Input Multiplicities in Nonlinear, Multivariable Control Systems

Input multiplicities in process control occur when more than one set of manipulated parameters m can produce the desired steady state outputs c. They are directly related to the stability and desirability of any intended loop pairing of m's and c's. A chemical reactor example illustrates the phenomena.

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SCOPE

This work is a study of the significance of the singularity condition of catastrophe theory in the design of nonlinear multivariable control systems. It explores the relationships among three concepts: the catastrophe condition; a widely used index of interaction developed by Bristol; and, the stability of a limiting version of typical industrial control systems.

Recent studies of multiple steady-state phenomena have produced interesting examples of such behavior in chemical engineering systems. In the typical framework, the process is assumed to be described by an equation of the form $f(x,a) = 0$, where a is a set of parameters and x is a set of process state variables. For example, in a stirred-tank reactor a may consist of parameters such as residence time, coolant temperature, activation energy, reaction velocity constant, etc., while x consists of the resulting steady-state concentration and temperature. Catasrophe theory has been shown to be very useful in delineating values of the parameters set a which can produce multiple steady states; i.e., at which more than one value of x will satisfy $f(x,a) = 0$.

In the process control framework, elements of the variables x are typically noted as output or controlled variables c, while those elements of the parameters a which are adjustable during operation are regarded as the manipulated variables m. In this nomenclature, $f(c,m) = 0$. In most applications, c and m each contain the same number of variables. These are paired, according to some control strategy, into feedback loops in which one of the manipulated variables m_j is manipulated to hold one of the controlled variables c_i at a desired value. Reset (integral) action is usually included in each loop. Under these circumstances, it is operationally impossible for the process to reach more than one steady state value of c, despite the existence of such alternate steady states. Alternate steady-states are eliminated by the integral action in the feedback controllers, which can come to rest only at the desired value of c.

In this work, we reverse the original question and ask whether more than one set of parameters a can produce the same values of the process state variables x. Mathematically, this is simply an interchange of nomenclature between a and x. However, in the process control framework, we are now asking whether more than one set of manipulated variables m can produce the same values of the controlled variables c. This is a conceptually different question. If such multiplicity can exist, the ramifications for process control are of great importance. The typical feedback control scheme described above can conceivably operate at any of these multiple steady states. Further, it may be difficult, if not impossible, for plant operating personnel to detect such an occurrence. This is true first because we usually monitor and record values of c, but not of m; and second because we expect the integral action to reset the values of m to overcome the effects of permanent, unmeasured disturbances. However, we neither expect nor desire such resetting if there have been no such disturbances.

The paring mentioned above, of components of c and m into feedback loops, has always been a key subject of process control. Bristol (1966) has developed a relative gain array, whose elements are sometimes referred to as interaction indices, as a useful guide in this pairing process. The relative gain array is constructed from the matrix of process gains $(\partial c/\partial m)$, and involves the inverse of this matrix. If the process gain matrix is singular, no information about loop pairing can be obtained from the relative gain array. But, a singularity of $(\partial c/\partial m)$ is one of the tests used by catastrophe theory to detect the possible existence of the input multiplicities discussed above. A study of this suggested relationship between loop pairings and input multiplcities is therefore a further objective of this work.

CONCLUSIONS AND SIGNIFICANCE

The process gain matrix $\partial c/\partial m$ for a nonlinear multivariable system may become singular at some steady states. A physical example of this occurrence is given for a stirred-tank chemical reactor. Under such conditions, catastrophe theory indicates the possibility of input multiplicity. More than one set of manipulated variable m may produce the same steady-state values of the controlled variables c. Bristol's relative gain array is not defined when $\partial c/\partial m$ is singular, and thus gives no direct guidance on loop pairings.

