C_p = specific heat
c = concentration
$\mathbf{F}$ = Jacobian matrix
$\hat{\mathbf{F}}$ = $\mathbf{F} + \mathbf{F}^T$
$\mathbf{f}$ = autonomous vector function
ΔH = heat of reaction
K = constant for Liapunov function contour
n = order of reaction
Q = activation energy divided by the gas constant
q = volumetric flow rate
r = rate of reaction per unit volume
T = temperature
t = time
U = overall heat transfer coefficient
V = reactor volume
$\mathcal{V}$ = Liapunov function
$\mathbf{x}$ = general state vector
y = normalized concentration
η = normalized temperature
ρ = density
τ = time constant defined in Equation (2)

Subscripts and Superscripts

$\wedge$ = deviation from steady state
$\cdot$ = total time derivative
$\|\ \|$ = norm of a vector
ss = steady state
A = heat sink
o = input
1,2,3 = specific values of K
T = transpose

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The Effect of Feedback Control on Chemical Reactor Stability

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In a previous paper (*1*) an analysis of a wide class of chemical reactors established criteria for computing a region of asymptotic stability (RAS). Sufficient conditions were given for treating arbitrary nonlinear kinetics for a system that can be described by two state variables, temperature and concentration. These criteria were established for the reactor operating without control, but in virtually all cases of practical interest some mode of control is desirable to help improve stability and performance. The choice of a particular control action is most often a decision based wholly on past experience with related problems. This paper is concerned with establishing criteria by which the stability effects of many linear or nonlinear control modes may be analyzed. The analysis is based on the second method of Liapunov and Krasovskii's theorem (3), techniques which are described fully in the reference cited above.

THE SYSTEM EQUATIONS

The system under consideration is a well-stirred reactor in which a homogeneous reaction is taking place. It can be described by energy and material balances which yield

$$\left.\begin{aligned}\rho V C_p \frac{dT}{dt} &= \Delta H V r - U A_R\,(T - T_A) - \rho q C_p\,(T - T_o)\\ V\frac{dc}{dt} &= -Vr - q\,(c - c_o)\end{aligned}\right\} \quad (1)$$

The dependent variables, temperature and/or concentration, are to be controlled in this system. A feedback controller responds to changes in these variables and improves system behavior through its effect on another variable of the system called a "manipulating" variable. A typical control scheme might control reactor temperature for example by manipulating the heat transfer coefficient. For this system there are eight possible combinations of the control variables (T, c) and the principle manipulating variables (T_o, T_A, c_o, U) if the controller input and output are taken one variable at a time. A sizable increase in this number will result if the control or manipulating variables are to act or respond in concert. Since such control schemes require very rapid computational facilities, this last consideration raises questions concerning the applicability of computers to control. In what follows all eight simple loops and some combination controls are discussed. It is simplest to study each possible manipulating variable in a sequence of cases. The flow variable q is not included; it is straightforward in principle but does not seem to be of any practical interest.

FEED TEMPERATURE AS A MANIPULATING VARIABLE

Let feed temperature T_o be an as yet unrestricted function of reactor temperature T and concentration c. Following the transformation procedure detailed in reference 1 the basic Equation (1) may be written in normalized form:

$$\left.\begin{aligned} \frac{d\hat{\eta}}{dt} &= \hat{r}/c_o - \frac{b}{a}\hat{\eta} + \frac{1}{\tau}\hat{\eta}_o \\ \frac{d\hat{y}}{dt} &= -\hat{r}/c_o - \frac{1}{\tau}\hat{y} \end{aligned}\right\} \quad (2)$$

Proceeding in accordance with Krasovskii's theorem it is essential to examine the Jacobian matrix:

$$\mathbf{F} = \begin{bmatrix} \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{b}{a} + \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}} & \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{y}} \\ -\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} & -\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) \end{bmatrix} \quad (3)$$

Then

$$-\hat{\mathbf{F}} = \begin{bmatrix} 2\left(\frac{b}{a} - \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}}\right) & \frac{1}{c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{y}} \\ \frac{1}{c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{y}} & 2\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) \end{bmatrix} \quad (4)$$

If the matrix $-\hat{\mathbf{F}}$ is positive definite, the function

$$V(\hat{\eta}, \hat{y}) = \left(\frac{d\hat{\eta}}{dt}\right)^2 + \left(\frac{d\hat{y}}{dt}\right)^2 \quad (5)$$

will be a Liapunov function, and the system can be guaranteed to be asymptotically stable. Examination of the matrix Equation (4) thus establishes the stability criteria:

$$\frac{b}{a} - \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}} > 0 \quad (6)$$

$$4\left(\frac{b}{a} - \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}}\right)\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) > \left[\frac{1}{c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{y}}\right]^2 \quad (7)$$

If the effect of control is to be an improvement in relative stability, the control-related terms in these criteria must act to expand the T, c region that satisfies the inequalities. Since the manipulating feed-temperature variable appears in the inequalities as separately dependent on each of the control variables, the effects may be studied one at a time.

