c_i = positive constant coefficient in generalized polynomial
F = weighted sum of convex functions
F_{ij} = $\partial^2 F/\partial x_j \partial x_i$
M_r = power mean
M_χ, M_ψ = functional means
r, s = constants
U = generalized polynomial
u, v, w, x, y = independent variables
Z = dependent variable

Greek Letters

α, β, λ = positive constants
α_i, γ_i = weighting factors
Δ_j = discriminants of modified Hessian matrix
μ = a constant
σ = ± 1
Φ = convex function
χ, ψ = continuous, strictly monotonic functions
χ^{-1}, ψ^{-1} = inverse functions

Superscript

— = value at stationary point

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Nonlinear Feedforward Control of Chemical Reactors

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This paper illustrates the synthesis of nonlinear feedforward controllers for chemical reactors. In most of the theoretical development and application of feedforward control only linear systems have been considered. There are, however, no inherent linear limitations in feedforward control. Since chemical reactors are usually nonlinear, the effectiveness of control should be improved by including nonlinearities in the design of feedforward controllers. This is particularly true for batch reactors because of the large changes in variables during a batch cycle. Continuous stirred-tank reactors are studied with single and consecutive reactions of first and higher order. Effectiveness of linear and nonlinear feedforward controllers is compared for disturbances of various magnitude and direction. Feedforward control of batch and tubular reactors is also discussed.

Feedforward control of chemical processes has received an increasing amount of attention in recent years. This interest is a result of the recognition of the advantages of feedforward control in many chemical engineering applications; improved knowledge and appreciation of the dynamics of chemical processes; and the availability of computers to permit realistic analysis, synthesis, and evaluation of control systems, both on line and off line.

Distillation columns and chemical reactors have received most of the attention. The general theory of feedforward controller synthesis was developed by Bollinger and Lamb

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(*1*) using matrix methods and assuming linear, autonomous systems. These methods were used in theoretical and small-scale experimental studies of distillation columns (*2, 2a, 8, 12*) and chemical reactors (*4, 6, 9, 13, 14*). Industrial scale applications have usually employed empirical methods (*7, 11*).

In most of these applications, linear transfer functions have been employed. Nonlinear systems are linearized around some steady state operating level. Some consideration has been given to feedforward nonlinearities (*10, 11*) but only in the steady state gain portion of the feedforward controller.

Haskin and Sliepcevich (*5*) have pointed out that there are no inherent linear limitations in feedforward control. They applied their nonlinear invariance principle to a jacketed-kettle heat exchanger where nonlinearities occurred in the convective terms of the energy equations.

This paper illustrates the synthesis of nonlinear feedforward controllers for continuous and batch reactors. Since chemical reactors are usually nonlinear, the effectiveness of control should be improved by including nonlinearities in the design of feedforward controllers. The basic notion that this paper attempts to convey is that nonlinear methods can and should be used in feedforward control. The approach is to examine some simple cases for which analytical solutions in the form of explicit algebraic or differential equations can be obtained. Theoretical feedforward controller equations are developed for several reactors and kinetics, and their application illustrated by computer simulation of an example chosen from the literature.

It is recognized that analytical solutions may prove intractable for more complex systems and computer solutions will be required. Iterative search or variational techniques can sometimes be used to determine the required functional relationships. Local linearization around a number of steadystate levels is probably the most straightforward technique. The nonlinear changes in gains and time constants can be determined with theoretical methods or empirical testing. The availability of a process computer offers the opportunity to do these calculations on-line.

The case of a single continuous stirred-tank reactor with irreversible first-order kinetics is studied in detail for various choices of manipulative and controlled variables and disturbances. Different selections are shown to result in drastically different forms of the feedforward controller. The two cases simulated are (a) reactor composition and temperature are controlled by manipulation of cooling jacket temperature and throughput, and (b) product composition is controlled by manipulation of cooling jacket temperature.

Feedforward controller equations for several other CSTR systems and kinetics are given: reversible reactions, n^{th}-order kinetics, two stages, consecutive reactions, and variable holdup.

Feedforward control of batch reactors, in which nonlinear methods are particularly important because of the large changes in variables with time, is also discussed. A few comments on feedforward control of tubular reactors are also included.

The specific numerical example used in the computer simulation is based on Harriott's problem 15-1 (*3*, p. 317). Values of parameters and steady state variables are:

F_S = 2,000 lb./hr. U = 150 B.t.u./(hr.)(sq. ft.)(°R.)
C_{OS} = 0.50 lb./lb.
T_{OS} = 530 °R. T_{JS} = 586.7 °R.
C_p = 0.75 B.t.u./(lb.)(°R.)
V = 2,400 lb.
λ = 600 B.t.u./lb.
E = 30,000 B.t.u./lb.-mole
α = 7.08×10^{10}/hr.
T_S = 600 °R.
C_S = 0.246 lb./lb.
k_S = 0.86/hr.
A = 100 sq.ft.

CONTINUOUS STIRRED-TANK REACTORS

System

The first system to be studied is a single-jacketed CSTR in which a first-order irreversible reaction occurs: $C \xrightarrow{k}$ Products. It is assumed that mixing is perfect in the reactor and in the cooling jacket and that holdup V, specific heat C_p, exothermic heat of reaction λ, heat transfer coefficient U, and area A are all constant.

Equations

Component continuity:

$$V\frac{dC}{dt} = F\,(C_O - C) - V\mathcal{R} \tag{1}$$

Energy:

$$V\,C_p\frac{dT}{dt} = F\,C_p(T_O - T) + \lambda V\mathcal{R} - UA\,(T - T_J) \tag{2}$$

Kinetic:

$$\mathcal{R} = C\,\alpha \exp\,(-E/RT) \tag{3}$$

These equations are highly nonlinear because of the exponential function as well as product terms.

Feedforward Controller Synthesis

Control of Composition and Temperature. In the case to be studied first, the feedforward control criteria are chosen to be the maintenance of constant reactor composition and temperature; that is, we wish to keep C equal to its steady state value C_S and T equal to its steady state value T_S. Since two controlled variables have been specified (C and T), at least two manipulative variables are required. Cooling jacket temperature T_J and reactor throughput F are selected.

