20.0$ until it approaches the neighborhood of point I after 45 sec. where the fluctuations of the coordinates are within the ranges indicated below:

$$30.65 \times 10^{-5} \leq X_1 \leq 30.59 \times 10^{-5}$$
$$450.17 \leq T_1 \leq 450.51$$

As was pointed out it is impossible to operate, even in a dynamic sense near point Q. Therefore the fact that the controller brings the system to points H or I is no bad reflection on the part of the controller but represents the best compromise between the choice of the performance function the dynamic limitations of the process.

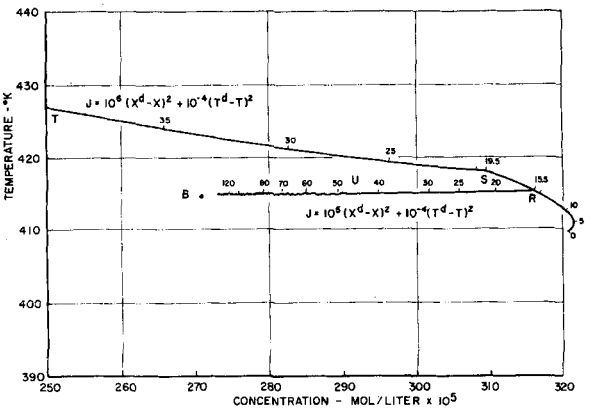

Fig. 11. The effect of the choice of weights on the optimum response to an initial displacement with the desired corresponding to an unstable steady state point.

The fact that the performance function is subjective, especially the choice of the relative values of the weights, is emphasized by points L and M. Here two different choices in the relative weights results in significantly different responses. When the desired state is a nonsteady state point, the optimum response depends on the choice of the relative weight. There is no prior way of selecting the exact weights, but the dynamic properties of the system can serve as a guide line. For example with the aid of Figure 7 it would seem reasonable to weigh the performance function in favor of the concentration in order to operate around point P. Since the trajectories for $F_{20} = 0$ turn around in this region, a strong penalization for concentration deviations will prevent the system from prematurely turning away from the region of point P.

As a final test for the control system a desired point is selected which corresponds to an unstable steady point such as point B in Figure 4 with

$$X_1^d = 270.7 \times 10^{-5} \text{ m./liter}$$

$$T_1^d = 414.94°\text{K.}$$

To see if it is possible to operate around point B, refer again to Figures 5 and 6 where the extreme effects of the control action on the dynamic behavior of the system can be seen. In Figure 5 point B is surrounded by trajectories which eventually go to the high temperature region, while in Figure 6 point B is surrounded by trajectories which eventually go to the low temperature region. Thus it may appear possible to operate about point B since control in the immediate vicinity is possible, but the margin of control is very narrow. If the temperature should become as little as 4 or 5 deg. higher than at point B, Figure 6 shows that the system will be in a region where the trajectories will move the system to the high temperature region. Thus even with the maximum cooling rate the system is beyond control.

An attempt to control the system is made with an initial disturbance at

$$X_1 = 320.7 \times 10^{-5} \text{ m./liter}$$

$$T_1 = 409.9°\text{K.}$$

The choice of weights in the performance function must severely penalize the temperature deviations in view of the narrow margin of operation in this variable. In Figure 11 is shown the response for two different sets of weights. With the usual values of $a_1 = 10^6$ and $a_2 = 10^{-4}$, the system follows trajectory $ORST$. For the first 19.5 sec. the control action calls for $F_{20} = 0$; then it calls for $F_{20} = 20$ starting at point S, but by this time the temperature is over 418°K. and the system is hopelessly carried away to the high temperature region. When $a_1 = 10^5$ and $a_2 = 10^{-4}$, the system follows trajectory $ORUB$. Thus the increase in the relative weight for the temperature deviation has the effect of switching the system at point R, which is a point at a lower temperature than point S. From point R to U the controller calls for $F_{20} = 20.0$. Beyond point U the control action oscillates with the system dynamically approaching point B at a slower and slower rate.

ACKNOWLEDGMENT

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NOTATION

a_i = one of several constants
$c(t)$ = control variable
E_a = activation energy
F = effluent flow rate from continuous stirred tank reactor
F_{10} = reactant stream flow rate
F_{20} = cooling water flow rate
ΔH_R = heat of reaction
J = performance criterion
$K = \frac{2\rho\sigma}{U}$
(k) = general index on the sampling period
$k = k_0 e^{-E/RT}$, reaction rate constant
$m_i(t)$ = general input variable
N = number of sampling periods large enough to include transient
N_e = number of sampling periods to reach steady state operation
$P(t)$ = performance function
P^1, P^2, P^3 = predicted performance functions
T = length of sampling period
T_1 = temperature of material in reactor
T_{10} = temperature of inlet stream
T_{c0} = temperature of inlet cooling water
T_c = temperature of exit cooling water
t = time
t_0 = initial time
t_1 = specific time, $t_1 > t_0$
U = overall heat transfer coefficient
V = volume of reactor, a constant
X_1 = concentration of reactant A
x_i = a general state variable, $i = 1,2,\ldots n$
x_i^d = desired value for state variable, $i = 1,2,\ldots m$
$\mathbf{x}^1, \mathbf{x}^2, \mathbf{x}^3$ = predicted states

Greek Letters

α = lower bound on input variable $c(t)$
β = upper bound on input variable $c(t)$
Γ_j = integrated function defined by Equation (12)
γ_i = general function of the ith input variable defined by Equation (11)
λ = time, used as a general designation for a range of times
ρ = density
σ = heat capacity
φ_i = general differential function as defined by Equation (1)
Φ_i = general integrated function

Subscripts

i = index
j = index
opt = optimum
min = minimum
max = maximum
int = intermediate
end = end regime

Superscript

o = optimum

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