Predictive Feedback Control of a Continuous Flow Stirred Tank Reactor

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A novel feedback control system, called a *predictive feedback control system*, is developed for the regulation of the exit composition of a continuous flow stirred tank reactor (CFSTR). The control system utilized two basic feedback signals. One is the effluent concentration of the composition to be controlled. This is measured by a batch type of composition analyzer such as a chromatograph. The other is a predictive feedback signal which continuously predicts the difference between the actual value of the controlled variable and the measurement supplied by the analyzer. The predictive signal is generated from a plant model which approximately relates the controlled variable and the continuously measured reactor temperature.

Unlike direct feedback control systems, the stability of the predictive system is unaffected by the periodic sampling and time delays introduced by the batch analyzer. Moreover, at steady state the predictive feedback signal disappears, and, like direct feedback systems, predictive feedback systems yield very accurate steady state control.

A computer simulation of the predictive feedback control of a particular CFSTR has shown that predictive control is considerably more effective in composition control than conventional direct feedback control, is more effective than conventional temperature control, and retains the advantages of direct feedback control while partially eliminating the undesirable effects caused by the batch analyzer.

Traditionally, the control of continuous flow, stirred tank, chemical reactors (CFSTR) has been based on the continuous measurement of reactor, or reactant mass, temperature. However, the increasing interest in higher product quality and optimum economic operation have resulted in a significant trend toward direct feedback reactor control. That is, control based on the direct, or actual, measurement of the composition of the reactor effluent.

The measurement of the composition of a multicomponent stream almost always implies the use of a batch type of composition analyzer such as a gas chromatograph or mass spectrometer. Such analyzers involve the periodic sampling of the reactor effluent, subsequent preparation and analysis of the sample, followed by the release of suitable signals representing the concentration of the particular components of interest.

Studies by Min and Williams (*4*, *8*), and Ross (*6*) indicate that when direct feedback control is used, the time delays and periodic sampler inherent in the batch analyzer can be highly detrimental to the system stability and the quality of control. The results presented by these authors indicate that this undesirable situation will almost certainly occur whenever the analysis delay and sampling period of the analyzer are of the same order of magnitude as the dominant time constants of the reactor. Thus, while direct feedback reactor control may seem desirable, in many cases the application of this type of control may be self-defeating.

To date, no work has been presented concerning the development of special reactor regulator systems which utilize direct feedback while eliminating or decreasing the undesirable effects caused by the batch analyzer. This paper describes such a control system, called a *predictive feedback control system*, for the regulation of the composition of a single component in the effluent of a CFSTR.

The work presented by Smith (*7*), Lupfer and Oglesby (*3*), and Reswick (*5*) regarding the control of plants containing dead time provided the stimulus for the work presented here.

C. I. Huber is with the E. I. du Pont Company, Buffalo, New York.

THE REACTOR MODEL

To facilitate the following presentation, a linearized model of a particular CFSTR will be used throughout this paper. The block diagram of the linearized reactor model is shown in Figure 1 as the portion enclosed by the dotted rectangle.

The linear mathematical model corresponding to the diagram of Figure 1 is the same as that used by Kermode and Stevens (*2*) and Huber (*1*) and includes the following assumptions:

1. The reactant mass is perfectly mixed and of constant volume.
2. The reaction is first order, exothermic, and irreversible, $A \rightarrow$ products, and the reaction rate constant is given by the Arrhenius equation.
3. The energy balance is based on an arithmetic mean temperature gradient between the coolant and reactant mass and a constant overall heat transfer coefficient.
4. The feed and coolant temperatures, and all flow rates except coolant rate, are constant.