Obviously other choices of manipulative and controlled variables could be made. Some other selections are considered later. The form of the feedforward controller varies drastically from case to case. Some care must be taken in the choice. For example, it would be impossible to use T_J and T_O as manipulative to control T and C because C is a function of only T, F, and C_O.

The disturbances for which the controller must compensate are feed composition C_O and feed temperature T_O. Thus the feedforward controller equations will give the manipulative variables T_J and F as functions of the disturbances C_O and T_O *such that* C and T are maintained constant.

$$\begin{aligned} T_J &= f_1\,(C_O, T_O) \\ F &= f_2\,(C_O, T_O) \end{aligned} \tag{4}$$

These functions are, in general, nonlinear since no linear restrictions have been imposed on the system nor linearization of equations employed. The resulting functions will contain both nonlinear dynamic and nonlinear steady state terms.

With the feedforward control criteria

$$\begin{aligned} C &= C_S \\ T &= T_S \end{aligned} \tag{5}$$

it is clear that

$$\frac{dC}{dt} = \frac{dT}{dt} = 0 \tag{6}$$

Substitution of Equations (5) and (6) into the system equations (1) to (3) gives the two nonlinear feedforward controller equations:

$$F = \frac{C_S k_S V}{C_O - C_S} \tag{7}$$

$$T_J = T_S - \frac{C_S k_S V}{UA}\left[\lambda - \frac{C_p(T_S - T_O)}{(C_O - C_S)}\right] \tag{8}$$

Measurement of disturbances C_O and T_O permits calculation of manipulative variables F and T_J. Equations (7) and (8) show several interesting points: the relationships between F and C_O and between T_J and C_O are nonlinear; the relationship between T_J and T_O is linear; no dynamic terms appear in either equation (steady state gain only); F is not a function of T_O.

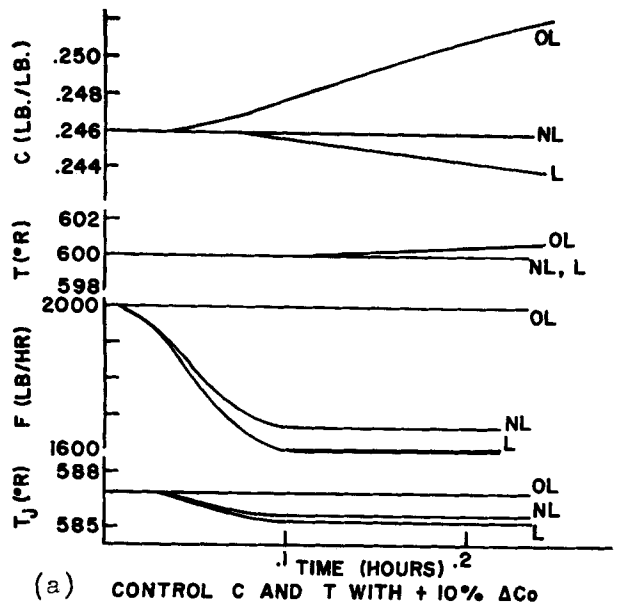
A linear feedforward controller will be derived next to compare nonlinear and linear techniques and results. Linearization of the system equations (1) to (3) around the steady state operating level leads to two linear, constant-coefficient, ordinary differential equations:

$$\left.\begin{aligned}\frac{dC}{dt} &= a_{11}C_O + a_{12}T_O + a_{13}C + a_{14}T + a_{15}F + a_{16}T_J \\ \frac{dT}{dt} &= a_{21}C_O + a_{22}T_O + a_{23}C + a_{24}T + a_{25}F + a_{26}T_J\end{aligned}\right\} \tag{9}$$

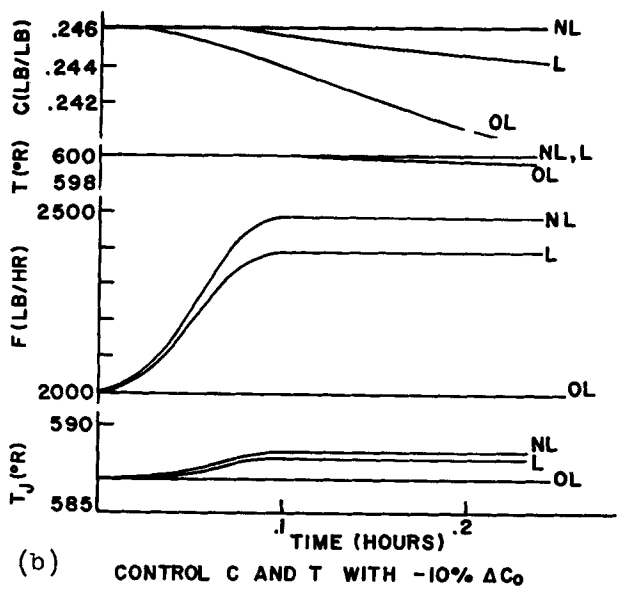
where

$a_{11} = F_S/V$
$a_{12} = 0$
$a_{13} = -k_S - F_S/V$
$a_{14} = -C_S k_S E/RT_S^2$
$a_{15} = C_{OS}/V$
$a_{16} = 0$
$a_{21} = 0$
$a_{22} = F_S/V$
$a_{23} = \lambda k_S/C_p$
$a_{24} = -F_S/V - UA/C_pV + \lambda C_S k_S E/C_p RT_S^2$
$a_{25} = -T_S/V + T_{OS}/V$
$a_{26} = UA/C_pV$

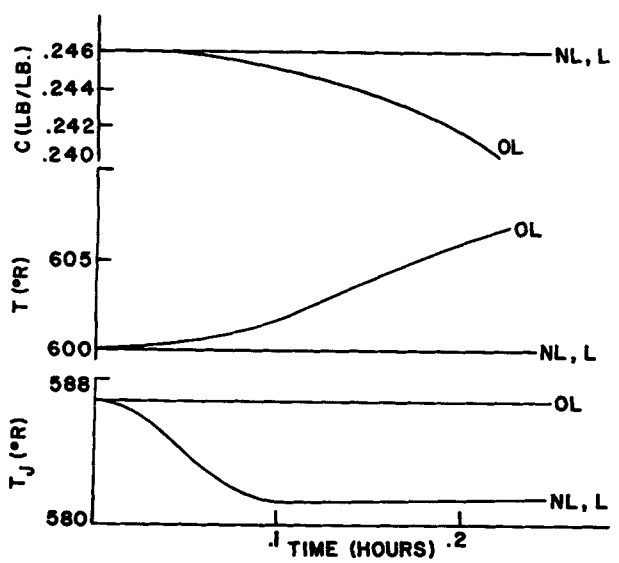
All variables in Equation (9) are now in perturbation form (deviations from steady state) so the feedforward control criteria become



