ACKNOWLEDGMENT

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NOTATION

A = a chemical compound or its concentration (mole/liter)
B = same
c = specific heat of the reacting mixture, calories/g.
C = concentration, mole/liter
e = volumetric C.S.T.R. (continuously stirred tank reactor) to batch efficiency ratio
F = flow rate, liters/hr.
h = reactor heat input, °K./hr.
H = reactor heat input, °K./hr.
ΔH_R = heat of reaction, calories/mole of A
I = control quality
j = pure imaginary, $\sqrt{-1}$
k = reaction-rate constant, different units.
K = proportionality constant for a proportional controller
M = a matrix
n = mole fraction, or number of reactors in a chain or reaction order
Q = modified heat of reaction, (°K.) (mole)/liter of A
R = general reaction rate
t = time, hr.
T = temperature, °K., or controller time constant
V = reactor volume, liters or variation vector
x = concentration of feed component, mole/liter
X = variation in concentration of feed component, mole/liter
y = concentration of product component, mole/liter
Y = variation in concentration of product component, mole/liter
Z = variation in reactor temperature, °K.
α, β, γ = stoichiometric coefficients
Δ = fractional control quality
θ = C.S.T.R. holding time, hr.
ρ = density of reacting mixture, g./liter
τ = reaction time for a tubular reactor, hr.
ω = signal frequency, radians/hr.

Subscripts

0, 1 = C.S.T.R. feed and product streams
D = derivative controller
I = integral controller
n = reactor number in a chain
P = proportional controller
s = steady state

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II. Frequency-response Relations for Reactor Chains, Tubular Reactors, and Unit Reactor Control Loops

REACTOR CHAINS

The results which were obtained in Part I for a single reactor can be used to calculate step by step the response of a chain of reactors. Interest in these calculations is twofold. First the safe operation of the whole chain may put upon a reactor in the chain more stringent control requirements than would individual operation, especially in the case of reactions highly sensitive to temperature. Second, these calculations can be used to determine simpler modes of control for the whole chain. In some cases, for instance, the feed flow is controlled by inlet sampling and the whole heating system by a sampling of the final product, the individual heat-control loop on each reactor thus being eliminated. The calculations are straightforward and the theory is easily developed with the introduction of matrices. It will be developed here on the basis of the example used previously, of a reaction involving components A and B, with a rate $R(x, T)$.

First Case: Variations in Concentration Only

Equations (17) and (18) of Part I are used with the feed concentration variations X_0 and Y_0

$$(1 + \alpha\theta R_x' + j\omega\theta)X = X_0 \qquad (1)$$

$$-\theta R_x'X + (1 + j\omega\theta)Y = Y_0 \qquad (2)$$

These may be written in matrix form, the variation vector V_i representing the variations in the composition of the feed to reactor $i + 1$:

$$V_i = \begin{vmatrix} X_i \\ Y_i \end{vmatrix}$$

and the matrix M_i of the variation coefficients being introduced.

In matrix notation Equations (1) and (2) may be written

$$\begin{vmatrix} 1 + \alpha\theta R_x' + j\omega\theta, & 0 \\ -\theta R_x', & 1 + j\omega\theta \end{vmatrix} \cdot \begin{vmatrix} X \\ Y \end{vmatrix} = \begin{vmatrix} X_0 \\ Y_0 \end{vmatrix}$$

and for the reactor i in a chain

$$\begin{vmatrix} 1 + \alpha\theta_i R_{xi}' + j\omega\theta_i, & 0 \\ -\theta_i R_{xi}', & 1 + j\omega\theta_i \end{vmatrix} \cdot \begin{vmatrix} X_i \\ Y_i \end{vmatrix} = \begin{vmatrix} X_{i-1} \\ Y_{i-1} \end{vmatrix}$$

or

$$V_{i-1} = M_i V_i \qquad (3)$$

with

$$M_i = \begin{vmatrix} 1+\alpha\theta_i R_{xi}'+j\omega\theta_i, & 0 \\ -\theta_i R_{xi}', & 1+j\omega\theta_i \end{vmatrix} \qquad (4)$$

Therefore, the relation between product and feed variations in composition is

$$V_n = (M_1 M_2 \cdots M_i \cdots M_n)^{-1} V_0 \qquad (5)$$

This formula gives the desired result, namely that the product composition varies as a function of feed-composition variations.