The dependence of $\hat{\eta}_o$ on $\hat{\eta}$ (the control function) will strengthen the inequalities (6) and (7) if

$$\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}} = \frac{\partial\hat{T}_o}{\partial\hat{T}} < 0 \quad (8)$$

The more negative $\left(\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}}\right)$ the more will the RAS be expanded. Inequality (8) requires that the functional dependence of T_o on T be an odd monotonic function restricted to the second and fourth quadrants in a plot of T_o vs. T. It may be noted that a large range of functions will fit this category. An important elementary control mode that meets the requirement is proportional control with negative feedback:

$$\hat{T}_o = -\mu\hat{T};\ \mu > 0 \quad (9)$$

By simple differentiation

$$\frac{\partial\hat{T}_o}{\partial\hat{T}} = \frac{d\hat{T}_o}{d\hat{T}} = -\mu < 0 \quad (10)$$

A controller operating in accordance with this equation will respond to a positive control temperature deviation by acting to lower the feed temperature in order to return the control variables to their steady state values. Two important nonlinear control modes that also satisfy inequality (8) are

$$\hat{T}_o = -\mu \operatorname{sgn} \hat{T} \quad (11)$$

$$\hat{T}_o = -\mu \operatorname{sat} \hat{T} \quad (12)$$

Equations (11) and (12) are illustrated graphically in Figure 1. Equation (11) represents a relay device. Following any disturbance a relay will always bring a maximum signal to bear on a system in order to restore it to the steady state. In this sense it is the most desirable type of control to enlarge the RAS since it maximizes inequality (8). This property has been demonstrated in general for linear systems, and is not new to the automatic control literature (2). Equation (12) represents an ideal linear device that has upper and lower limits on the signal that it can produce. A saturating linear valve is typical of such devices.

It is also possible to show that derivative control can be satisfactorily utilized to increase the RAS. Consider

$$\hat{T}_o = \mu\frac{d\hat{T}}{dt} \quad (13)$$

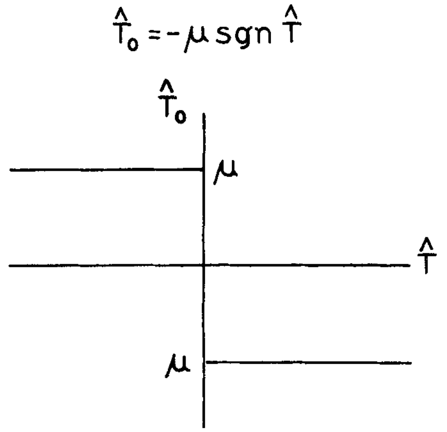
In terms of normalized variables

$$\hat{\eta}_o = \mu\frac{d\hat{\eta}}{dt} \quad (14)$$

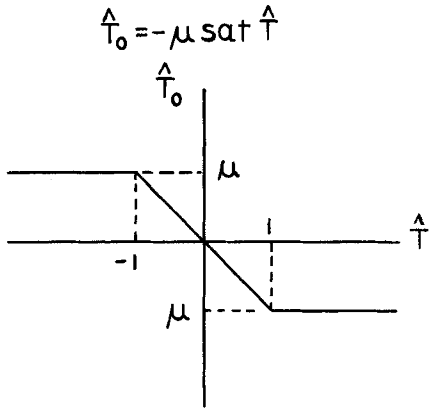
Substituting the first of Equations (2) one obtains

$$\hat{\eta}_o = \mu\left[\hat{r}/c_o - \frac{b}{a}\hat{\eta}\right] + \frac{\mu}{\tau}\hat{\eta}_o \quad (15)$$

$$\hat{\eta}_o = \left[\frac{\mu}{1 - \mu/\tau}\right]\left[\hat{r}/c_o - \frac{b}{a}\hat{\eta}\right] \quad (16)$$



THE RELAY FUNCTION



THE SATURATING FUNCTION

Fig. 1. Nonlinear control modes satisfying inequality (8).

$$\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}} = -\left[\frac{\mu}{1-\mu/\tau}\right]\left[b/a - \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}}\right] \tag{17}$$

By virtue of the first criterion for stability in the uncontrolled case (1)

$$b/a - (1/c_o)\frac{\partial\hat{r}}{\partial\hat{\eta}} > 0 \tag{18}$$

Thus derivative control will satisfactorily increase the RAS if

$$\tau > \mu > 0 \tag{19}$$

From the point of view of stability the gain on the derivative controller should be as close as possible to the flow time constant of the system without exceeding it. Just how close it is to be set is best dictated by performance criteria.