The initial, or preload, steady state conditions and transfer functions for this model are (*1*):

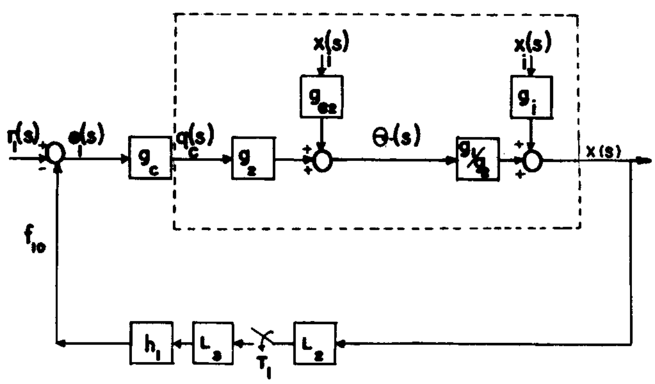

Fig. 1. Typical direct feedback regulator system.

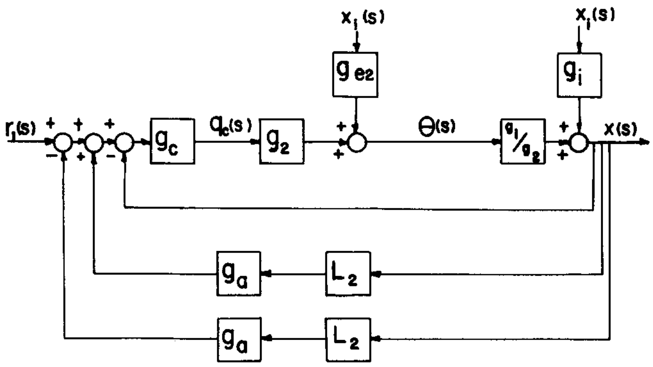

Fig. 2. Equivalent continuous analogue.

$$x_{iss} = 0.5000 \text{ (lb. mole/cu.ft.)}$$

$$x_{ss} = 0.2716 \text{ (lb. mole/cu.ft.)}$$

$$q_{css} = 0.2000 \text{ (cu.ft./sec.)}$$

$$\theta_{ss} = 710.0105 \text{ (°R.)}$$

$$g_1(s) = \frac{x(s)}{q_c(s)} = \frac{(0.1847)(0.5110)}{(s+a)(s+b)}; \tag{1}$$

$$g_2(s) = \frac{\theta(s)}{q_c(s)} = \frac{-(0.5110)(s+33.1369)}{(s+a)(s+b)} \tag{2}$$

$$g_i(s) = \frac{18.0000}{(s+33.1369)}; \; g_{e2}(s) = \frac{\theta(s)}{x_i(s)} = \frac{(18.00)(5{,}045.6193)}{(s+a)(s+b)} \tag{3}$$

where

$$a = -21.1109 \text{ (hr.}^{-1}\text{)}; \; b = 15.9570 \text{ (hr.}^{-1}\text{)} \tag{4}$$

$$\tau_a = -2.84 \text{ (min.)} \quad \tau_b = 3.76 \text{ (min.)}$$

Note that the reactor is inherently unstable.

A TYPICAL DIRECT FEEDBACK REGULATOR SYSTEM

Figure 1 is the block diagram of a typical direct feedback reactor regulator system. The object of the system is the regulation of x to the set point r_1 in the face of disturbances, or loads, in x_i. The manipulated variable, or control effort, is the coolant flow rate q_c, and G_c is the transfer function of a conventional continuous controller. It is assumed that the loads in x_i are not directly measurable.

The analyzer model consists of a periodic sampler, followed by a pure time delay L_3 and a zero-order hold device h_1. It is assumed that the analyzer is connected to the reactor effluent by a continuous sampling line, and that this line introduces transport lag L_2 into the feedback loop. The transfer functions for the transport lag, analyzer lag, and hold device are

$$L_2(s) = e^{-sT_2}; \; L_3 = e^{-sT_3}$$

$$h_1 = \frac{1 - e^{-sT_1}}{s}$$

where

$$T_1 = T_3 = 2.00 \text{ min.}; \; T_2 = 0.50 \text{ min.}$$

Note that the sampling period T_1 and the analysis lag T_3 are of the same order of magnitude as the plant time constants τ_a and τ_b [see Equation (4)]. Therefore, as noted earlier, it is unlikely that the direct feedback regulator system will result in satisfactory system stability and control quality.