Illustration 4

The foregoing formula will be applied to the case of a first-order reaction

$$A \rightarrow B$$

performed isothermally in a chain of reactors of equal size. The rate of the reaction is

$$R(x) = \frac{dB}{dt} = -\frac{dA}{dt} = kx$$

Therefore $R_x'(x) = k$ and the quantity $\theta R_x' = \theta k$ is constant for all reactors. All the matrices M_i are therefore the same, and Formula (5) may be written as $V_n = M^{-n}V_0$ or

$$\begin{vmatrix} X_n \\ Y_n \end{vmatrix} = \begin{vmatrix} 1 + \theta k + j\omega\theta, & 0 \\ -\theta k, & 1 + j\omega\theta \end{vmatrix}^{-n} \begin{vmatrix} X_0 \\ Y_0 \end{vmatrix} \qquad (6)$$

Matrix multiplication and division yields

$$\begin{vmatrix} 1 + \theta k + j\omega\theta, & 0 \\ -\theta k, & 1 + j\omega\theta \end{vmatrix}^{-n}$$

$$= \begin{vmatrix} \dfrac{1}{(1 + \theta k + j\omega\theta)^n}, & 0 \\ \Omega, & \dfrac{1}{(1 + j\omega\theta)^n} \end{vmatrix}$$

the term Ω being

$$\Omega = \theta k \sum_{\lambda=0}^{\lambda=n-1} (1 + \theta k + j\omega\theta)^{\lambda-n} \cdot (1 + j\omega\theta)^{-1-\lambda} \qquad (7)$$

Developing matrix expression (6) shows the relation between variations in concentration of A in the feed and product streams to be

$$X_n = \frac{1}{(1 + \theta k + j\omega\theta)^n} X_0 \qquad (8)$$

and the variation in the concentration of B in the product stream Y_n, caused by concentration variations X_0, Y_0 in the feed stream,

$$Y_n = \Omega X_0 + \frac{1}{(1 + j\omega\theta)^n} Y_0$$

Usually $Y_0 = 0$, no product being present in the feed stream, and thus

$$Y_n = \Omega X_0,$$

or

$$Y_n = \theta k \sum_{\lambda=0}^{\lambda=n-1} (1 + \theta k + j\omega\theta)^{\lambda-n} \cdot (1 + j\omega\theta)^{-1-\lambda} X_0 \qquad (9)$$

or, summing the geometric series,

$$\frac{Y_n}{X_0} = (1 + j\omega\theta)^{-n} - (1 + j\omega\theta + \theta k)^{-n}$$

This is an interesting result, as it relates the variations in product composition to those in feed composition for a reactor chain. To illustrate this relationship better, a numerical example is presented. A chain of n equal-sized reactors operates on the first-order reaction

$$A \rightarrow B$$

with a 95% conversion of compound A. The inlet and outlet concentrations are

compound A
$x_0 = 1.00$ mole/liter, $x_n = 0.05$ mole/liter

product B
$y_0 = 0.00$ mole/liter, $y_n = 0.95$ mole/liter

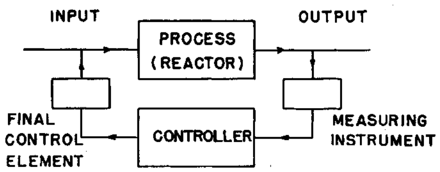


Fig. 4. Block diagram of a control system.

The operation is isothermal, with a rate constant

$$k = 19.0 \text{ hr.}^{-1}$$

The holding time, θ, for a reactor of the chain is found from a mass balance over the system, given by

$$\theta = \frac{1}{k}\left[\left(\frac{x_0}{x_n}\right)^{1/n} - 1\right] \qquad (10)$$

The maximum amplitude ratio is attained at vanishing frequency. Its value, calculated from Formula (9) for $\omega = 0$, is

$$\left|\frac{Y_n}{X_0}\right|_{max} = 1 - \frac{1}{(1 + \theta k)^n} = 1 - \frac{x_n}{x_0} = 0.95$$

It is therefore a constant, independent of the number of reactors.

While vanishing frequency results are the easiest to calculate, more information about system behavior may be derived from the values of the phase angle and amplitude ratio of the concentration variations at a frequency physically related to system properties, that is, for instance, such as $\omega n\theta = 1$. Such results, calculated by means of Equation (9), are presented in the accompanying table.