As noted above the dependence of $\hat{\eta}_o$ on $\hat{y}$ (another control function) may be studied independently. A sufficient condition for increased RAS is found from inequality (7) in which $(\partial\hat{\eta}_o)/(\partial\hat{y})$ appears. In order to strengthen this inequality the sign of the term $\left(\frac{\partial\hat{r}}{\partial\hat{\eta}}-\frac{\partial\hat{r}}{\partial\hat{y}}\right)$ must be known. The subcases are

$$\left.\begin{array}{l}
\frac{\tau}{c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}}-\frac{\partial\hat{r}}{\partial\hat{y}}\right) > \frac{\partial\hat{\eta}_o}{\partial\hat{y}} > 0, \quad \left(\frac{\partial\hat{r}}{\partial\hat{\eta}}-\frac{\partial\hat{r}}{\partial\hat{y}}\right) > 0 \\
\frac{\tau}{c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}}-\frac{\partial\hat{r}}{\partial\hat{y}}\right) < \frac{\partial\hat{\eta}_o}{\partial\hat{y}} < 0, \quad \left(\frac{\partial\hat{r}}{\partial\hat{\eta}}-\frac{\partial\hat{r}}{\partial\hat{y}}\right) < 0 \\
\frac{\partial\hat{\eta}_o}{\partial\hat{y}} = 0, \quad \left(\frac{\partial\hat{r}}{\partial\hat{\eta}}-\frac{\partial\hat{r}}{\partial\hat{y}}\right) = 0
\end{array}\right\} \tag{20}$$

For any of these subcases the greatest possible extension of the RAS will result from

$$\frac{\partial\hat{\eta}_o}{\partial\hat{y}} = \frac{\tau}{c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}}-\frac{\partial\hat{r}}{\partial\hat{y}}\right) \tag{21}$$

This last function is in essence again a statement of proportional control, but this time the proportional gain is limited in magnitude and ambiguous as to sign. Whether the feedback is to be positive or negative is fixed by the sign of $\left(\frac{\partial\hat{r}}{\partial\hat{\eta}}-\frac{\partial\hat{r}}{\partial\hat{y}}\right)$. This last point may be interpreted geometrically for any choice of $r(\hat{\eta}, \hat{y})$; $\frac{\partial\hat{r}}{\partial\hat{\eta}} = \frac{\partial\hat{r}}{\partial\hat{y}}$ will determine a line in the T, c plane. For nth order Arrhenius kinetics for example where

$$r = A\ e^{-Q/T}\ c^n \tag{22}$$

the equality $(\partial\hat{r}/\partial\hat{\eta}) = (\partial\hat{r}/\partial\hat{y})$ is valid along the parabola:

$$c = \frac{n\rho C_p}{\Delta HQ}T^2 \tag{23}$$

Above this line feedback should be positive, and below it feedback should be negative. For this specific kinetic equation it is possible to integrate Equation (21) formally. The resulting control function is

$$\hat{\eta}_o = \frac{\tau}{c_o}\left\{\left[\left(\frac{\Delta HQ}{\rho C_p\ (n+1)}\right)\frac{c}{T^2} - 1\right][\hat{r}] + \left[\left(\frac{\Delta HQ}{\rho C_p(n+1)}\right)\right]\left[\frac{c}{T^2} - \frac{c_{ss}}{T^2_{ss}}\right][r_{ss}]\right\} \tag{24}$$

This will simultaneously satisfy inequality (8) if

$$\rho C_p(n+1)\ T^2 > \Delta HQc \tag{25}$$

Geometrically this parabolic inequality further restricts the possible states in the T, c plane and may be the limiting factor in fixing the RAS. Obviously a feedback controller operating according to this equation will necessarily be a computer.

COOLANT TEMPERATURE AS A MANIPULATING VARIABLE

In many cases of practical interest reactors are heated or cooled by immersed coils or external jackets. Especially if the coolant or heating fluid undergoes a phase change (steam heated, refrigerant cooled) its temperature may be a valuable manipulating variable. Let the ambient temperature T_A be a function of reactor temperature and concentration. The normalized system equations are

$$\left.\begin{aligned} \frac{d\hat{\eta}}{dt} &= \hat{r}/c_o - \frac{b}{a}\hat{\eta} + \left(\frac{b}{a} - \frac{1}{\tau}\right)\hat{\eta}_A \\ \frac{d\hat{y}}{dt} &= -\hat{r}/c_o - \frac{1}{\tau}\hat{y} \end{aligned}\right\} \quad (26)$$

Since $\left(\frac{b}{a} - \frac{1}{\tau}\right) = (UA_R/\rho V C_p) > 0$, the analysis for this mode of control is entirely analogous to the use of feed temperature as the manipulating variable. The results are

$$\frac{\partial\hat{\eta}_A}{\partial\hat{\eta}} = \frac{\partial\hat{T}_A}{\partial\hat{T}} < 0 \quad (27)$$

$$\left.\begin{aligned} &\frac{\rho V C_p}{UA_R\, c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) > \frac{\partial\hat{\eta}_A}{\partial\hat{\eta}} > 0, \left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) > 0 \\ &\frac{\rho V C_p}{UA_R\, c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) < \frac{\partial\hat{\eta}_A}{\partial\hat{\eta}} < 0, \left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) < 0 \\ &\frac{\partial\hat{\eta}_A}{\partial\hat{\eta}} = 0, \left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) = 0 \end{aligned}\right\} \quad (28)$$