Exact mathematical singularity of a matrix of partial derivatives of an approximate process model is a somewhat hypothetical occurrence. Therefore, it is necessary to examine the behavior of process control in the general vicinity of such indicated singularities of $\partial c/\partial m$. This can be done by examining the stability of a limiting case. For some chosen single-loop feedback pairings of c and m variables, it is assumed that very slow reset action is used in each loop, and the stability of the resulting movements between quasi-steady-states is examined in the time domain. A further condition, called plausibility, is added. This condition requires that each of the individual feedback loops have limiting stability. A necessary condition for simultaneous stability and plausibility is derived. The catastrophe condition arises naturally as the boundary of this necessary condition. It then follows that a given pairing can be both stable and plausible only on one side of the catastrophe boundary. This boundary, together with other related boundaries, is shown to divide the control space into the regions in which different pairings can be simultaneously stable and plausible.

A simple necessary condition for stability and plausibility, Eq. 18, gives important information about any desired multi-

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variable pairing. This condition can be evaluated from only a steady-state process model; dynamic information is unnecessary.

The ultimate danger under the existence of input multiplicities is the undetected transition of the process control system from one steady-state to another. Such an example is illustrated for a chemical reactor. The example is then analyzed in terms of the aforementioned stability-plausibility regions.

The results indicate the necessity of careful examination of the process steady-state behavior to detect any input multiplicities, before deciding on a control strategy. The possibility of an undetected transition to an unanticipated, and perhaps economically undesirable, steady-state operating condition is best eliminated at the system design stage.

STATEMENT OF THE PROBLEM

We will be concerned here only with the steady-state behavior of the process, and not its dynamics. Temporarily, we assume an explicit functional dependence for this steady-state behavior

$$c = c(m) \tag{1}$$

where c is a vector of n functions of time, which represent the plant variables to be controlled, and m is a vector of n functions of time, which represent the plant variables which will be manipulated to achieve control of c. In typical process terms, m represents the valve positions and c the instrument feedback signals.

In many situations, explicit dependence to represent the steady-state behavior may not be available, and we have instead the more general relationship

$$f(c,m) = 0 \tag{2}$$

where f is a vector of n functional relations between the components of c and of m. We defer discussion of this situation to later.

The form of control to be analyzed is at first appearance very restrictive. Specifically it is

$$m(t) = G_r \int_0^t [c^* - c(t')]dt' + m_0 \tag{3}$$

where c^* is a constant vector whose n components represent the desired steady-state values of the corresponding components of c; G_r is a diagonal matrix of n reset rates, g_i;

$$G_r = \begin{pmatrix} g_1 & & & \\ & g_2 & & 0 \\ & & \ddots & \\ 0 & & & g_n \end{pmatrix} \tag{4}$$

m_0 is an arbitrary initial value of m; and, t' is an integration variable. Physically, this control represents single-loop pairings of the manipulated variables m with the controlled variables c, and use of pure integral feedback control in each loop. Henceforth, we assume without loss of generality that the components of c and m have been ordered to match the intended pairings indicated by the control action in Eq. 3.

Discussion of this restricted form of control is in order. It is similar to that used by Bristol (1966) in the discussion of his well-known interaction index, μ. It is of interest for several reasons. Reset or integral feedback action is used in most process control situations to assure precise control at steady state, despite undetectable changes in various loads which might otherwise alter the steady-state conditions. Too, Eq. 3 is a limiting representation of the behavior of the usual two-mode (proportional-plus-reset) and three-mode (proportional-plus-reset-plus-derivative) control actions used in the loops of single-loop pairing strategies. These strategies are frequently used in multivariable process control situations. The limit referred to occurs when all the reset rates, g_i, are sufficiently small that the rates at which the reset control changes the manipulated variables $m(t)$ are much slower than the process dynamics. In other words, at the limit very slow reset action has been superimposed on the proportional and/or derivative control actions. The purpose of such slow reset is simply to trim the long-term steady-state of the process to the desired conditions. As an example, a reset rate of one repeat per hour might be used in a loop with a process whose largest effective time constant is a few seconds. Under these conditions, process dynamics and the other control modes are unimportant in analyzing the reset behavior, since their transients finish very quickly relative to the rate of movement of the manipulated variables by the reset control. For practical purposes the reset control moves the process through a series of quasi-steady-states, hopefully on the way to the desired steady state c^*. One feels intuitively that, unless the desired steady state can be reached in an orderly manner by this very slow reset control, one cannot be optimistic about the performance of the system when more rapid reset rates are used. It is conceivable that, for a particular transient, process dynamics and the reset transients could interact favorably and produce a total response more favorable than that of the reset control alone. But, in general, if the very slow reset action produces unstable behavior, one would not wish to risk much on the hope that increasing its speed, and thereby exciting the process dynamics, will improve the situation. Finally, there is at least one physically important situation in which very slow reset control finds frequent application. This is cascade control in which the outer loop involves a very slow measurement, such as by a chromatograph. This composition measurement is used in a feedback manner to reset the set point of the inner controller. The inner controller maintains close transient control of a secondary process variable, such as temperature, whose value is only a rough indicator of composition, but is quickly measurable.