POLAR-PLOT DATA FOR A REACTOR CHAIN, FOR $\omega n\theta = 1$

Number of reactors, n	Unit holding time, θ	Total holding time, $n\theta$	Amplitude ratio $\lvert Y_n/X_0 \rvert$ for $\omega n\theta = 1$	Phase angle for $\omega n\theta = 1$, deg.
1	1.000 hours	1.000 hours	0.671	−48
2	0.183	0.366	0.763	−56
3	0.090	0.271	0.813	−57
5	0.043	0.216	0.861	−58
10	0.018	0.184	0.904	−58
∞	0.000	0.158	0.950	−57.3

These values give an indication of the transformation of the shape of the Nyquist plot with reactor number. From a nearly circular plot touching the imaginary axis at the origin for a single reactor, the plots evolve toward a circle centered at the origin for the limiting case of the tubular reactor.

Formula (5) gives the relation between feed- and product-composition variations for a chain of n stirred-flow reactors. It may be interesting to examine what happens when the number of reactors increases indefinitely, the total holding time remaining constant. This limiting case is represented by a tubular reactor with uniform conditions in a cross section.

Limiting Case of the Tubular Reactor

All holding times are assumed equal and $\tau = n\theta$ is the tubular-reactor holding time. Therefore

$$\theta_i = \frac{\tau}{n} = \Delta\tau_i$$

where the increment $\Delta\tau_i$ is thus defined. Then Expression (4) of the matrix M_i may be written

$$M_i = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} + \begin{vmatrix} \alpha R_{xi}' + j\omega, & 0 \\ -R_{xi}', & j\omega \end{vmatrix} \Delta\tau_i$$

Neglecting second-order terms in $\Delta\tau_i$ gives

$$M_i = \exp\left\{ \begin{vmatrix} \alpha R_{xi}' + j\omega, & 0 \\ -R_{xi}', & j\omega \end{vmatrix} \Delta\tau_i \right\}$$

Therefore

$$V_0 = M_1 M_2 \cdots M_i \cdots M_n V_n$$

$$V_0 = \exp\left\{ \sum_{i=1}^{i=n} \begin{vmatrix} \alpha R_{xi}' + j\omega, & 0 \\ -R_{xi}', & j\omega \end{vmatrix} \Delta\tau_i \right\} V_n$$

Passing to the limit gives

$$V_n = \exp\left\{ - \begin{vmatrix} \alpha \int_0^\tau R_x' dt + j\omega\tau, & 0 \\ -\int_0^\tau R_x' dt, & j\omega\tau \end{vmatrix} \right\} V_0 \qquad (11)$$

The exponential form of the transfer functions characterizing the behavior of systems with dead time may be recognized. The matrices

$$\begin{vmatrix} j\omega\tau, & 0 \\ 0, & j\omega\tau \end{vmatrix} \quad \text{and} \quad \begin{vmatrix} \alpha \int_0^\tau R_x' \, dt, & 0 \\ -\int_0^\tau R_x' \, dt, & 0 \end{vmatrix}$$

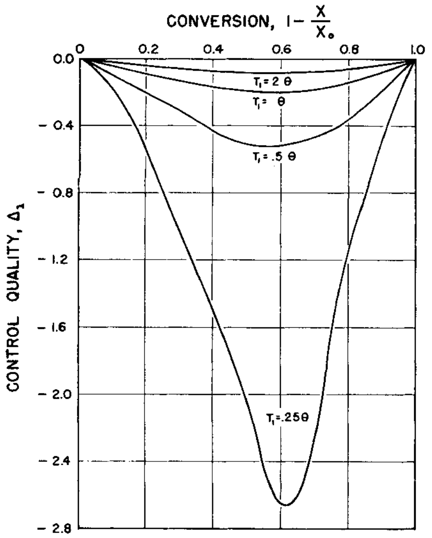


Fig. 5. Fractional control quality against conversion for integral control of a first-order reaction in a C.S.T.R.

commute; therefore Expression (11) may be written

$$V_n = \exp\left\{-\begin{vmatrix} j\omega\tau, & 0 \\ 0, & j\omega\tau \end{vmatrix}\right\}$$

$$\cdot\exp\left\{-\begin{vmatrix} \alpha\int_0^\tau R_x'\,dt, & 0 \\ -\int_0^\tau R_x'\,dt, & 0 \end{vmatrix}\right\} V_0$$

or

$$V_n = \exp\{-j\omega\tau\}\begin{vmatrix} \exp\left\{-\alpha\int_0^\tau R_x'\,dt\right\}, & 0 \\ 1-\exp\left\{-\int_0^\tau R_x'\,dt\right\}, & 1 \end{vmatrix} V_0 \qquad (12)$$

Developing this matrix expression one finds the formula for a tubular reactor (with any order reaction) which corresponds to Expression (9) for a reactor chain:

$$Y_n = \left(1 - \exp\left\{-\int_0^\tau R_x'\,dt\right\}\right) \cdot\exp\{-j\omega\tau\}X_0 \qquad (13)$$

The Nyquist diagram, which represents Y_n/X_0, is a circle centered at the origin of the complex plane.