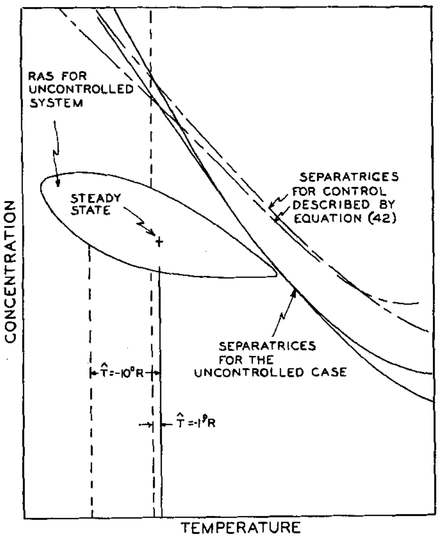


Fig. 2. The effect of heat transfer coefficient as a manipulating variable on the region of stable steady states.

INLET CONCENTRATION AS A MANIPULATING VARIABLE

The only concentration which can serve as a manipulating variable is the inlet concentration. Let

$$c_o = c_{oss} + \hat{c}_o = c_o\,(T, c) \quad (29)$$

The system equations then become

$$\left.\begin{aligned} \frac{d\hat{\eta}}{dt} &= \hat{r}/c_{oss} - \frac{b}{a}\hat{\eta} \\ \frac{d\hat{y}}{dt} &= -\hat{r}/c_{oss} - \frac{1}{\tau}\hat{y} + \frac{1}{\tau}\hat{y}_o \end{aligned}\right\} \quad (30)$$

Once again Krasovskii's theorem may be applied:

$$\mathbf{F} = \begin{bmatrix} -\left(\frac{b}{\alpha} - \frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}}\right) & \frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} \\ -\frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}} + \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{\eta}} & -\left(\frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) + \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{y}} \end{bmatrix} \quad (31)$$

$$-\hat{\mathbf{F}} = \begin{bmatrix} 2\left(\frac{b}{a} - \frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}}\right) & \frac{1}{c_{oss}}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{\eta}} \\ \frac{1}{c_{oss}}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{\eta}} & 2\left(\frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) - \frac{2}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{y}} \end{bmatrix} \quad (32)$$

The stability criteria are

$$\left.\begin{aligned} &\frac{b}{a} - \frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}} > 0 \\ &4\left(\frac{b}{a} - \frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}}\right)\left[\left(\frac{1}{c_{oss}}\frac{\partial\hat{r}}{d\hat{y}} + \frac{1}{\tau}\right) - \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{y}}\right] > \\ &\left[\frac{1}{c_{oss}}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{y}}\right]^2 \end{aligned}\right\} \quad (33)$$

In this case the first stability criterion is not affected by control; the effect of the control mode can be seen in the second criterion. For nth order Arrhenius kinetics it has been shown (*1*) that

$$\frac{1}{c_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau} > 0 \quad (34)$$

Therefore a sufficient condition for improving RAS for the system is

$$\frac{\partial\hat{y}_o}{\partial\hat{y}} = \frac{\partial\hat{c}_o}{\partial\hat{c}} < 0 \quad (35)$$

Inequality (35) represents the same type of restriction as inequality (8). Hence proportional, relay, saturating, linear, and derivative modes of control are admissible, provided the constants are appropriately restricted.

The effect of $(\hat{y}_o, \hat{\eta})$ control on the RAS is as before dependent on the sign of $\left(\frac{\partial \hat{r}}{\partial \hat{\eta}} - \frac{\partial \hat{r}}{\partial \hat{y}}\right)$. The limitations on permissible control are similar to those dictated by Equation (20).

HEAT TRANSFER COEFFICIENT AS A MANIPULATING VARIABLE

The heat transfer coefficient may be used as a manipulating variable if the coolant (or heating fluid) flow rate is made a function of some control variable. Again consider the general case of dependence on both control variables:

$$U = U_{ss} + \hat{U} = U(T, c) \tag{36}$$

The normalized system equations are

$$\left.\begin{aligned} \frac{d\hat{\eta}}{dt} &= \hat{r}/c_o - \frac{b}{a}\hat{\eta} - \hat{U}\beta A_R - \hat{U}\hat{\eta}A_R/a \\ \frac{d\hat{y}}{dt} &= -\hat{r}/c_o - \frac{1}{\tau}\hat{y} \end{aligned}\right\} \tag{37}$$