We will begin by analyzing the stability of the slow reset control action of Eq. 3, when applied to the general nonlinear process described by Eq. 1. This analysis will ultimately lead us to consideration of multiple-steady-phenomena of concern for process control, namely, input multiplicities. The result is equivalent to one derived by Niederlinski (1971), but arises from physical arguments amplifying the relationship to input multiplicity.

STABILITY ANALYSIS

Differentiation of Eq. 3 with respect to time yields

$$\frac{dm}{dt} = G_r(c^* - c) \tag{5}$$

Substitution from Eq. 1 yields

$$\frac{dm}{dt} + G_r c(m) = G_r c^* \tag{6}$$

The nonlinearity of $c(m)$ prevents general stability analysis of Eq. 6. We use instead the typical technique of linearization around steady-state

$$c(m) \approx c^* + \frac{\partial c}{\partial m}(m - m^*) \tag{7}$$

where

$$\frac{\partial c}{\partial m} = \begin{Bmatrix} \frac{\partial c_1}{\partial m_1} & \frac{\partial c_1}{\partial m_2} & \cdots & \frac{\partial c_1}{\partial m_n} \\ \frac{\partial c_2}{\partial m_1} & \frac{\partial c_2}{\partial m_2} & \cdots & \frac{\partial c_2}{\partial m_n} \\ \vdots & \vdots & & \vdots \\ \frac{\partial c_n}{\partial m_1} & \frac{\partial c_n}{\partial m_2} & \cdots & \frac{\partial c_n}{\partial m_n} \end{Bmatrix} \tag{8}$$

is the Jacobian matrix of partial derivatives evaluated at the desired steady-state c^*. The elements of $\partial c/\partial m$ are the local steady-state gains of the process. The elements of m^* are steady-state values of the manipulated variables m which will produce the desired values c^*. Defining the usual deviation variable

$$M = m - m^* \tag{9}$$

and substituting Eq. 7 into Eq. 6, we obtain in a straight-forward manner

$$\frac{dM}{dt} = -G_r \frac{\partial c}{\partial m} M \tag{10}$$

This equation describes the transient behavior of the control system, when it is very close to the desired steady-state.

As is well-known from stability theory, the necessary and sufficient condition for Eq. 10 to be stable is that all eigenvalues of the matrix $G_r(\partial c/\partial m)$ have positive real parts. Stability of the locally valid Eq. 10 is necessary, but not sufficient, for stability of the original nonlinear Eq. 6. Nevertheless, necessary conditions will be adequate for our purposes, since Eq. 6 itself only represents a limiting behavior of the intended control system. As discussed above, we do not mathematically demonstrate that stability of Eq. 6 is even a necessary condition for stability of a more likely control system in which the reset rates are sufficient to excite the process dynamics. Therefore, there would be little point establishing sufficient conditions for stability of Eq. 6, even in the unlikely event this could be achieved.