Second Case: Variation in Concentration and Temperature with a Steady Heat Input

The treatment for this case is similar to that above, the equations to be considered being

$$(1 + \alpha\theta R_x' + j\omega\theta)X + \alpha\theta R_T'Z = X_0$$

$$-\theta R_x'X + (1 + j\omega\theta)Y - \theta R_T'Z = Y_0$$

$$-\alpha Q\theta R_x'X + (1 + j\omega\theta - \alpha Q\theta R_T')Z = Z_0$$

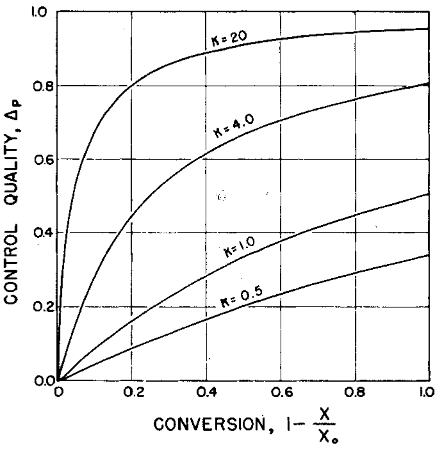


Fig. 6. Fractional control quality against conversion for proportional control of a first-order reaction in a C.S.T.R.

obtained from the basic expressions (17), (18), (19) of Part I.

The matrix M_i similar to (4) is now

$$M_i = \begin{vmatrix} 1 + \alpha\theta_i R_{xi}' + j\omega\theta_i, & 0, & \alpha\theta_i R_{T_i}' \\ -\theta_i R_{xi}', & 1 + j\omega\theta_i, & -\theta_i R_{T_i}' \\ -\alpha Q\theta_i R_{xi}', & 0, & 1 - \alpha Q\theta_i R_{T_i}' + j\omega\theta_i \end{vmatrix} \qquad (14)$$

and the relation between feed and product variations for a chain of n reactors is as before

$$V_n = (M_1M_2\cdots M_i\cdots M_n)^{-1}V_0 \qquad (15)$$

where the vectors V_i are defined now as

$$V_i = |\,X_i,\ Y_i,\ Z_i\,|$$

Numerical calculations on Formula (15) are best carried out step by step.

The determinant of Matrix (14) is

$$D_i \equiv (1 + j\omega\theta_i)^2[1 + \alpha\theta_i(R_{xi}' - QR_{T_i}') + j\omega\theta_i]$$

The factor

$$1 + \alpha\theta_i(R_{xi}' - QR_{T_i}') + j\omega\theta_i$$

is recognized as one that appeared in Expression (24) of Part I.

The stability of the reactor chain is obtained when all units of the chain are stable. Following the discussion in Part I the condition on the holding times

$$\theta_i < \frac{1}{(QR_{T_i}' - R_{xi}')\alpha}$$

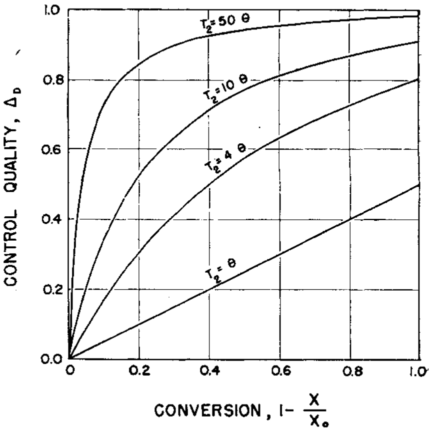


Fig. 7. Fractional control quality against conversion for derivative control of a first-order reaction in a C.S.T.R.

is obtained, which must be satisfied in the case of a highly exothermic reaction ($Q > R_{xi}'/R_{T_i}'$) in order to have stable operation. This is again an example of the restrictions which control requirements may impose on reactor design.

REACTOR CONTROL

In the preceding page only the calculation of the frequency response of continuously stirred tank reactors has been considered. This section will combine for illustrative purposes, the frequency-response functions thus obtained with different controller-response functions to find the quality of the control circuit formed by reactor and controller. The control system considered may be represented by Figure 4.