By Krasovskii's theorem

$$\mathbf{F} = \begin{bmatrix} -\left[\frac{b}{a} - \frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{\eta}} + \left(\beta A_R + \frac{A_R}{a}\hat{\eta}\right)\frac{\partial \hat{U}}{\partial \hat{\eta}} + \hat{U}A_R/a\right] & \frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{y}} - A_R\,(\beta + \hat{\eta}/a)\frac{\partial \hat{U}}{\partial \hat{y}} \\ -\frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{\eta}} & -\left(\frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{y}} + \frac{1}{\tau}\right) \end{bmatrix} \tag{38}$$

$$-\hat{\mathbf{F}} = \begin{bmatrix} 2\left[\frac{b}{a} - \frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{\eta}} + \left(\beta A_R + \frac{A_R}{a}\hat{\eta}\right)\frac{\partial \hat{U}}{\partial \hat{\eta}} + UA_R/a\right] & \frac{1}{c_o}\left(\frac{\partial \hat{r}}{\partial \hat{\eta}} - \frac{\partial \hat{r}}{\partial \hat{y}}\right) + A_R\,(\beta + \hat{\eta}/a)\frac{\partial \hat{U}}{\partial \hat{y}} \\ \frac{1}{c_o}\left(\frac{\partial \hat{r}}{\partial \hat{\eta}} - \frac{\partial \hat{r}}{\partial \hat{y}}\right) + A_R\,(\beta + \hat{\eta}/a)\frac{\partial \hat{U}}{\partial \hat{y}} & 2\left(\frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{y}} + \frac{1}{\tau}\right) \end{bmatrix} \tag{39}$$

The two stability criteria are

$$\left.\begin{aligned} &\left(\frac{b}{a} - \frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{\eta}}\right) + \left(\beta A_R + \frac{A_R}{a}\hat{\eta}\right)\frac{\partial \hat{U}}{\partial \hat{\eta}} + \frac{UA_R}{a} > 0 \\ &4\left[\frac{b}{a} - \frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{\eta}} + (\beta A_R + A_R\,\hat{\eta}/a)\frac{\partial \hat{U}}{\partial \hat{\eta}} + \frac{UA_R}{a}\right]\left[\frac{1}{c_o}\frac{\partial \hat{r}}{\partial \hat{y}} + \frac{1}{\tau}\right] > \left[\frac{1}{c_o}\left(\frac{\partial \hat{r}}{\partial \hat{\eta}} - \frac{\partial \hat{r}}{\partial \hat{y}}\right) + \right. \\ &\left. + A_R\,(\beta + \eta/a)\frac{\partial \hat{U}}{\partial \hat{y}}\right]^2 \end{aligned}\right\} \tag{40}$$

Inspection of both inequalities shows that a sufficient condition for increased RAS is

$$(\beta + \hat{\eta}/a)\frac{\partial \hat{U}}{\partial \hat{\eta}} + \hat{U}/a > 0 \tag{41}$$

For any given function $\hat{U}(\hat{\eta}, \hat{y})$ this differential inequality defines a separatrix which divides the T, c plane into two areas, an area in which stability is improved and an area in which it is made worse. The uncontrolled reactor whose stability was previously analyzed numerically (*1*) may be taken as an example. Suppose that it is desired to control the reactor by feeding back a temperature signal to regulate the coolant flow rate. Assuming that the heat transfer coefficient varies as the 0.8 power of coolant flow rate, and that the flow rate is in turn proportional to the feedback temperature, one obtains

$$\hat{U} = \lambda\,[(\eta_{ss} + \hat{\eta})^{0.8} - \eta_{ss}^{0.8}] \tag{42}$$

Substituting into inequality (41) one gets

$$0.8\beta + \frac{\eta_{ss}}{a} + \frac{1.8\hat{\eta}}{a} - \frac{\eta_{ss}^{0.8}}{a}(\eta_{ss} + \hat{\eta})^{0.2} > 0 \tag{43}$$

which has the solution

$$\hat{T} > -1°\text{R}. \tag{44}$$

This result indicates that for all temperature disturbances greater than $-1°$R. the control acts to increase the known region of stable steady states. For temperature disturbances less than $-1°$R. the control will reduce this region, as shown by the dashed separatrices in Figure 2.

The effect of this control function on the RAS will depend on whether it causes the limiting separatrix to become more or less confining to the $\mathcal{V}$ contour. It appears in Figure 2 that while this particular choice is satisfactory in expanding the RAS, it is nevertheless not the most desirable from this point of view. If by a suitable choice of feedback parameters Equation (42) can be made into proportional control, the stability picture can be improved still further. If

$$\hat{U} = \lambda\,\hat{\eta} \tag{45}$$

solution of Equation (45) with inequality (41) gives

$$\hat{T} > -10°\text{R}. \tag{46}$$

This line is also shown on Figure 2 for comparison with the previous result; the new result evidently allows more of an improvement on the RAS. For the more general case where $U = U(T, c)$ inequality (41) will not produce a vertical straight line but some more general locus in the T, c plane. As in previous cases the conditions imposed on the second contribution of the general function $U(T, c)$ will depend on the sign of $\left(\frac{\partial \hat{r}}{\partial \hat{\eta}} - \frac{\partial \hat{r}}{\partial \hat{y}}\right)$.