The necessary stability condition involves the $n \times n$ matrix $G_r(\partial c/\partial m)$, which depends both on the process properties through $\partial c/\partial m$, and also on the particular choice of the reset gains g_i. It is desirable to eliminate this dependence on the particular values of g_i, and relate the stability condition only to the process itself through $\partial c/\partial m$. To this end, and for physical reasons, we will define a further desirable aspect of the control scheme of Eq. 3, and will refer to it as plausibility.

The gains on the diagonal of $\partial c/\partial m$ represent the direct process gains, i.e., the gains between the pairs of manipulated and controlled variables which have been selected as pairs for the individual control loops. In tuning each of the individual loops, most engineers will naturally insist that the overall gain of each individual loop be positive. Mathematically, this is stated

$$g_i \frac{\partial c_i}{\partial m_i} > 0 \qquad i = 1, 2, \ldots, n \tag{11}$$

and will be referred to as the ***plausibility*** condition. It is true that stability of Eq. 6 can be achieved by using reset control gains g_i which do not satisfy this condition. A physical example of this will be demonstrated later. However, if the condition is violated for any loop, then that loop is dependent for its stability on interaction with the other closed loops. If the other loops were opened to manual control for any reason, the offending loop would be unstable because its controller gain would have the wrong sign; i.e., would produce positive feedback. We will assume this to be a physically undesirable situation, and therefore exclude it from consideration on plausibility grounds.

It is clear that plausibility is closely related to integrity. This latter property guarantees stand-alone stability of each of the individual loops in a multivariable control system. It is a stronger property than plausibility, because of the definite statement of stability. Plausibility guarantees only *limiting* stand-alone stability of each of the individual loops. In fact, all plausibility says is that the sign of the reset gain is the same as that which would be needed for integrity. However, in contrast to integrity, plausibility makes no statement about the magnitude of the reset gain. The arbitrary nonlinearity of the process assumed here prevents magnitude statements. Therefore, a different term is useful to emphasize the relative weakness of this property. We now proceed to derive necessary conditions for both stability *and* plausibility, which conditions will depend only on properties of the process through $\partial c/\partial m$.

Well-known properties of the eigenvalues of a $(n \times n)$ matrix A are (Halmos, 1958)

$$|A| = \sum_{i=1}^{n} \lambda_i$$

$$\mathrm{tr}\, A = \sum_{i=1}^{n} \lambda_i \tag{12}$$

where $|A|$ is the determinant, tr A is the trace, or the sum of all n diagonal terms, and $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the n eigenvalues, not necessarily distinct. From Eq. 12 it follows that necessary conditions for all eigenvalues of a real matrix A to have positive real parts are

$$|A| > 0 \qquad \mathrm{tr}\, A > 0 \tag{13}$$

We have noted above that necessary conditions for stability of Eq. 6 are that all eigenvalues of $G_r \partial c/\partial m$ have positive real parts. Applying Eq. 13 to this matrix we obtain

$$|G_r| \cdot \left|\frac{\partial c}{\partial m}\right| > 0$$

$$g_1 \frac{\partial c_1}{\partial m_1} + g_2 \frac{\partial c_2}{\partial m_2} + \ldots + g_n \frac{\partial c_n}{\partial m_n} > 0 \tag{14}$$

The second of these conditions is already guaranteed by the assumption of plausibility, and may be eliminated from further consideration. Since G_r is diagonal, the first condition may be simplified to

$$(g_1 g_2 \ldots . g_n) \cdot \left|\frac{\partial c}{\partial m}\right| > 0 \tag{15}$$

We now further use the plausibility assumption to eliminate the product involving the gain. Define the matrix $(\partial c/\partial m)_+$ as follows: If the ith diagonal term of $\partial c/\partial m$ is negative, multiply each term in the ith column of $\partial c/\partial m$ by (-1); otherwise leave the ith column unchanged. Thus, $(\partial c/\partial m)_+$ is a version of $\partial c/\partial m$ in which all diagonal terms have been made positive. Multiplication of a column of a determinant by a constant is equivalent to multiplying the value of the determinant by that constant. Hence,

$$\left|\left(\frac{\partial c}{\partial m}\right)_+\right| = (1)^p \left|\frac{\partial c}{\partial m}\right| \tag{16}$$

where p is the number of diagonal terms in $\partial c/\partial m$ which were negative. By the plausibility condition in Eq. 11, the gain g_i corresponding to each of these originally negative diagonal terms must be negative, and other gains must all be positive. Therefore we may write

$$(g_1 g_2 \ldots g_n) = (-1)^p \cdot |g_1| \cdot |g_2| \ldots . |g_n| \tag{17}$$