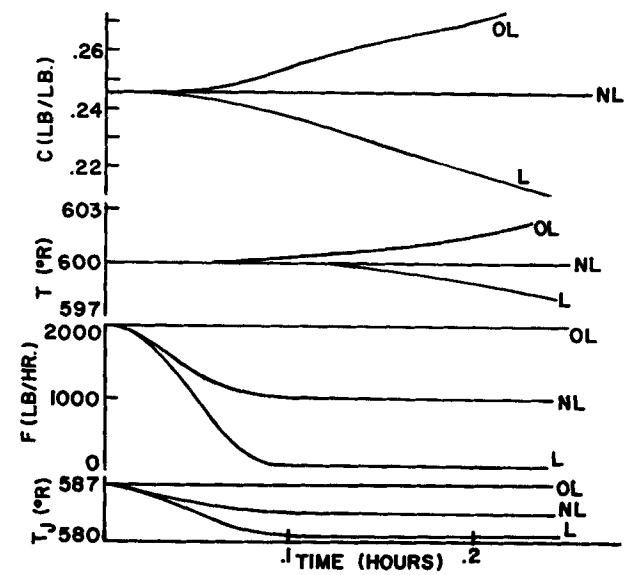
(a) CONTROL C AND T WITH + 10% ΔC_O



(b) CONTROL C AND T WITH -10% ΔC_O



(c) CONTROL C AND T WITH +10% ΔT_O



(d) CONTROL C AND T WITH +50% ΔC_O

Fig. 1. Transient responses.

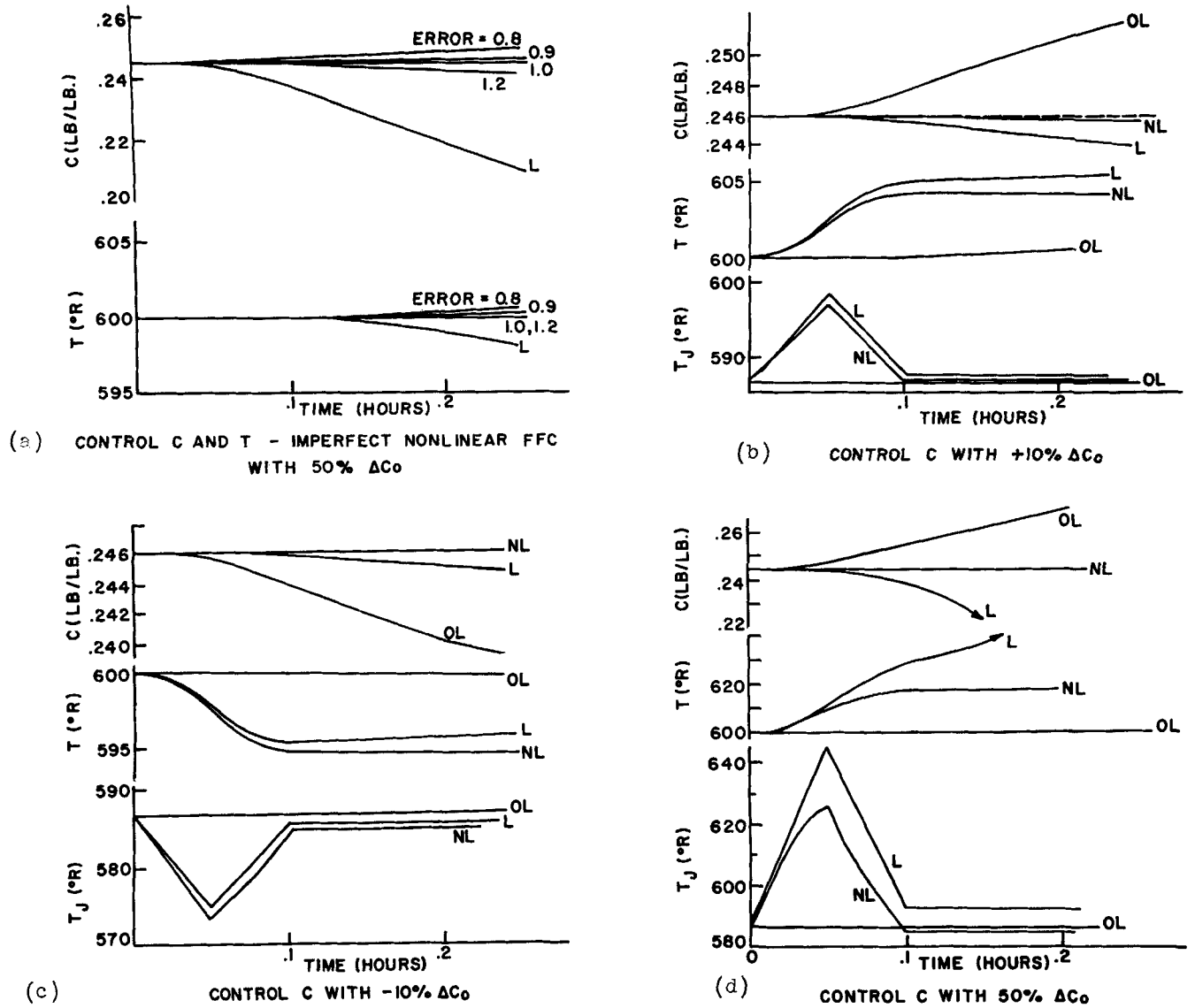


Fig. 2. Transient responses.

$$C = T = 0 \tag{10}$$

Solving for the linear feedforward controller, we obtain

$$F = \left[\frac{-F_S}{C_{OS} - C_S}\right] C_O \tag{11}$$

$$T_J = \left[\frac{-C_p F_S}{UA}\right] T_O + \left[\frac{-C_p F_S (T_S - T_{OS})}{UA(C_{OS} - C_S)}\right] C_O \tag{12}$$

The transfer function between T_J and T_O is exactly the same as in the nonlinear case [Equation (8)] when the proper change from perturbation to total variables is made.