COMBINATION CONTROL

There may arise certain circumstances under which it is advantageous to control a chemical reactor by more than one manipulating variable. It is therefore of interest to see how combination control affects reactor stability. When one considers the case of feed temperature and concentration as simultaneous manipulating variables, the normalized state equations are

$$\left.\begin{aligned} \frac{d\hat{\eta}}{dt} &= \hat{r}/C_{oss} - \frac{b}{a}\hat{\eta} + \frac{1}{\tau}\hat{\eta}_o \\ \frac{d\hat{y}}{dt} &= -\hat{r}/C_{oss} - \frac{1}{\tau}\hat{y} + \frac{1}{\tau}\hat{y}_o \end{aligned}\right\} \qquad (47)$$

Then

$$\mathbf{F} = \begin{bmatrix} \left(\frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{b}{a} + \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}}\right) & \left(\frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{y}}\right) \\ \left(-\frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}} + \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{\eta}}\right) & -\left(\frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau} - \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{y}}\right) \end{bmatrix} \qquad (48)$$

$$-\hat{\mathbf{F}} = \begin{bmatrix} 2\left(\frac{b}{a} - \frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}}\right) & \frac{1}{C_{oss}}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\left(\frac{\partial\hat{y}_o}{\partial\hat{\eta}} + \frac{\partial\hat{\eta}_o}{\partial\hat{y}}\right) \\ \frac{1}{C_{oss}}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\left(\frac{\partial\hat{y}_o}{\partial\hat{\eta}} + \frac{\partial\hat{\eta}_o}{\partial\hat{y}}\right) & 2\left(\frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau} - \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{y}}\right) \end{bmatrix} \qquad (49)$$

The stability criteria are

$$\left.\begin{aligned} &\frac{b}{a} - \frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}} > 0 \\ &4\left(\frac{b}{a} - \frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{\partial\hat{\eta}_o}{\partial\hat{\eta}}\right)\left(\frac{1}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau} - \frac{1}{\tau}\frac{\partial\hat{y}_o}{\partial\hat{y}}\right) > \\ &\left[\frac{1}{C_{oss}}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \frac{1}{\tau}\left(\frac{\partial\hat{y}_o}{\partial\hat{\eta}} + \frac{\partial\hat{\eta}_o}{\partial\hat{y}}\right)\right]^2 \end{aligned}\right\} \qquad (50)$$

By inspection two previously derived criteria fall out immediately:

$$\left.\begin{aligned} \frac{\partial\hat{\eta}_o}{\partial\hat{\eta}} &= \frac{\partial\hat{T}_o}{\partial\hat{T}} < 0 \\ \frac{\partial\hat{y}_o}{\partial\hat{y}} &= \frac{\partial\hat{c}_o}{\partial\hat{c}} < 0 \end{aligned}\right\} \qquad (51)$$

The use of the combination control is particularly valuable in establishing criteria for the hybridized modes, where a concentration variable is used to control temperature and vice versa. In this case the hybridized modes appear as $\left(\frac{\partial\hat{\eta}_o}{\partial\hat{y}}\right)$ and $\left(\frac{\partial\hat{y}_o}{\partial\hat{\eta}}\right)$ Of the several possible interpretations one can be selected for illustration. Let

$$\frac{\tau}{C_{oss}}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) - \left(\frac{\partial\hat{y}_o}{\partial\hat{\eta}} + \frac{\partial\hat{\eta}_o}{\partial\hat{y}}\right) = 0 \qquad (52)$$

This is one way in which the second of inequalities (50) may be strengthened. Associate each hybridized mode with the rate term differentiated with respect to the same variable:

$$\left.\begin{aligned} \frac{\partial\hat{y}_o}{\partial\hat{\eta}} &= +\frac{\tau}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{\eta}} \\ \frac{\partial\hat{\eta}_o}{\partial\hat{y}} &= -\frac{\tau}{C_{oss}}\frac{\partial\hat{r}}{\partial\hat{y}} \end{aligned}\right\} \qquad (53)$$

Equations (53) may be restated as

$$\left.\begin{aligned} \frac{\partial\hat{c}_o}{\partial\hat{T}} &= +\tau\frac{\partial\hat{r}}{\partial\hat{T}} \\ \frac{\partial\hat{T}_o}{\partial\hat{c}} &= -\frac{\tau\,\Delta H}{\rho C_p}\frac{\partial\hat{r}}{\partial\hat{c}} \end{aligned}\right\} \qquad (54)$$

Integrating each equation from the steady state one obtains

$$\left.\begin{aligned} \hat{c}_o &= +\tau\hat{r} \\ \hat{T}_o &= -\frac{\tau\,\Delta H}{\rho C_p}\hat{r} \end{aligned}\right\} \qquad (55)$$

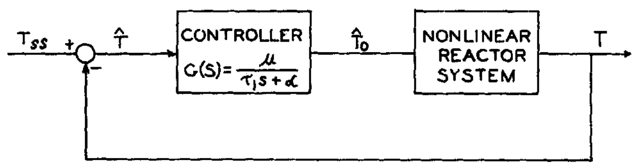


Fig. 3. Closed loop block diagram for a first-order controller.