STRUCTURE OF PREDICTIVE FEEDBACK REGULATORS

The purpose of this section is to describe the development of a reactor control system that includes direct feedback while decreasing the undesirable effects that a batch type of composition analyzer has on control.

The continuous analogue of the direct feedback regulator system is equivalent to Figure 1 with unity feedback and f_{10} equal to x. In the continuous analogue, any lags and samplers due to the batch analyzer have been deleted. This control system is hypothetical (not physically realizable) because to date there are no analyzers capable of continuously measuring the composition of a multicomponent effluent from a reactor. This system, however, does represent the ultimate or best direct feedback control system in the sense that all undesirable characteristics of the batch analyzer have been removed.

The objective of this section may be restated in terms of the continuous analogue system as follows: starting with the continuous analogue, develop a feedback control system which is both physically realizable and as nearly as possible equivalent to the continuous analogue. The control system is developed by applying a logical sequence of operations to the block diagram of the continuous analogue system (Figure 1 with unity feedback), remembering that for the control system to be physically realizable, any direct measurement of concentration must be produced by a batch type of analyzer, and the load variable x_i is not measurable.

Figure 2 is an equivalent block diagram representation of the continuous analogue. The outermost loop of this diagram represents the actual measurement of the controlled variable by the batch analyzer and, therefore, must be a part of the final realizable control system. The positive feedback loop is included so that the system is equiva-

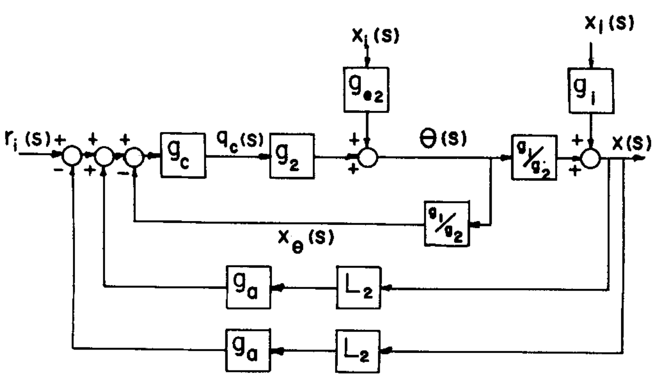

Fig. 3. First modification of continuous analogue.

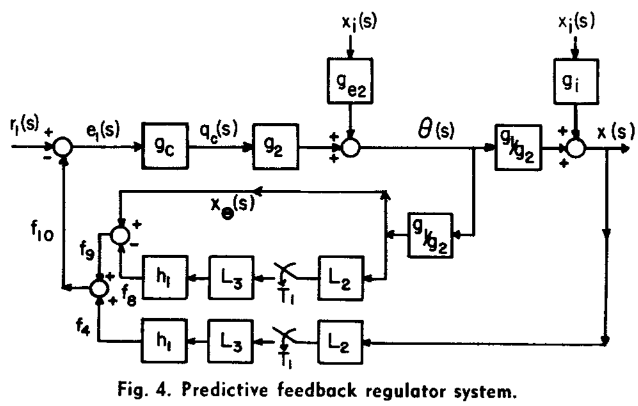

Fig. 4. Predictive feedback regulator system.

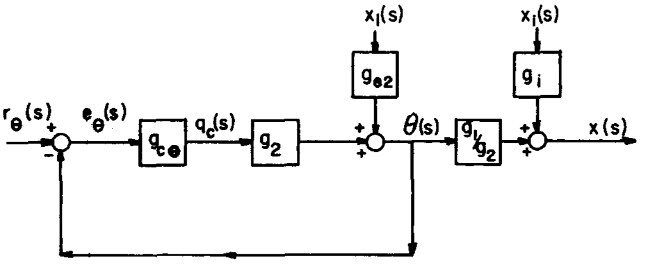

Fig. 5. Conventional temperature control system.

lent to the continuous analogue. The innermost loop of Figure 4 is not physically realizable and, therefore, cannot exist as it is in the final realizable control system.