A variable in the reactor outlet stream, for instance product concentration, is measured and is compared with the desired value in the controller which sends out a signal acting on the controlled variable in the reactor inlet stream, for instance feed concentration, through a final control element. Detailed information about such diagrams and control theory in general may be found in references *1* and *2*.

A negligible lag is assumed in measurement and in the final control element, in order to isolate the effect of controller-response characteristics on the system. For present purposes the three usual idealized types of controllers are examined (*1*). Actual controllers often approach combinations of these and can be treated in the same manner; such a case will be illustrated in the analogue example.

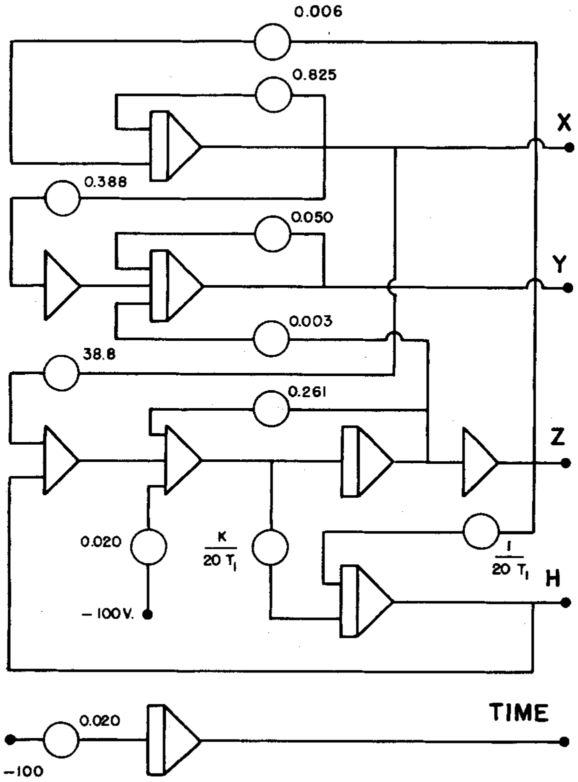


Fig. 8. R.E.A.C. circuit for temperature control in a C.S.T.R. Data of illustration 3.

Controller	Frequency response $G(j\omega)$
Integral	$-P/E = 1/j\omega T_1$
Proportional	$-P/E = K$
Derivative	$-P/E = j\omega T_2$

In the preceding expressions of controller response to a cyclic disturbance of frequency ω, E designates the error signal and P the controller output. The quantities T_1, K, T_2 are constants characteristic of controller operation.

Control quality may be expressed by the quantity

$$I = \int_0^\infty |\, W(t)\,|^2\, dt \qquad (16)$$

where $W(t)$ is the system response to a unit impulse applied to system input at time zero. The choice of this criterion takes into consideration the importance of the deviation amplitude caused by the perturbation and also the length in time of the deviation. This expression will be used in the study of control quality.

The integral I may be evaluated in terms of the frequency-response function of the controlled system $Y(j\omega)$. From reference *2*

$$W(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega e^{j\omega t}\, Y(j\omega) \qquad (17)$$

Therefore

$$I = \int_0^\infty |\, W(t)\,|^2\, dt$$
$$= \frac{1}{\pi}\int_0^\infty Y(j\omega)\, Y(-j\omega)\, d\omega \qquad (18)$$

Example

A control loop will be considered on the basis of measurement of product concentration in the outlet stream and control of feed concentration in the inlet stream. Reactor operation is assumed to be isothermal and data of Illustration 4 are used. Thus the frequency-response function for a chain of n equal-sized reactors is given by Expression (9):

$$G_n(j\omega) = \frac{Y_n}{X_0} = \theta k \sum_{\lambda=0}^{\lambda=n-1} (1 + \theta k + j\omega\theta)^{\lambda-n}(1 + j\omega\theta)^{-1-\lambda}$$

$G_n(j\omega)$ is the frequency-response function for the reactor chain without control.

For the controlled system (Figure 4) the input to the reactor is equal to the input to the system X_0 minus the output of the final controller. The input to the controller is the output of the reactor Y_n. Hence if $G(j\omega)$ represents the frequency-response function for the controller, the output of the controller is $G(j\omega)Y_n$; the input to the reactor is $X_0 - G(j\omega)Y_n$; and the output of the reactor is $Y_n = G_n(j\omega)[X_0 - G(j\omega)Y_n]$. Solving this for Y_n yields

$$Y_n = \frac{G_n(j\omega)}{1 + G(j\omega)G_n(j\omega)}\, X_0 \qquad (19)$$

The frequency-response function for the system with control is therefore

$$Y(j\omega) = \frac{Y_n}{X_0} = \frac{G_n(j\omega)}{1 + G(j\omega)G_n(j\omega)} \qquad (20)$$

Control quality may then be determined from formula (18), where $Y(j\omega)$ is replaced by its expression (20).