Equations (55) suggest that improved stability can be achieved by proportional control of the manipulating variables through the chemical reaction rate. The analysis to this point places no restriction on the form of the rate equation. Again it is clear that a high speed computer is called for in computing the rate from the measured variables.

HIGHER ORDER CONTROL MODES

The control functions which have been considered do not affect the order of the system, but it is not difficult to extend the arguments to the case of a controller which can be represented by a first order transfer function as shown in Figure 3. The treatment given here will be general for a third-order system. The three equations are

$$\left.\begin{aligned}
\frac{d\hat{\eta}}{dt} &= \hat{r}/c_o - \frac{b}{a}\hat{\eta} + \frac{1}{\tau}\hat{\eta}_o \\
\frac{d\hat{y}}{dt} &= -\hat{r}/c_o - \frac{1}{\tau}\hat{y} \\
\frac{d\hat{\eta}_o}{dt} &= -(\mu/\tau_1)\hat{\eta} - (\alpha/\tau_1)\hat{\eta}_o
\end{aligned}\right\} \tag{56}$$

For simplicity the analysis will be restricted to the case of $\hat{\eta}_o$ as a function of only $\hat{\eta}$. By Krasovskii's theorem the **F** and $\hat{\mathbf{F}}$ matrices will be third order

$$\mathbf{F} = \begin{bmatrix}
\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{b}{a} + \frac{1}{\tau}\frac{d\hat{\eta}_o}{d\hat{\eta}}\right) & \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} & \frac{1}{\tau} \\
-\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} & -\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) & 0 \\
-\frac{\mu}{\tau_1} - \frac{\alpha}{\tau_1}\frac{d\hat{\eta}_o}{d\hat{\eta}} & 0 & -\frac{\alpha}{\tau_1}
\end{bmatrix} \tag{57}$$

$$-\hat{\mathbf{F}} = \begin{bmatrix}
2\left(\frac{b}{a} - \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{d\hat{\eta}_o}{d\hat{\eta}}\right) & \frac{1}{c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) & \left(\frac{\mu}{\tau_1} - \frac{1}{\tau} + \frac{\alpha}{\tau_1}\frac{d\hat{\eta}_o}{d\hat{\eta}}\right) \\
\frac{1}{c_o}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right) & 2\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) & 0 \\
\frac{\mu}{\tau_1} - \frac{1}{\tau} + \frac{\alpha}{\tau_1}\frac{d\hat{\eta}_o}{d\hat{\eta}} & 0 & \frac{2\alpha}{\tau_1}
\end{bmatrix} \tag{58}$$

There will now be three basic stability criteria:

$$\left.\begin{aligned}
&\frac{b}{a} - \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{d\hat{\eta}_o}{d\hat{\eta}} > 0 \\
&4\left(\frac{b}{a} - \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{d\hat{\eta}_o}{d\hat{\eta}}\right)\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) > \frac{1}{c_o^2}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right)^2 \\
&8\frac{\alpha}{\tau_1}\left(\frac{b}{a} - \frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{1}{\tau}\frac{d\hat{\eta}_o}{d\hat{\eta}}\right)\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) > 2\left(\frac{\mu}{\tau_1} - \frac{1}{\tau} + \frac{\alpha}{\tau}\frac{d\hat{\eta}_o}{d\hat{\eta}}\right)^2 \\
&\left(\frac{1}{c_o}\frac{\partial\hat{r}}{\partial\hat{y}} + \frac{1}{\tau}\right) + \frac{2\alpha}{\tau_1 c_o^2}\left(\frac{\partial\hat{r}}{\partial\hat{\eta}} - \frac{\partial\hat{r}}{\partial\hat{y}}\right)^2
\end{aligned}\right\} \tag{59}$$

The first two are similar to inequalities (6) and (7). A sufficient condition for increased RAS is

$$\frac{d\hat{\eta}_o}{d\hat{\eta}} < 0 \tag{60}$$

A judicious choice of control function would be

$$\frac{d\hat{\eta}_o}{d\hat{\eta}} = \frac{1}{\alpha}\left(\frac{\tau_1}{\tau} - \mu\right) \tag{61}$$

since this would reduce the third of inequalities (59) to the second, leaving inequality (60) as the only restriction on the controller.