Figure 1, *a* to *d*, compares open-loop (OL), nonlinear feedforward (NL), and linear feedforward (L) responses for disturbances in C_O and T_O. An S-shaped disturbance of 0.1 hr. duration was used so that a true derivative (as required later) could be obtained. Changes of ± 10% and + 50% in C_O were used to illustrate the effects of magnitude and direction on a nonlinear system. Only 10% changes in T_O are shown since the feedforward controlled system is linear in T_O, and therefore results are independent of disturbance magnitude and direction. For T_O disturbances, perfect control of C and T is achieved by both linear and nonlinear systems.

As expected, performance of the linear feedforward controller is worse for larger disturbances in C_O, that is, C is not held constant. Little change in T is seen for both linear and nonlinear cases until the C_O disturbance is large. The linear feedforward controller overcorrects for positive C_O changes and undercorrects for negative C_O changes, as expected from the shape of the curves given by Equations (7) and (8).

Errors in process modeling and measurement would result in imperfect feedforward control. Previous work has shown that these effects are not critical in linear systems. The effect of such errors in a nonlinear system was explored by imposing deliberate errors of − 10% and ± 20% in the measurement of a + 50% change in C_O. Figure 2*a* shows that imperfect nonlinear feedforward control is still effective and is even better than linear control for large disturbances.

Control of Composition. For control of composition only, allowing reactor temperature to be uncontrolled, the feedforward control criterion is

$$C = C_S \tag{13}$$

and therefore

$$\frac{dC}{dt} = 0 \tag{14}$$

Since only one variable has been specified, only one manipulative variable is required. Cooling jacket temperature T_J is chosen. The disturbances for which the controller must compensate are feed composition C_O, feed temperature T_O, and feed rate F. The feedforward controller equations must now give the nonlinear relationships between the manipulative variable T_J and the disturbances C_O, T_O, and F *such that* C is held constant:

$$T_J = f\,(C_O, T_O, F) \tag{15}$$

Substitution of Equations (13) and (14) into the system equations (1) to (3) gives

$$T_J = \left[1 + \frac{FC_p}{UA}\right]\left[\frac{-E/R}{\log\left(\frac{F(C_O - C_S)}{VC_S\alpha}\right)}\right] - \left[\frac{FC_pT_O}{UA}\right] - \left[\frac{\lambda F(C_O - C_S)}{UA}\right] + \left[\frac{VC_pR/UA}{EF(C_O - C_S)}\right]\left[\frac{-E/R}{\log\left(\frac{F(C_O - C_S)}{VC_S\alpha}\right)}\right]^2 \left[F\frac{dC_O}{dt} + (C_O - C_S)\frac{dF}{dt}\right] \tag{16}$$

The feedforward controller is highly nonlinear in C_O and F but is linear in T_O. It now has both steady state and dynamic elements. Derivatives of the disturbances $\dot{C}_O$ and $\dot{F}$ are required. Since perfect differentiation at all frequencies is physically unrealizable, feedforward control would not be theoretically possible. However, use of conventional lead networks should normally enable adequate control over the low frequency range of real interest.

To derive the linear feedforward controller, the criterion $C = 0$ is substituted into the linearized system equation (9), yielding

$$T_J = K_1(\tau_1 S + 1)C_O + K_2(\tau_2 S + 1)\,F + K_3 T_O \tag{17}$$

where

$$K_1 = \frac{C_pRF_ST_S^2}{UAVC_SEk_S}\left(F_S + \frac{UA}{C_p}\right) - \frac{\lambda F_S}{UA}$$

$$\tau_1 = \frac{VC_p}{C_pF_S + UA - \lambda VC_SEk_S/RT_S^2}$$

$$K_2 = \frac{C_pRT_S^2\,(C_S - C_{OS})}{UAVC_SEk_S}\left(F_S + \frac{UA}{C_p}\right) - \frac{\lambda(C_S - C_{OS})}{UA} + \frac{C_p(T_S - T_{OS})}{UA}$$

$$\tau_2 = \left[\left(\frac{F_S + \frac{UA}{C_p}}{V}\right) - \frac{C_SEk_S\,\lambda}{RT_S^2C_p} + \frac{C_SEk_S}{RT_S^2}\left(\frac{T_S - T_{OS}}{C_S - C_{OS}}\right)\right]^{-1}$$

$$K_3 = \frac{C_pF_S}{UA}$$

For the numerical example

$K_1 = 23.5$, °R./(lb./lb.)
$\tau_1 = 0.48$, hr.
$K_2 = 0.00648$, °R./(lb./lb.)
$\tau_2 = 0.225$, hr.
$K_3 = -0.1$, °R./°R.

Figures 2, *b* to *d*, and 3, *a* to *d*, compare open-loop, linear feedforward, and nonlinear feedforward responses for disturbances in C_O, T_O, and F. Perfect control for T_O disturbance is again obtained with both linear and nonlinear controllers. The slight drift in C is due to the system open-loop instability. The discontinuity in the slope of T_J is due to the S-shaped forcing function.

Performance of the nonlinear feedforward controller is again superior to the linear controller. The linear controller overcorrects for positive C_O and F changes and undercorrects for negative C_O and F changes. For the large 50% change in C_O the linear controller even ends up at steady state with T_J changed in the wrong direction. This results from the marked nonlinearity of the system, yielding a curve of steady state T_J vs. C_O that is not monotonic.

Other CSTR Cases

Nonlinear feedforward controller equations are given for a number of other CSTR configurations, reaction kinetics, and choice of manipulative variables.