Substitution of Eqs. 16 and 17 into Eq. 15 yields the final form of the necessary condition for stability and plausibility

$$\left|\left(\frac{\partial c}{\partial m}\right)_+\right| > 0 \tag{18}$$

As desired, this condition depends only on properties of the process.

Mathematically, $(\partial c/\partial m)_+$ is a process gain matrix resulting from a transformation of $(\partial c/\partial m)$. This transformation makes every diagonal gain element have a positive value. There is a simple physical explanation of the transformation, and of the process gain matrix $(\partial c/\partial m)_+$, relative to the original process gain matrix $(\partial c/\partial m)$. The matrix $(\partial c/\partial m)_+$ is that which would result if the physical control system were designed so that each of the loops needed a positive controller gain for plausibility, i.e., for stand-alone stability. This could hypothetically be done, for example, through appropriate selection of air-to-open vs. air-to-close valves for each loop. Obviously, the selection of valve types is based on more important considerations, such as a fail-safe situation in the event of loss of valve-motive power. However, the point is that the inherent stability of a control system is obviously unaffected by change of one of the control valves from one type to another. Such a change merely requires a change in the sign of the corresponding controller gain, and most newer instruments provide facility for this change in sign of the gain. Thus, stability results based on the special case in which all loops are designed for positive controller gains, i.e., based on $(\partial c/\partial m)_+$, must yield the correct conclusion for stability of every other possible case.

Equation 18 may be easily checked for alternative pairings. Switching pairings between any two loops is equivalent to interchanging the columns of $\partial c/\partial m$ corresponding to these two loops. This will change the sign of $|(\partial c/\partial m)|$. However, it may be necessary to multiply one or both of the interchanged columns by (-1) in forming $|(\partial c/\partial m)_+|$, to satisfy plausibility. Each such multiplication effects a further sign change. Thus, for alternative pairings the only possible change in $|(\partial c/\partial m)_+|$ is in the sign, making such tests computationally quite simple.

RELATION WITH BRISTOL's INTERACTION INDEX

Bristol (1966) has developed an interaction index which has gained widespread recognition for its utility in analyzing multivariable control situation. The elements of Bristol's μ matrix for a linearized representation of the process of Eq. 1, are calculated according to

$$\mu_{ij} = \left(\frac{\partial c}{\partial m}\right)_{ij} \left[\left(\frac{\partial c}{\partial m}\right)^{-1}\right]^T_{ij} \tag{19}$$

In other words, the ij element of μ is the product of the corresponding elements in two matrices: $\partial c/\partial m$, and the matrix resulting from $\partial c/\partial m$ by inverting and then transposing. The value of μ_{ij} gives some insight into the desirability of pairing c_i and m_j in one of the n control loops. Bristol's index is also called the relative gain array, and can give further insight, particularly for linear systems, than will be discussed here. But, we can note from Eq. 19 that the determinant $|\partial c/\partial m|$, used in the stability arguments above, also appears in the denominator of each element of μ. This occurs in the calculation of the inverse of the process matrix.

THE CATASTROPHE CASE

If $|(\partial c/\partial m)_+|$ is zero, Eq. 18 fails to conclude anything about the nonlinear system behavior. The only conclusion which can be reached is from Eq. 12 which shows that the linearized system, Eq. 10, has at least one zero eigenvalue and is therefore marginally stable. From the definition of $(\partial c/\partial m)_+$, it is clear that its determinant can differ from that of $\partial c/\partial m$ by at most a sign. Therefore, if $|(\partial c/\partial m)_+|$ is zero, so must be $|(\partial c/\partial m)|$. The borderline condition can therefore be rewritten more simply as

$$\left|\frac{\partial c}{\partial m}\right| = 0 \tag{20}$$

When Eq. 20 is true, Bristol's index μ is also undefined, as may be seen from Eq. 19. Thus, neither Bristol's index nor the stability approach gives any information about the potential performance of the chosen pairing of c and m variables.