Unlike concentration, the temperature (θ) of the reactant mass can be measured continuously. Thus to transfrom the innermost loop of Figure 2 into a realizable form, it is shrunk in size so that it originates at θ, rather than at x, as shown in Figure 3. Now, the innermost loop of the system represents the continuous measurement of changes in reactor temperature and the transformation of this measurement into a signal x_θ which represents the corresponding changes in the controlled variable.

The control system shown in Figure 3 differs from the previous system in that the innermost loop does not sense the portion of the load represented by the signal $x_i g_i$. There is no way that this signal can be introduced into the innermost loop, because the loop originates before the signal enters the system and because x_i is not directly measurable. Consequently, the innermost loop is only partially loaded and produces the signal $x_\theta(s) = \theta(g_1/g_2)$ rather than $x(s) = x_\theta + x_i g_i$. As a result of this partial loading, the control system in Figure 3 is no longer equivalent to the continuous analogue. Thus in the evolution of the control system from the equivalent continuous analogue to Figure 3, the continuous analogue configuration has been sacrificed for the sake of physical realizability.

Next, the positive feedback loop in Figure 3 is shrunk so that it too originates at θ, yielding a physically realizable but partially loaded loop.

The two partially loaded loops are then combined to form the system of Figure 4, where g_a has been replaced by the batch analyzer model. This regulator system represents the final stage in the evolution of the hypothetical continuous analogue system into a physically realizable system.

The final control system (Figure 4) is easily recognizable as the direct feedback system (Figure 1) with an

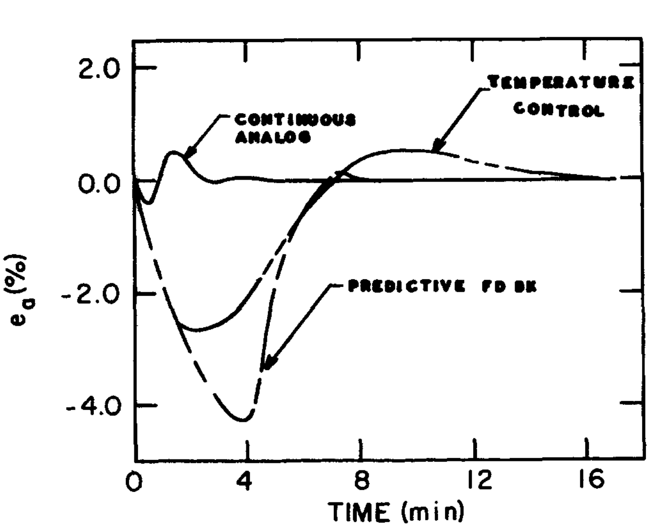

Fig. 6. Dynamic error response.

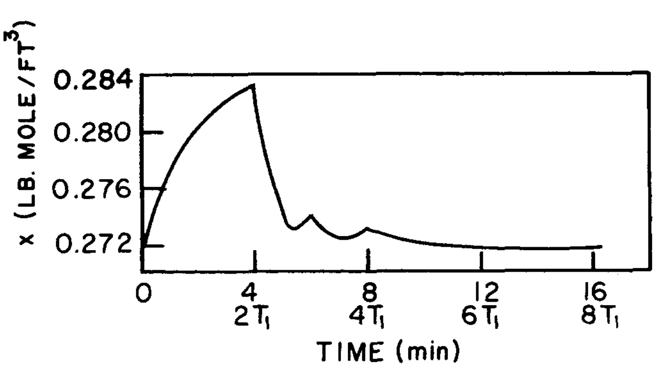

Fig. 7a. Dynamic response of X.

additional inner, or minor, feedback loop originating at the temperature variable. This minor feedback loop will be referred to as the *predictive feedback* loop or simply the *predictor* loop. The control system as a whole will be called the *predictive feedback regulator system.* Of course, in order to physically implement this control system, the transfer functions in the predictor loop must be generated by electronic or pneumatic devices. Note that, unlike the continuous analogue and direct feedback systems, the predictive system requires two sensing devices, both temperature and composition.