1. Use T_J and C_O for manipulative variables (control C and T for disturbances in F and T_O):

$$\left.\begin{aligned} C_O &= C_S\,(1 + k_SV/F) \\ T_J &= T_S - \frac{VC_Sk_S}{UA} + \frac{C_pF}{UA}\,(T_S - T_O) \end{aligned}\right\} \tag{18}$$

2. n^{th} order kinetics (control C and T with T_J and F): With $\mathcal{R} = C^n\,\alpha\,\exp\,(-E/RT)$

$$\left.\begin{aligned} F &= VC_S{}^nk_S/(C_O - C_S) \\ T_J &= T_S - \frac{VC_S{}^nk_S}{UA}\left[\lambda - \frac{C_p(T_S - T_O)}{(C_O - C_S)}\right] \end{aligned}\right\} \tag{19}$$

3. Reversible reactions (control C and T with T_J and F, first-order kinetics):

With Reactions $C \underset{k'}{\overset{k}{\rightleftarrows}}$ Product

$$\begin{aligned} F &= \frac{Vk_S}{C_O - C_S}\beta \\ T_J &= T_S + \frac{C_pVk_S(T_S - T_O)}{UA(C_O - C_S)}\beta - \frac{Vk_S\lambda}{UA}\beta \end{aligned} \tag{20}$$

where

$$K = k/k'$$

$$\beta = C_S - \frac{1 - C_S}{K}$$

4. Variable holdup (control C and T with F and T_J): With variable holdup ($F_O \neq F$) the system equations are

$$\frac{dV}{dt} = F_O - F$$

$$\frac{d(VC)}{dt} = F_OC_O - FC - VC\,\alpha\,\exp\,(-E/RT)$$

$$C_p\frac{d(VT)}{dt} = C_p(F_OT_O - FT) + \lambda\,VC\,\alpha\,\exp\,(-E/RT) - UA(T - T_J)$$

Solution for the nonlinear feedforward controller yields

$$\left.\begin{aligned} F &= F_O - \left(\frac{F_O}{C_Sk_S}\right)\frac{dC_O}{dt} - \left(\frac{C_O - C_S}{C_Sk_S}\right)\frac{dF_O}{dt} \\ T_J &= T_S + \frac{F_O}{UA}\left[C_p(T_S - T_O) + \lambda\,(C_O - C_S)\right] \end{aligned}\right\} \tag{21}$$

5. Two stages (control T_1, T_2, and C_2 with T_{J1}, T_{J2}, and F):

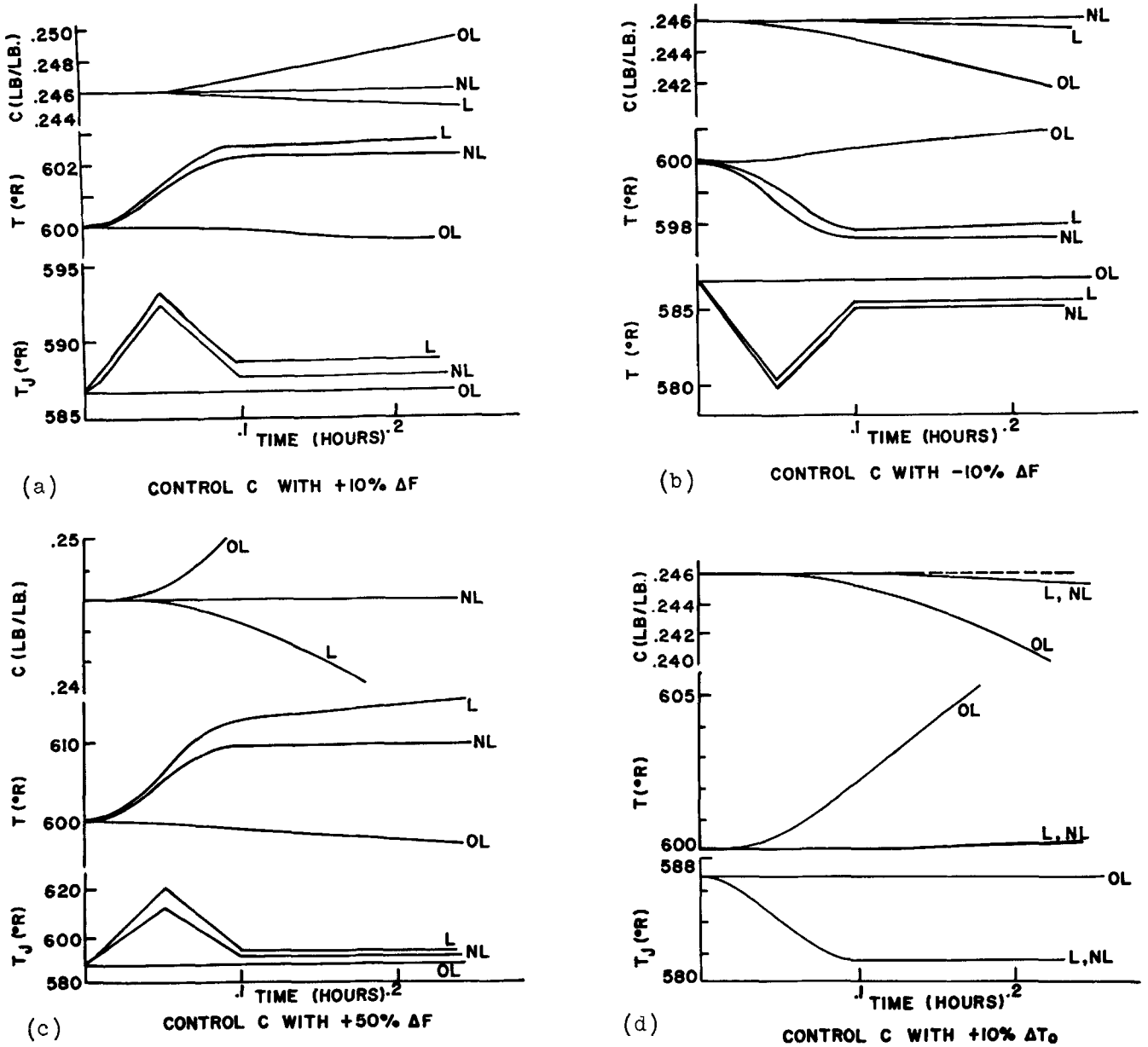


Fig. 3. Transient responses.

$$\frac{dF}{dt} + \left[\frac{C_O - C_{2S}}{V_1V_2C_{2S}k_{2S}}\right] F^3 - \left[\frac{V_1k_{1S} + V_2k_{2S}}{V_1V_2k_{2S}}\right] F^2 - [k_{1S}]\, F = 0$$

$$T_{J1} = T_{1S} + \frac{FC_p(T_{1S} - T_O)}{U_1A_1} - \frac{\lambda V_2k_{1S}C_{2S}}{U_1A_1}\left(1 + \frac{V_2k_{2S}}{F}\right)$$

$$T_{J2} = T_{2S} + \frac{FC_p(T_{2S} - T_{1S})}{U_2A_2} - \frac{\lambda V_2C_{2S}k_{2S}}{U_2A_2} \qquad (22)$$

where subscripts 1 and 2 refer to the first and second tanks, respectively.