The case of a single reactor will be examined in more detail. The expression of control quality for a single reactor with different controllers or no control are, from the foregoing development,

integral control

$$I_I = \frac{1}{\pi}\int_0^\infty \frac{\theta^2 k^2 \omega^2 T_1{}^2\, d\omega}{k^2\theta^2 - 2\omega^2 k T_1 \theta^2(2 + \theta k) + \omega^2 T_1{}^2(1 + \omega^2\theta^2)[(1 + \theta k)^2 + \omega^2\theta^2]}$$

proportional control

$$I_P = \frac{1}{\pi}\int_0^\infty \frac{\theta^2 k^2\, d\omega}{K^2\theta^2 k^2 + 2K(1 + \theta k - \omega^2\theta^2)\theta k + (1 + \omega^2\theta^2)[(1 + \theta k)^2 + \omega^2\theta^2]}$$

derivative control

$$I_D = \frac{1}{\pi}\int_0^\infty \frac{\theta^2 k^2\, d\omega}{k^2\theta^2\omega^2 T_2{}^2 + 2\omega^2\theta^2 T_2(2 + \theta k)k + (1 + \omega^2\theta^2)[(1 + \theta k)^2 + \omega^2\ \theta]}$$

These expressions are valid only for stable systems. The value of I would be infinite for an unstable system, as in this case response $W(t)$ is undamped or ever increasing in amplitude.

When there is no control, that is to say,

$$\frac{1}{T_1} = K = T_2 = 0$$

these integrals reduce to

$$I_0 = \frac{1}{\pi}\int_0^\infty \frac{\theta^2 k^2\, d\omega}{(1+\omega^2\theta^2)[(1+\theta k)^2+\omega^2\theta^2]}$$
$$= \frac{\theta k^2}{2(1+\theta k)(2+\theta k)}$$

The integrals expressed above are calculated by integration in the complex plane or use of tables in the appendix of reference *2*. The results have been expressed here in terms of the system with no control in fractional form:

$$\Delta = 1 - \frac{I}{I_0}$$

which better shows the gain in control quality due to the controller. The value of Δ when the control loop is broken is zero and reaches unity for perfect control. The expressions for the respective fractional control qualities are for integral *control*

$$\Delta_I = \frac{k\theta^2}{k\theta^2 - (1 + \theta k)(2 + \theta k)T_1},$$

$$\text{for } T_1 > \frac{k\theta^2}{(2 + \theta k)(1 + \theta k)}$$

for proportional control

$$\Delta_P = \frac{K\theta k}{1 + \theta K + K\theta k}$$

for derivative control

$$\Delta_D = \frac{T_2 k}{2 + \theta k + T_2 k}$$

Fractional control quality has been represented for the different modes of control Δ_I, Δ_P, Δ_D against conversion in Figures 5, 6, and 7. Curves are given for different values of the characteristic control parameters T_1, K, and T_2. Conversion in this case is

$$1 - \frac{x}{x_0} = \frac{\theta k}{1 + \theta k}$$

where x_0, x are the concentrations of reactant A in the feed and the product.

The plots of Figures 5, 6, and 7 show an increase in control quality by the same instrument when the conversion decreases, which is evident *a priori*, since at low conversion a disturbance on the feed will have only a small effect on outlet product concentration. The plots are characteristic of the three simplified modes of control examined. Idealized components have been used in this loop analysis and the results in practice must be tempered with a knowledge of the performance of the components and system actually available.

ANALOGUE SIMULATION OF CONTROLLED SYSTEMS

The equations describing the operation of the three types of controllers which have been considered in this study are