RELATIVE STABILITY OF PREDICTIVE FEEDBACK REGULATORS

The characteristic equations for the direct feedback, continuous analogue, and predictive feedback systems are:

Direct feedback: $1 + [L_2(s)L_3(s)h_1(s)g_c(s)g_1(s)]^*$ (5)

Continuous analogue: $1 + g_c(s)g_1(s)$ (6)

Predictive feedback: $1 + g_c(s)g_1(s)$ (7)

where the symbols $[\ ]^*$ indicate that the terms within the brackets are sampled by the analyzer. Equations (5) and (7) can readily be obtained from Figures 1 and 4, respectively. Characteristic Equation (6) can be determined from Figure 1 if it is modified as previously outlined to give the continuous analogue.

Note that the characteristic equation for the direct feedback system is sampled and contains both the analyzer and transport lags. Characteristic equations which contain lags generally indicate poor system stability.

Indeed, Min and Williams (*4, 8*) have demonstrated that as the magnitude of the analysis lag or sampling period approaches the magnitude of the dominant system time constant, the stability of direct feedback systems decreases drastically.

A comparison of Equations (6) and (7) shows that the characteristic equation for the predictive feedback system is the same as that for the hypothetical continuous analogue.

Thus, unlike direct feedback systems, the stability of predictive feedback systems is unaffected by the sampling and lags inherent in the batch analyzer. Therefore, in general, predictive feedback regulator systems should be significantly more stable than the corresponding direct feedback system.

The effect the predictor loop has on control and the effectiveness of predictive feedback control is best illustrated by means of a numerical example.

A NUMERICAL EXAMPLE

Continuous PID mode controllers were designed for

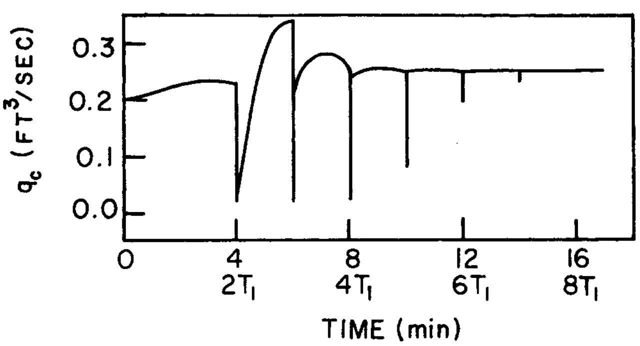

Fig. 7*b*. Dynamic response of q_c.

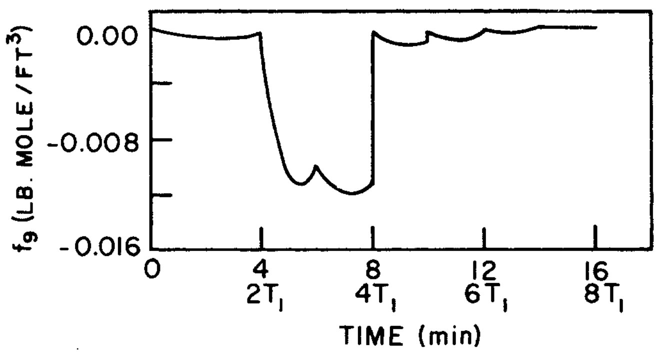

Fig. 7*d*. Dynamic response of f_9.

the continuous analogue and the predictive feedback regulator systems by means of simulation on a Control Data Corporation G21 digital computer. The transfer function (g_c) used for the controller was

$$g_c(s) = K_p + (K_I/s) + K_D s \tag{8}$$

For both systems, the load change was 5% step change in x_i, and the controllers were designed to satisfy the following performance criteria:

Minimize the objective function

$$\text{ITAE} = \int_0^{t_s} e_a(t)\,t\,dt \tag{9}$$

subject to the following constraints:

$$\lim_{t\to\infty} e_a(t) = 0 \tag{10}$$

$$0.02 \text{ (cu.ft./sec.)} \leq q_c(t) \leq 0.38 \text{ (cu.ft./sec)} \tag{11}$$

where e_a is the actual error defined by

$$e_a(t) = r_1 - x(t) \tag{12}$$

$$= x_{ss} - x(t) \tag{13}$$

The settling time is defined as the time when the percent error is less than one-tenth of 1%:

$$t \geq t_s{:}\ \frac{e_a(t)}{x_{ss}} 100 \leq 0.1\% \tag{14}$$

The objective function (ITAE) is the well-known integral of the time weighted absolute value of the error.