Note that an explicit analytical equation for $F(C_O, T_O)$ is not obtained. On-line, real time solution of the nonlinear differential equation would be required with analog or digital techniques.

6. Consecutive first-order reactions (control B and T with T_J and F):

With Reactions $A \xrightarrow{k_1} B \xrightarrow{k_2} C$

and for pure A_O feed.

$$\frac{dF}{dt} + \left(k_{1S} + k_{2S} - \frac{k_{1S}A_O}{B_S}\right) F + \left(\frac{1}{V}\right) F^2 + Vk_{1S}k_{2S} = 0 \qquad (23)$$

$$T_J = T_S + \frac{FC_p(T_S - T_O)}{UA} - \frac{\lambda_1B_S(F + Vk_{2S}) + \lambda_2Vk_{2S}B_S}{UA}$$

The nonlinear differential equation for F is of the Riccati type and could be transformed into a second-order, linear, differential equation and a series solution obtained. Computer solution is probably easier.

7. Control T only (with T_J for disturbances in F, C_O, T_O):

$$T_J = T_S + \frac{C_pF_{(t)}}{UA}(T_S - T_{O(t)}) - \frac{\lambda Vk_S}{UA}C_{(t)} \qquad (24)$$

where

$$C_{(t)} = \exp(-k_S t) \exp\left(-\frac{1}{V}\int F_{(t)}\,dt\right)$$

$$\left[\frac{1}{V}\int F_{(t)} C_{O(t)} \exp(k_S t) \exp\left(\frac{1}{V}\int F_{(t)}dt\right)dt + C_S\right]$$

BATCH REACTORS

Introduction

Application of feedforward control to batch chemical processes has received little attention. Undoubtedly one reason for this neglect is the greater popularity of continuous plants in many process industries. However many batch processes still survive in the chemical and other industries where reaction rates are slow, production volume is small, or multiproducts are manufactured. Another equally important reason for the lack of batch feedforward control application is the inherent highly nonlinear nature of batch processes. Most of the process variables undergo large changes. Therefore linear techniques, both feedforward and feedback, are of limited utility.

Batch reactor control is a servomechanism problem, as compared with the regulation problem in continuous processes. The feedforward controller's job is to compensate for set point changes instead of load changes. For a single-loop linear system (for $C = 1$ in Figure 4*a*) with no load disturbances, the feedforward control for perfect control ($C = C^{Set}$) can be derived:

$$F_{(S)} = \frac{1}{G_{(S)}} \tag{25}$$

Physical realizability would theoretically limit control even in the linear case.

For multivariable linear systems, Equation (25) can be generalized to give

$$[F]_{C\times C} = [G]^{-1}_{C\times C} \tag{26}$$

However the problem to be studied here is the nonlinear one. For purposes of illustration consider the same example as before with first-order kinetics. The batch reactor equations are

$$V\frac{dC}{dt} = -VC\,\alpha \exp(-E/RT)$$

$$VC_p\frac{dT}{dt} = \lambda VC\,\alpha \exp(-E/RT) - UA\,(T - T_J) \tag{27}$$

Composition changes over the course of a batch. Two control criteria will be considered. First, as is commonly the case, a specific temperature-time relationship is assumed to be desired, that is, $T^{Set}{}_{(t)}$ is given. Second, a composition-time relationship will be specified. Jacket temperature T_J is the manipulative variable.

Specific Temperature Profile

In the first case the feedforward control problem is to determine T_J as a nonlinear function of T^{Set} *such that* reactor temperature follows T^{Set} exactly. If T^{Set} is a specified function of time, T_J can be determined as a function of time directly. Thus both T^{Set} and T_J would be fed into the system as fixed functions. If the feedforward controller were perfect and no load changes occurred, T would follow T^{Set} with no error. Naturally perfection is never realized, so a feedback controller would be required to trim up the temperature loop (see Figure 4*b*). Feedforward compensation for load changes could also be included but are not considered in this paper.

Isothermal Batch Reactor. The simplest temperature profile would be $T = T_S$, a constant. From Equation (27)

$$C_{(t)} = C_O \exp(-k_S t) \tag{28}$$

where C_O is the initial concentration of C at t = 0. Since $T = T_S$ and $dT/dt = 0$, Equation (27) can be solved to give

$$T_{J(t)} = T_S - \frac{\lambda VC_O k_S e^{-k_S t}}{UA} \tag{29}$$

Thus, T_J must change exponentially with time.