Integral control

$$E = -T_1 \frac{dP}{dt}$$

Proportional control

$$E = -\frac{1}{K} P$$

Differential control

$$P = -T_2 \frac{dE}{dt}$$

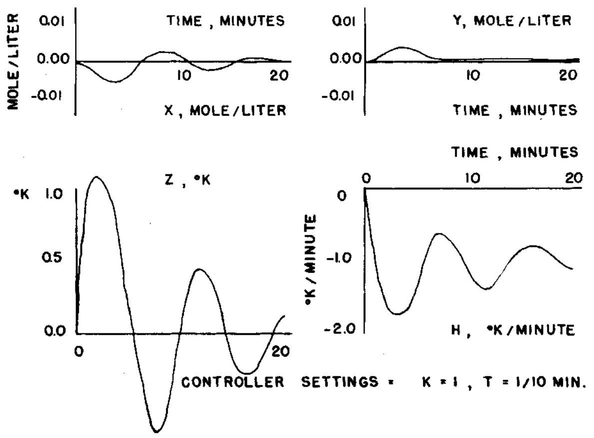
These equations, written for an appropriate control loop, may be associated with the linearized equations describing reactor behavior: [Equations (12), (13), (14) of Part I].

$$\theta \frac{dX}{dt} + (1 + \alpha\theta R_x')X + \alpha\theta R_T'Z = X_0 \qquad (21)$$

$$\theta \frac{dY}{dt} - \theta R_x'X + Y - \theta R_T'Z = Y_0 \qquad (22)$$

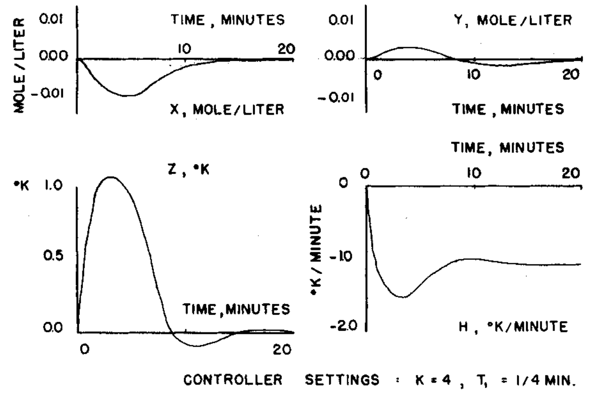
$$\theta \frac{dZ}{dt} - \alpha Q\theta R_x'X + (1 - \alpha Q\theta R_T')Z = \theta\Delta H + Z_0 \qquad (23)$$

The system thus obtained may be solved to obtain the response of the controlled



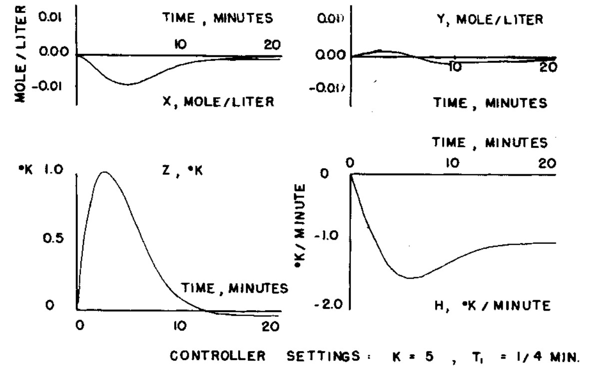
CONTROLLER SETTINGS = K = 1, T = 1/10 MIN.

Fig. 9. Example of C.S.T.R. temperature control (underdamped case).



CONTROLLER SETTINGS : K = 4, T_1 = 1/4 MIN.

Fig. 10. Example of C.S.T.R. temperature control (correct controller settings).



CONTROLLER SETTINGS : K = 5, T_1 = 1/4 MIN.

Fig. 11. Example of C.S.T.R. temperature control (overdamped case).

reactor to a given disturbance. The analytical solution will, however, in many cases be cumbersome and in practice, especially when more complex performance functions are needed, the use of an analogue computer is of great advantage. An example will be solved with the analogue technique.

Considered here is the case of a temperature-control loop with a controller combining the proportional and integral control modes. A constant feed composition is assumed, that is to say $X_0 = Y_0 \equiv 0$, and a disturbance caused by a change in feed temperature, Z_0. The equations which describe this system are (21), (22), (23) and the controller equation for the temperature-control loop becomes

$$\frac{dH}{dt} = -K\frac{dZ}{dt} - \frac{1}{T_1}Z \qquad (24)$$

With the values of Illustration 2 for a second-order exothermic reaction

$$2A \rightarrow B + D$$

with $\Delta H_R = -50{,}000$ cal./mole of A these equations take the following form:

$$0.33\frac{dX}{dt} + 16.50X + 0.1245Z = 0$$

$$0.33\frac{dY}{dt} - 7.750X + Y - 0.0622Z = 0$$

$$0.33\frac{dZ}{dt} - 775.X - 5.224Z = 0.33\Delta H + Z_0$$

$$0.33\frac{dH}{dt} = -0.33K\frac{dZ}{dt} - \frac{0.33}{T_1}Z$$

The analogue circuit which represents these equations with a time scale changed from hours to minutes is given as an illustration on Figure 8. The symbols of the circuit diagram are standard and may be found in reference *3*.