Equation (10) implies zero steady state actual error. Equation (11) is a result of the assumed physical limitations on the control effort q_c.

For the purpose of comparison, a conventional temperature control system, shown in Figure 5, was considered. The control objective for this system is the same as the objective for the predictive and continuous analogue systems, namely, the regulation of x to its initial steady state value x_{ss} in the face of load changes in x_i. Unlike the predictive and continuous analogue regulator systems, the control exerted by the temperature control system is based solely on the measurement of a variable other than the controlled variable.

By using the above performance criteria, a proportional controller was designed for the temperature control system by simulation on a Control Data Corporation G21 computer. As before, the load change was a 5% step change in x_i. It should be noted that integral control can't be used as it would attempt to force the temperature error to zero, which is not the objective of this control system. A proportional derivative controller was tried; however, no improvement over proportional control was noted.

The dynamic response and response characteristics of the actual error (e_a) for the predictive feedback and continuous analogue systems are shown in Figure 6 and Table 1, respectively. Both clearly indicate that the predictive system results in significantly larger peak error, settling time, and ITAE. However, like the continuous analogue, the predictive feedback system does result in zero steady state error.

An investigation of the behavior of the various signals generated by the predictive feedback system indicates why this type of system will generally be less effective than its continuous analogue and also supplies information regarding the operation of the predictor loop.

The dynamic response of the signals generated by the predictive system, shown in Figures 7, indicates that the response of the control system to the load change does not become significant until the first change occurs in the analyzer feedback f_4. In other words, significant control effort does not begin until the batch analyzer has sensed a change in the controller variable. To further amplify this point, consider the response of the signal f_{10} formed,

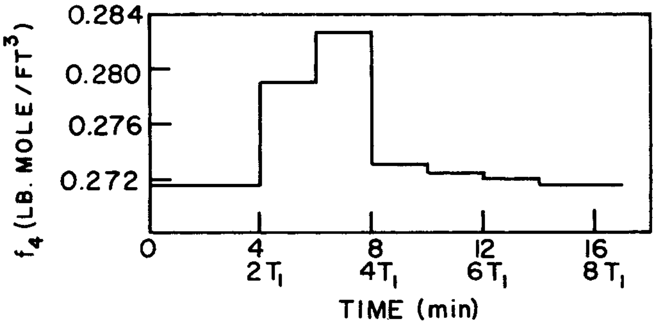

Fig. 7*c*. Dynamic response of f_4.

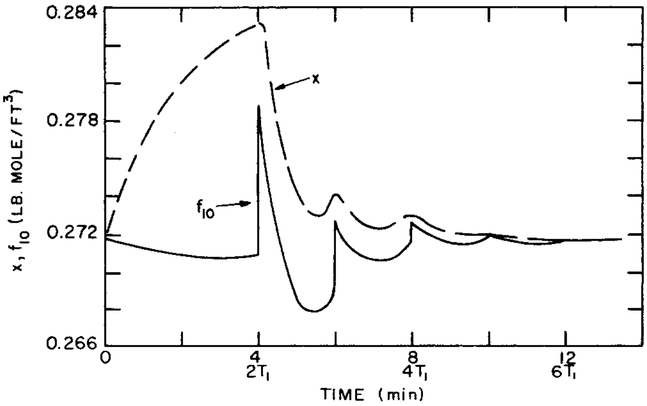

Fig. 7*e*. Dynamic response of X and f_{10}.