Temperature Ramp. It is sometimes desirable to have reactor temperature change steadily with time. In this case

$$T_{(t)} = T_O + K_B t \tag{30}$$

Solution of Equation (27) for C gives

$$C_{(t)} = C_O \exp\left[-\int_o^t \alpha \exp\left[\frac{-E/R}{T_O + K_B t}\right] dt\right]$$

and solving for T_J, we get

$$T_{J(t)} = T_O + K_B t + \frac{VC_pK_B}{UA} - \left[\frac{\lambda V\alpha}{UA}\exp\left(\frac{-E/R}{T_O + K_B t}\right)\right] C_O \exp\left[-\int_o^t \alpha \exp\left(\frac{-E/R}{T_O + K_B t}\right)dt\right] \tag{31}$$

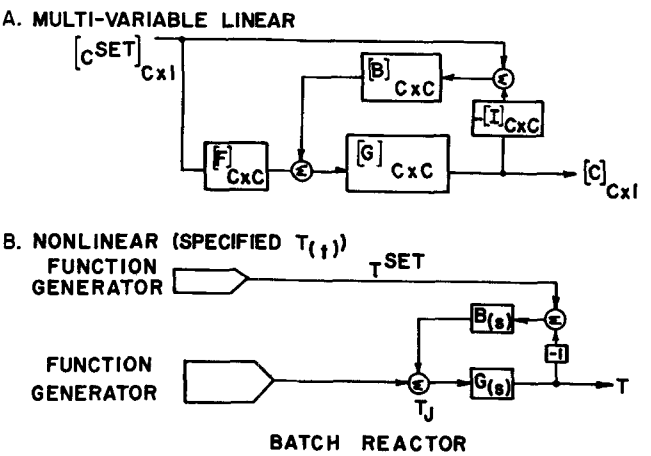


Fig. 4. Feedforward control with set point changes.

This reduces to the isothermal case when $K_B = 0$. Typical curves are shown in Figure 5 for different values of K_B and T_O. The last term in Equation (31) is the heat of reaction (λCk). The first two terms follow the temperature ramp. The third term is the dynamic offset of the jacket temperature. The jacket temperature is higher by (VC_pK_B/UA) than it would be at a constant value of reactor temperature due to the sensible heat of the reactor. One interesting aspect of this dynamic lag is the effect if the temperature range is stopped. An instantaneous decrease in T_J (or increase in Q) is required (see Figure 5*d*). This effect is, of course, not unique to chemical reactors. For example, it is experienced when heating or cooling a stirred tank.

Arbitrary Function. Generalizing one step further, assume the reactor temperature to be an arbitrary function of time $\phi_{(t)}$. Then T_J can be found to be

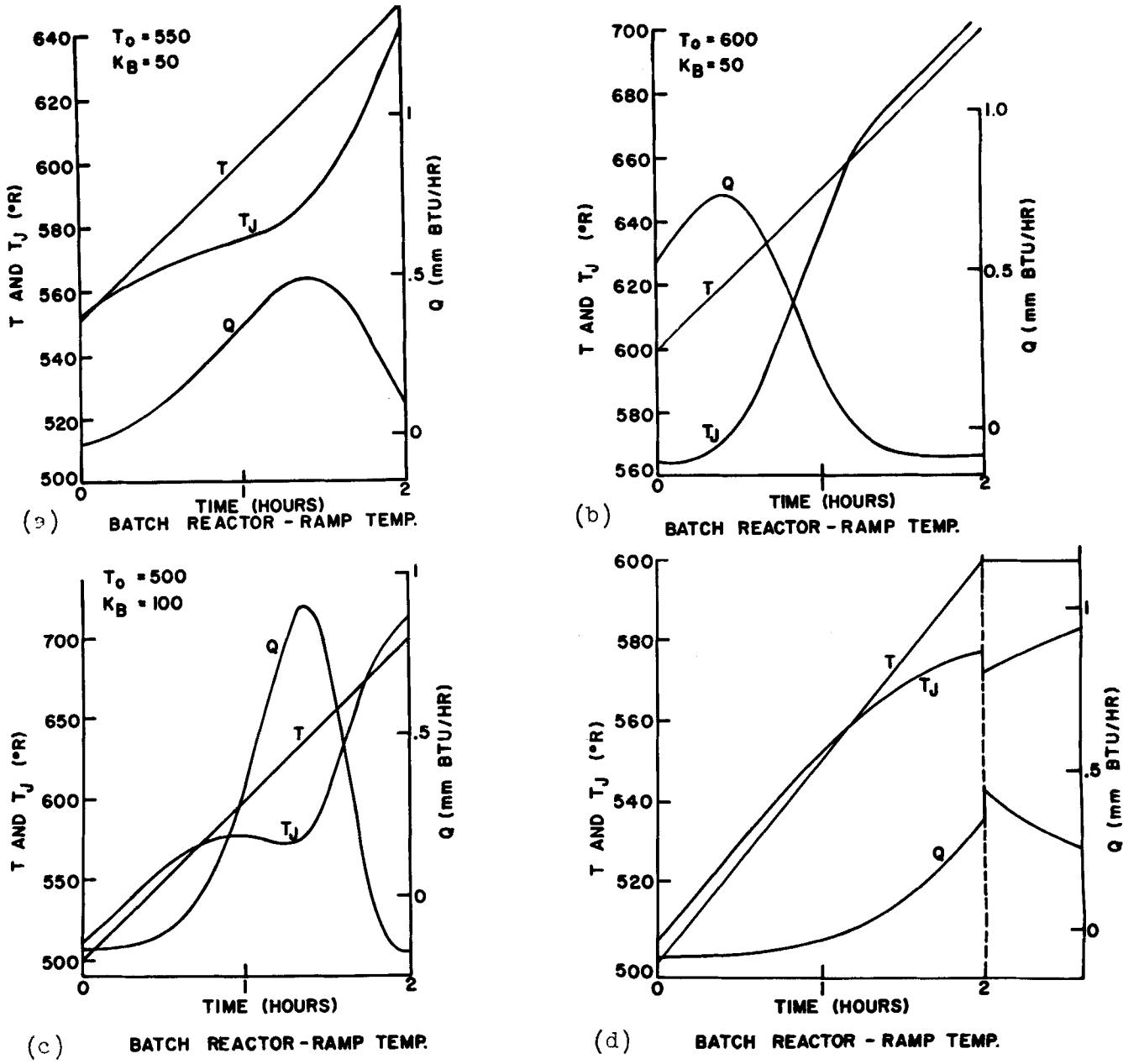


Fig. 5. Batch curves with feedforward control of T_J.

$$T_{J(t)} = \phi_{(t)} + \frac{VC_p}{UA}\frac{d\phi_{(t)}}{dt} - \left[\frac{\lambda V\alpha}{UA}\exp\left(-\frac{E}{R\phi_{(t)}}\right)\right] C_O \exp\left[-\int_o^t \alpha \exp\left(\frac{-E}{R\phi_{(t)}}\right) dt\right] \quad (32)$$