It is of some interest to consider the limiting case as α goes to zero and the system is subjected to pure integral control. In the limit the third criterion of (59) becomes

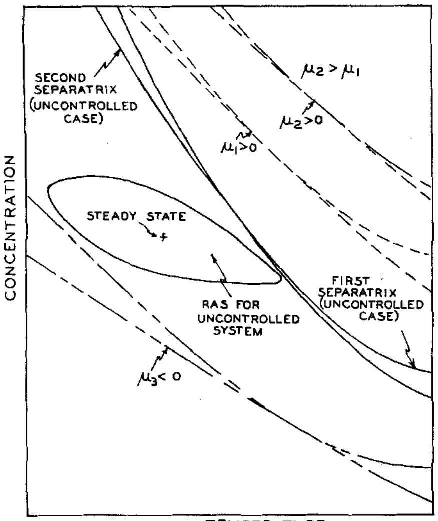


Fig. 4. The effect of proportional control $\hat{T}_o = -\mu\hat{T}$ on the region of stable steady states.

$$0 > (\mu/\tau_1 - 1/\tau)^2 \left(\frac{1}{c_o} \frac{\partial \hat{r}}{\partial \hat{y}} + \frac{1}{\tau} \right) \qquad (62)$$

This inequality can only be satisfied if $(\partial \hat{r}/\partial \hat{y}) < 0$, a relatively rare occurrence. In more usual cases the stability of the system when subjected to integral control will be indeterminate by this Liapunov function.

DISCUSSION

Above all it should be emphasized that the various criteria developed above apply only to stability considerations. No conclusions can be drawn from this analysis with regard to system performance. Perhaps the greatest utility of these results is in indicating what control functions might provide fruitful areas for a performance investigation. Furthermore a guarantee of asymptotic stability is useful to the designer, since he can be assured that results of a linearized analysis will not lead to unexpected limit cycles or unstable behavior.

Another consideration of importance relates to the Liapunov function modifications that would result from any control choice. Analytically the proper Liapunov function is found by Equation (5). In general the effect of a control mode on the form of this function would have to be ascertained in detail if the extended RAS were needed numerically.

In all the cases considered above hybridized control depends primarily on what may be termed a relative reaction sensitivity, $\left(\frac{\partial \hat{r}}{\partial \hat{\eta}} - \frac{\partial \hat{r}}{\partial \hat{y}} \right)$ In order to utilize hybridized control effectively the kinetics of the reaction must be known, and facilities must be available to calculate the relative reaction sensitivity. In effect this will usually mean a high speed computer, probably an analogue. Some simplification of hybridized control may be achieved by using combination control, as was shown.

Two interesting observations can be made with respect to the nonhybridized proportional control modes with $\hat{\eta}_o$ and $\hat{y}_o$ as manipulating variables. In the temperature control case it can be seen from Figure 4 that the system will always possess an RAS regardless of gain $\mu > 0$. As the gain becomes infinite, the system becomes globally stable. This result is not unexpected, since second-order linear systems are always stable when subjected to negative linear feedback. Apparently this nonlinear system possesses this same property. The system stability becomes indeterminate if the feedback is made sufficiently positive as is also shown in Figure 4.

The nonhybridized concentration control exhibits somewhat different behavior. From inequalities (33) it is evident that this control mode affects the second stability criterion but not the first stability criterion. Interpreted graphically this means that by increasing the proportional gain the second separatrix can be moved in the T, c plane until the first separatrix becomes the limiting stability boundary. From a stability point of view there is no reason to increase the proportional gain in this control mode past the point where the first separatrix becomes the limiting factor; however performance considerations may require this.

ACKNOWLEDGMENT

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NOTATION

A	=	frequency factor
A_R	=	reactor area
a	=	$\rho V C_p$
b	=	$UA_R + \rho q C_p$
C_p	=	specific heat
c	=	concentration
$\mathbf{F}$	=	Jacobian matrix
$\hat{\mathbf{F}}$	=	$\mathbf{F} + \mathbf{F}^T$
ΔH	=	heat of reaction
n	=	order of reaction
Q	=	activation energy divided by the gas constant
q	=	volumetric flow rate
r	=	rate of reaction per unit volume
T	=	temperature
t	=	time
U	=	overall heat transfer coefficient
V	=	reactor volume
$\mathcal{V}$	=	Liapunov function
y	=	(c/c_o), normalized concentration

Greek Letters

α	=	symbol in Figure 4
β	=	$(T_{ss} - T_A)/\Delta H V c_o$
η	=	$(\rho C_p/\Delta H c_o)T$, normalized temperature
λ	=	proportionality constant
ρ	=	density
τ	=	V/q, flow time constant
τ_o	=	$\rho V C_p/UA_R$
τ_1	=	controller time constant

Subscripts and Superscripts

$\wedge$	=	deviation from steady state
ss	=	steady state
A	=	heat sink
o	=	input
T	=	transpose

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