This circuit was used to determine the response of the controlled reactor to a change in feed temperature

$$Z_0 = 1°C.$$

for three different settings of the controller characteristics K and T_1. The results are given on Figures 9, 10, and 11. Figure 9 represents a case with low damping ($K = 1$, $T_1 = 1/10$ min.). The system oscillates around the steady state. Figure 10 represents a more damped case ($K = 4$, $T_1 = ¼$ min.), which would be acceptable in practice. The system represented in Figure 11 is overdamped ($K = 5$, $T_1 = ¼$ min.) but may still be acceptable in practice. Such examples could be multiplied for various combinations of controller types. Discussion of them is easy, and they will not be developed further here.

CYCLING IN SYSTEMS WITH DEAD TIME

If the number of stirred flow reactors in a chain is increased indefinitely, the over-all holding time remaining constant, at the limit the case of a tubular reactor is obtained. The frequency-response functions for the isothermal tubular reactor without volume change have been obtained in Expression (12). For the case of a first-order reaction the expression of the frequency-response function relating product-concentration variations Y_n to feed concentration variations X_0 has been found:

$$Y_n = (1 - e^{-k\tau})e^{-i\omega\tau}X_0$$

The presence of the imaginary exponential in the expression of the frequency-response function is characteristic of systems with dead time. Thus a measuring instrument placed at the reactor outlet will perceive feed perturbations only a time after they happen and any corrective action will be delayed by that much. This dead time in the reactor system increases with the number of reactors in the chain and approaches a maximum time in a tubular reactor, and so in the latter design control may be more difficult than in a continuously stirred tank reactor (C.S.T.R.). Also control by stages may more readily be applied to the selected elements of a chain.

Dead time may easily lead to cycling of the controlled system if the control is improperly designed. Only an example of such a case will be given, for proportional control applied to a tubular reactor by measurement of product concentration at the outlet and control of inlet-feed concentration.

If $A(t)$ designates the disturbance on the feed concentration at the reactor inlet, the disturbance on product concentration at the outlet is $(1 - e^{-k\tau})A(t - \tau)$ and the equation of the proportional-control loop is

$$A(t) + K(1 - e^{-k\tau})A(t - \tau) = 0 \qquad (25)$$

where K is the characteristic constant of the proportional controller. Equation (25) is of the difference type, and methods of solution are well known. Thus introducing a solution

$$A(t) = e^{st}$$

into Equation (25) results in a characteristic equation which gives the values of s for which e^{st} is a solution of (25):

$$1 + K(1 - e^{-k\tau})e^{-s\tau} = 0$$

It is found that

$$s = \frac{1}{\tau}\left[\ln K(1 - e^{-k\tau}) + j\pi(1 + 2\lambda)\right]$$

where λ may take any integer value. The system is stable if the exponential e^{st} is damped:

$$\frac{1}{\tau}\ln K(1 - e^{-k\tau}) < 0$$

or

$$K(1 - e^{-k\tau}) < 1$$

Thus a limitation exists on the values of the proportional factor K which may be used. If controller action is too powerful (high K), cycling may develop.

COMMENT

It should be realized that in the practice of automatic control the results of frequency-response analyses can today be used to advantage principally for guidance rather than for the exact prediction of the performance to be expected of a practical control system. In the first place the disturbances occurring in an industrial operation will not usually be regular or periodic, although of course the typically random disturbance will excite all frequencies. Furthermore, the differences found between theory and practice are often the result of deviations from the simplified characteristics which are usually assumed for the sensing and the control elements. Furthermore largely indeterminate lags often occur in industrial installations. Nevertheless the equations obtained as a result of the application of frequency response theory offer real advantages in simplicity of treatment and clarity of exposition, have proved extremely helpful in understanding the control process itself, and have guided the engineer to practical solutions to automatic-control problems. As more precise characterizations of modern commercial instruments and of lag systems become available, better predictions are to be expected.

Numerical examples have been worked out in this paper and especially in Part I in order to demonstrate clearly the method of application of frequency-response analysis to continuous-flow reactions. These should also serve to clarify the characteristics of the chemical reactor control process itself. It was shown for example that such important factors as temperature-sensitive rates of reaction can be readily analyzed by these methods.

NOTATION

See page 256.

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