TABLE 1. CHARACTERISTICS OF DYNAMIC ERROR RESPONSES

System	e_{ap}, %	t_s, min.	e_{ass}, %	ITAE, (lb. mole) (min.^{2})/ cu.ft.
Continuous analogue	0.55	2.50	0.00	0.00247
Predictive feedback	−4.24	8.00	0.00	0.13920
Temperature control	−2.84	14.50	0.00	0.15930

as shown in Figure 4, by adding f_9 to f_4. Note that the regulation of x is based solely on the feedback signal f_{10}. Therefore, how well f_{10} approximates the behavior of x is certain to affect the ability of the controller to regulate x.

The response curves for x and f_{10} are shown in Figure 7*e*. A comparison of these curves indicates that for the first 4 min. after a load change f_{10} changes very little and is a very poor representation of the response of x. Indeed, during this interval f_{10} actually decreases slightly while x increases rapidly.

After the first 4 min., the analyzer feedback signal f_4 and the predictor loop output f_9 begin to react to the load change and changes in q_c. As a result, f_{10} approximates the response of x much more closely, both in magnitude and form.

In view of the behavior of f_{10}, it is not surprising that the control exerted by the predictive feedback system is generally less effective than the control exerted by its continuous analogue. Furthermore, when we consider the difference between x and f_{10} during the early part of the system response, it is clear why the peak error for the predictive system is relatively large.

Now consider the effect that the predictor loop has on the control exerted by the predictive system. As shown in Figure 7*d*, the predictor loop output signal (f_q) does not respond to the load change in a significant manner until the first change in f_4 occurs (that is, at $t = 2T_1 = 4$ min.). A comparison of signals x, f_{10}, and f_4 (Figures 7*e* and 7*c*) indicates, however, that after this time the action of the predictor loop dramatically improves the quality of the information supplied to the controller, compared with the information which would be supplied by the f_4 alone. In a sense the predictor loop modulates the signal from the analyzer, which during the early part of the system response is a very poor representation of x, thereby producing the signal f_{10} which is a much better representation of x.

Figures 7*e* and 7*d* indicate that as the quality of the information supplied by the analyzer improves substantially (at $t = 4T_1 = 8$ min.), the effect of the predictor loop decreases sharply. At steady state f_{10} equals f_4, the effect of the predictor loop has completely disappeared, and control is based solely on the actual measurement of the controlled variable supplied by the batch analyzer.

A comparison of the response curve characteristics for the predictive feedback and temperature control systems (see Figure 6 and Table 1) indicates that predictive control results in significantly smaller settling time and ITAE and temperature control results in significantly smaller peak error. Both systems yield zero steady state error.

It has been shown (*1*), however, that the steady state error by using temperature measurement to control composition is extremely sensitive to errors in the measurement of reactor temperature and small drifts in the value of the proportional constant. For example, to insure a steady state actual error of less than 0.1% in outlet composition, the error in the measurement of reactor temperature must be less than 0.02% (0.05°F.). Thus it is unlikely that a conventional temperature control system will, in reality, produce an acceptable steady state error (that is, an error less than 0.1% in composition).

It is important to note that, unlike the temperature control system, the steady state effectiveness of the predictive feedback regulator system does not depend on how closely the reactor temperature is measured. As previously mentioned, for this system the regulation of the controlled variable x at steady state is based solely on the actual measurement of x. Of course, errors in the measurement of the controlled variable x will affect the ability of the predictive feedback system to produce zero steady state error, or an acceptable steady state error. These errors are not magnified, however; that is, an error of 0.1% in the measurement of x causes a 0.1% steady state error rather than a larger error.

Min and Williams (*4, 8*) and Ross (*6*) have shown that if the analyzer sampling period and analysis lag are of the same order of magnitude as the dominant plant time constant, direct feedback control results in a settling time which is twenty to twenty-five times larger than that which would occur if the continuous analogue were used. The results shown in Table 1 indicate that the settling time for the predictive feedback system is less than four times that of the continuous analogue.

Min and Williams (*4, 8*) also showed that a direct feedback regulator system should result in a peak error of 80 to 100% of the magnitude of the step load applied. The predictive feedback system considered herein results in a peak actual error which is 84.8% of the applied step load (5%). Thus, the direct feedback and predictive feedback regulator systems can be expected to yield peak errors which are approximately the same. This conclusion is hardly surprising in view of the fact that neither predictive feedback nor direct feedback systems begin to exert significant control until the analyzer in the direct feedback loop first senses a change in the controlled variable.