Equation 20 has further significance, defined by the mathematics of catastrophe theory. Recent discussions of this theory have appeared in the chemical engineering literature (Chang and Calo, 1979; Chang and Calo, 1980; Calo and Chang, 1980; Aris, 1979). The reader is referred to these works for a more in-depth discussion of the mathematics, and also illustrative applications of catastrophe theory. For our purposes, it will be sufficient to note that whenever Eq. 20 is true we must consider the possibility of multiple steady states. We cannot be confident that the inverse function of $c(m)$, namely $m(c)$, exists as a one-to-one mapping from values of c to values of m. In physical terms, there may be more than one set of manipulated variables m which can produce the same, desired, steady state variable c. Therefore, Eq. 20 will be referred to as the catastrophe condition.

We will call this form of multiple steady states *input* multiplicity. This is to distinguish it from previous applications in which the multiplicity was visualized in a form in which one value of m could produce more than one set of steady-state values of c. The existence of this latter form of multiplicity may not be of great concern in the design of control systems. Reset feedback action is included in most process control systems. This action will not allow the control system to come to rest at any but the desired steady state value of c. For example, consider the classical continuous stirred tank reactor studied by Aris and Amundson (1958) and shown to have multiple steady states. Uppal et al. (1974) and Chang and Calo (1979) have further developed and explored this system. The seemingly simple case of a first-order, irreversible, exothermic reaction, with heat removal, has been shown to have a fascinating multiplicity of steady states. The same values of heat removal and residence time can produce more than one set of values of steady-state temperature and concentration in the reactor. However, if we consider this example in a control system framework, we would probably regard heat removal and residence time as manipulations m, and reactor temperature and concentration as controlled variables c. If reset feedback is used in the controllers, only one of the multiple values of c is a possible rest point of the control system, namely, the value which is used for the set points of the reset feedback controllers. Even if such reset action is not used, this form of multiplicity has a built-in observability in the process control framework. Since the control system monitors, and usually records, values of c, existence of multiple values of c can be observed from process operating data.

The possible existence of input multiplicity is a cause for considerable concern in the design of control systems. Suppose the reverse of the above example were true for some system. Namely, more than one set of values of the residence time and heat removal, m, could produce the desired set of reactor conditions (temperature and concentration), c. If so, pitfalls exist even when reset feedback control is used. The control system can conceivably come to rest at any of the possible steady states, as may be seen from Eq. 3. The economics of these steady states may differ considerably. In the reactor example, we would have different production rates and different utility costs at the different steady states. Further, operating plants do not normally monitor and record values of m. This would make difficult the detection of input multiplicity from plant operating data. To make matters worse, even if we elect to record values of m in an effort to detect input multiplicity, success may be elusive. This is because of the very nature of why we use, and what we expect from, reset feedback control. Specifically, we expect that permanent and unmeasured load changes will occur in the operating environment of the plant. We employ the reset feedback primarily to overcome the effects of these inevitable load changes. It does this by resetting the steady-state values of m to values necessary to maintain the original, desired, steady-state values of c. This is not input multiplicity. Instead, it is a recognition that the process models of Eqs. 1 and 2 are incomplete. The complete form would be $f(c,m,u) = 0$, where u represents the load variables. Therefore, if we wish to detect input multiplicity by simply observing m from operating data, we must apparently be prepared to monitor and record all disturbances u which might affect c. This is unrealistic for obvious reasons.