Specified Composition Profile

In this case the batch feedforward control problem is to determine T_J as a nonlinear function of C^{Set} *such that* reactor composition follows C^{Set} exactly. It is assumed that a ramp change in composition is desired.

$$C_{(t)} = C_O - K_B t, \text{ for } O \geq t > \frac{C_O}{K_B} \quad (33)$$

Solving for the feedforward controller, we get

$$T_J = \left[\frac{-E/R}{\log\left(\frac{K_B/\alpha}{C_O - K_B t}\right)}\right] - \frac{\lambda V K_B}{UA} - \frac{VC_p E K_B/UAR}{[C_O - K_B t]\left[\log\left(\frac{K_B/\alpha}{C_O - K_B t}\right)\right]^2} \quad (34)$$

TUBULAR REACTORS

Several discussions of feedforward control of tubular reactors have appeared in the literature. Lamb and coworkers (*13, 14*) used linear methods and frequency domain solution to obtain the dynamics of a packed tubular reactor and to synthesize feedforward controllers. Koppel (*6*) studied the case of an isothermal, plug-flow tubular reactor that was parametrically forced by throughput. He obtained an analytical solution for the dynamics and discussed feedforward manipulation of throughput to control outlet concentration.

The complexity of Koppel's solution, even in his simplified case, indicates the mathematical and practical difficulties of these distributed parameter systems. For-

tunately there is a great deal of research activity in this area, and it is hoped that techniques will soon be developed for handling realistic tubular reactor control problems. In the interim, empirical or linear methods appear to be the only techniques available for practical problems.

A simplified treatment of a nonisothermal, plug-flow, constant-throughput tubular reactor problem is developed below. Reactor temperature T is chosen as the manipulative variable. The feedforward control problem is to find how $T_{(t,Z)}$ should be changed to hold outlet concentration $C_{(t,L)}$ constant in the face of inlet feed concentration disturbances $C_{O(t)}$. The equations describing the system are

$$\left.\begin{aligned} &\frac{\partial C}{\partial t} + v\frac{\partial C}{\partial Z} + Ck = 0 \\ &k = \alpha \exp\left(-E/RT\right) \end{aligned}\right\} \qquad (35)$$

The steady state solution of Equation (35) with a given inlet concentration C_O and a constant reactor temperature (yielding a constant k_S) is

$$C_{S(Z)} = C_O \exp\left(-\frac{k_S}{v}Z\right) \qquad (36)$$

and the outlet concentration is

$$C_{S(L)} = C_O \exp\left(-\frac{k_S L}{v}\right) \equiv C_L$$

One way to hold $C_{S(L)}$ equal to a constant C_L for various values of C_O, at least steady state, would be to change k such that $k_S = (v/L)\log(C_O/C_L)$. Note that there may be other steady state values of $k_{S(Z)}$ that could also give C_L.

Now in the dynamic case, one can reason intuitively that if a slice of fluid enters the reactor with a composition $C_O{}^1$ and if this slice is held at a reactor temperature all the way down the reactor such that $k^1 = (v/L)\log(C_O{}^1/C_L)$, the concentration of the slice will be C_L at the end of the reactor. Therefore the dynamic change of k with time and length to hold $C_{(t,L)} = C_L$ with variable feed composition $C_{O(t)}$ is

$$k_{(t,Z)} = \frac{v}{L}\log\left[\frac{C_{O(t-Z/v)}}{C_L}\right] \qquad (37)$$

$$O \leq Z \leq L, t > O$$

and solving for reactor temperature, we get

$$T_{(t,Z)} = \frac{E/R}{\log\left(\frac{v}{\alpha L}\log\left[C_L/C_{O(t-Z/v)}\right]\right)} \qquad (38)$$

Unfortunately one runs into practical problems in implementing this feedforward control equation because reactor temperature must be varied continuously with time and reactor length. Most commercial tubular reactors are limited to a small number of cooling jacket sections and hence continuous manipulation of reactor temperature with Z is impossible. Although control may not be perfect, improvements over feedback control may be realized.

CONCLUSIONS

1. The effectiveness of feedforward control of chemical processes, particularly chemical reactors, can be improved by using nonlinear methods.
2. Analytical equations can be derived for the simple cases considered in this paper, but computer solutions will probably be required for complex systems.
3. Nonlinear methods are essential in application of feedforward control to batch reactors.
4. Uncertainties in controller equations and errors in measurement of disturbances appear to worsen only slightly the effectiveness of nonlinear feedforward control in the specific numerical example considered.

NOTATION

A = heat transfer area, sq.ft.
a = constant coefficient in linear equation
B = concentration of intermediate in consecutive reactions, lb./lb.
$B_{(S)}$ = feedback controller transfer function
$[B]$ = feedback controller transfer matrix
C = concentration of reactant, lb./lb.
C_p = specific heat, B.t.u./(lb.)(°R.)
E = activation energy, B.t.u./lb.-mole
F = feed rate, lb./hr.
f = function
$F_{(S)}$ = feedforward controller transfer function
$[F]$ = feedforward controller transfer matrix
$G_{(S)}$ = process transfer function
$[G]$ = process transfer matrix
$[I]$ = identity matrix
J = cooling jacket
K = equilibrium constant in reversible reaction
K_B = batch reactor ramp rate, °R./hr. or lb./(lb.)(hr.)
k = specific reaction rate, hr.$^{-1}$
L = length tubular reactor, ft.
n = reaction order
O = feed or initial conditions
Q = heat removal rate, B.t.u./hr.
R = perfect gas constant, B.t.u./(lb.-mole)(°R)
$\mathcal{R}$ = reaction rate, hr.$^{-1}$
S = steady state value or Laplace transform variable
T = reaction temperature, °R.
T_J = cooling jacket temperature, °R.
t = time, hr.
U = heat transfer coefficient, B.t.u./(hr.)(sq.ft.)(°R.)
V = reactor holdup, lb.
v = tubular reactor velocity, ft./hr.
α = pre-exponential factor, hr.$^{-1}$
λ = heat of reaction, B.t.u./lb.
τ = time constant, hr.
1 = first tank or first reaction
2 = second tank or second reaction
Z = tubular reactor axial coordinate, ft.

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