Finally, the controller constants for the predictive feedback system were used with a direct feedback controller. The system response was found to be highly unstable. No attempt was made to search for a set of constants which provided stable control. This instability coupled with the preceding analysis indicates that direct feedback control is significantly less effective than predictive feedback control for this system.

ACKNOWLEDGMENT

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NOTATION

a, b = roots of CFSTR characteristic equation, hr.$^{-1}$
e_a = actual error = $r_1 - x$
e_1 = measured error
f_4, f_8, f_9, f_{10} = signals generated by predictive feedback system
g_a = analyzer transfer function
g_c = transfer function of continuous controller
g_1, g_2, g_i, g_{e2} = transfer functions of CFSTR
h_1 = transfer function of zero-order hold device
K_p, K_I, K_D = proportional, integral, and derivative mode controller constants
L_2, L_3 = transfer functions of transport and analysis lag, respectively
q_c = coolant flow rate
r_1 = setpoint for concentration of component A

s = Laplace transform variable
t = time
t_s = settling time
T_1 = magnitude of analyzer sampling period
T_2 = magnitude of transport lag
T_3 = magnitude of analysis lag
x = concentration of component A in effluent
x_i = concentration of component A in feed
θ = temperature of reactant mass
τ_a, τ_b = reactor time constants

Subscripts

ss = steady state values

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Optimal Control of a Continuous Flow Stirred Tank Chemical Reactor

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The time optimal control problem for jacket cooled continuous flow stirred tank reactor (CSTR) with an exothermic, irreversible, second-order, homogeneous, liquid-phase reaction (the saponification of ethyl acetate) was solved with the maximum principle and phase plane analysis. Both experimental studies and analogue computer simulation studies were conducted.

The overall performance of the experimental system agreed very well with the performance of the corresponding system simulated on an analogue computer. However, there were enough differences in the observed and predicted operating states and switching curves to warrant the conclusion that the experimental performance can be significantly improved if experimental results are used to modify the results predicted with computer analysis. These differences were attributed to uncertainties in the model and the values of the model parameters as well as nonrandom (and unforeseen) measurement errors.

In recent years, the chemical engineering journals have contained an increasing number of articles on optimization and optimal control. Nearly all of these papers have been theoretical in nature. When applications of the theory are presented, they usually involve only the study of a system simulated on a digital or analogue computer. The words "data" and "results" are only rarely preceded by the word "experimental;" instead, computer data and computer results for systems simulated on a computer are used to verify theory. This study was motivated by the belief that the experimental verification of theory should accompany the development of theory.

The system studied in this work consists of a jacket cooled continuous flow stirred tank reactor (CSTR), with a homogeneous liquid-phase, exothermic, irreversible chemical reaction. The reaction is the saponification of ethyl acetate. The optimal control problem considered here is the following:

Using the heat transfer coefficient between the reaction mixture and the coolant as the control variable, what is the control law which drives the reactor system from a given initial state to a specified final state in minimum time?

This problem is significant in three practical applications: reactor start-up, changing from one steady state to another, and regulating specified final state conditions.

PREVIOUS WORK

The basic theoretical reference on the maximum principle is the book by Pontryagin and his co-workers (*1*). A good elementary account of the maximum principle can be found in the papers of Rozonoer (*2*).

While many significant applications of the maximum principle have been demonstrated in other engineering fields, it is only during the past few years that chemical engineers have begun to apply this mathematical theory to problems of chemical engineering importance. One of the first and most extensive of all studies in this area was accomplished by Aris and Siebenthal (*3, 4*). The work in this paper is based to a large extent on their study of the time-optimal control problem for a CSTR. Their studies were conducted with a simulated reactor system (with a general first-order reaction) on a digital computer; no experimental work was attempted.

Cotter and Takahashi (*5*) considered time-optimal control for a CSTR with feed flow rate and coolant flow rate

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