To recapitulate, the occurence of the condition in Eq. 20, namely vanishing of the Jacobian determinant, prevents conclusions about the performance of potential control system pairings from either arguments about the stability of slow reset control or from Bristol's index. Furthermore, it raises the possibility of input multiplicity, a phenomenon which must be of concern for control system design. Thus, the condition is centrally important in nonlinear multivariable process control.

Exact satisfaction of Eq. 20 is of course unlikely in physical applications. A very small numerical value of $|(\partial c/\partial m)|$ is also meaningless, because the quantity is dimensional and thus affected by scale choices such as system of units. We could define a normalized dimensionless value, for example by dividing by the product of all terms on the diagonal. However, for our purposes it is sufficient merely to seek changes in the sign of $|(\partial c/\partial m)|$. If we differentiate the process model of Eq. 1 at a variety of steady-states, either numerically or analytically, and detect changes in the sign of $|(\partial c/\partial m)|$, we must consider the possibility of input multiplicity.

The process model may well be in the implicit form of Eq. 2. In fact, this form of the model is generally assumed for mathematical studies of catastrophe theory (Chang and Calo, 1979). This is because the form of Eq. 1 already has a built-in assumption, namely that there is a one-to-one mapping from m to c, and thus there is no output multiplicity. If the model is implicit, then the catastrophe condition corresponding to Eq. 20 is (Chang and Calo, 1979)

$$\left|\frac{\partial f}{\partial m}\right| = 0 \tag{21}$$

There is no great change in using Eq. 21 rather than Eq. 20 as the catastrophe condition.

CHEMICAL REACTOR EXAMPLE

Physical Description

The physical example we will use is the stirred-tank reactor with control scheme in Figure 1. The reactions involved are

$$A \underset{4}{\overset{1}{\rightleftarrows}} R \underset{3}{\overset{2}{\rightleftarrows}} S \tag{22}$$

with R the desired product. The variables ultimately to be controlled are the concentrations of A and R in the product. The former assures desired total conversion, and the latter assures desired selectivity for product R. However, the control scheme illustrated takes advantage of the ability to quickly measure two related variables, temperature and residence time. With a nominally accurate kinetic model, we will have reasonable initial estimates of the temperature and residence time (product flow rate) needed to achieve the desired values of C_A and C_R. However, due both to model inaccuracies and to process distrubances, these temperature and residence time values will need updating. This is achieved by the feedback control scheme illustrated, involving a typically slow chromatographic measurement of C_A and C_R. These composition measurements are used in cascade loops, with slow reset action, to adjust the set points of the temperature and residence time controllers. The relatively rapid control of temperature and flow rate which can be achieved by the inner loops is adequate to keep the process close to desired conditions. The outer cascade loops involve relatively slow measurements, and function primarily to trim the set points for temperature and flow rate to values which are precise for the desired concentrations, despite possible changes in load variables. Under such circumstances, slow reset action in the outer loops is prudent. Increasing the reset rates to the point where the dynamics of the outer loops interact with those of the inner loops may offer little potential gain in overall quality of control. In any event, as we have already discussed, if the very slow reset action will not allow stable, plausible control loops, it is difficult to be optimistic about the chances for improvement of the performance by using faster reset action. Therefore, depending on the particular circumstances, one can regard the results of the type of analysis we are going to perform as either an evaluation of the actual performance of the intended control scheme; or, as a preliminary screening technique for the existence of inverse multiplicities and for guidance on loop pairings. In the latter case, we are not specifying anything about the intended control algorithm other than that it will include reset feedback between the temperature and residence time manipulations and the concentration outputs.

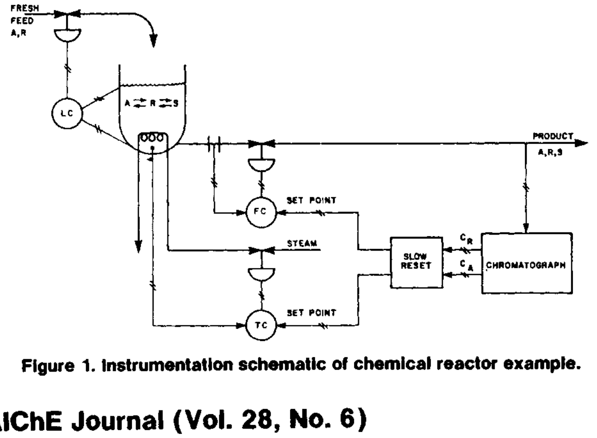

Figure 1. Instrumentation schematic of chemical reactor example.

Note that in Figure 1 we have not yet indicated the intended pairings between c_A, c_R and T, τ (temperature and residence time). Our purpose is to analyze both possibilities. Also note that we have allowed for the possibility of some product R in the fresh feed. This is done to provide a convenient disturbance variable for illustrating process transients. It causes no real change in the inherent behavior of the process.

Kinetic Model

Each of the four reactions will be assumed to be first order. The reaction rate constants will be taken in the Arrhenius form:

$$k = k_0 e^{-E/RT} \tag{23}$$

However, so that we may easily assess the relative velocities of all four reactions of Eq. 22, we will rewrite each rate constant expanded around a centrally chosen absolute temperature T_0.

$$k_i = k_{i0}[e^{-E_i/RT_0}]^{(\frac{1}{u}-1)} \tag{24}$$

where

$$u = \frac{T}{T_0} \tag{25}$$

is the normalized absolute temperature, E_i is the activation energy for the ith reaction, and k_{i0} is the reaction rate constant for the ith reaction at $T = T_0$ or $u = 1$. Values of k_{i0} thus indicate relative strengths of the four reactions at the centrally chosen absolute temperature T_0.

The usual mass-balance derivations on A, R, and S proceed in a straightforward way to yield

$$\begin{aligned} c_A &= C_{A_0} - p_1 c_A + p_4 c_R \\ c_R &= (1 - c_{A_0}) + p_1 c_A + p_3 c_S - (p_2 + p_4) c_R \\ c_S &= 1 - c_A - c_R \end{aligned} \tag{26}$$

where each c has been normalized to the total entering concentration of A and R,

$$c_i = \frac{C_i}{C_{A_0} + C_{R_0}} \tag{27}$$

Further, we have defined

$$p_i = k_i \tau \tag{28}$$

where τ is the residence time.

These normalized equations may be solved algebraically for the controlled concentrations, to yield

$$c_R = \frac{(1 + p_1 - c_{A_0})(1 + p_3)}{(1 + p_1)(1 + p_3) + p_2(1 + p_1) + p_4(1 + p_3)} \tag{29}$$

$$c_A = \frac{(1 + p_3)(p_4 + c_{A_0}) + p_2 c_{A_0}}{(1 + p_1)(1 + p_3) + p_2(1 + p_1) + p_4(1 + p_3)} \tag{30}$$

These equations are the process model in the explicit form, $c = c(m)$. The components of c are c_A and c_R, and the components of m are u and τ (which determine the values of the constants p_i).

Values of Parameters

The following values were chosen for the kinetic and other parameters:

$$k_{10} = 1$$
$$k_{20} = 0.7$$
$$k_{30} = 0.1$$
$$k_{40} = 0.006$$
$$E_1/RT_0 = 5{,}000/600 \tag{31}$$
$$E_2/RT_0 = 6{,}000/600$$
$$E_3/RT_0 = 30{,}000/600$$
$$E_4/RT_0 = 50{,}000/600$$
$$c_{A_0} = 0.8$$

The values of E_i/RT_0 are left as ratios of integers merely to facilitate interpretation and comparison. At the central temperature, $u = 1$, the forward reactions are dominant by at least one order of magnitude. The reverse reactions are much more temperature sensitive, and therefore will tend to become important at higher temperatures.

These effects can be illustrated by the plot of Figure 2 which shows the variation of concentrations with temperature, at a typical residence time, $\tau = 3$. As expected, the yield of desired product R initially increases, until reaction 2 becomes important and more R is lost to S. However, as temperature increases further, reaction 3 occurs and more R is formed at the expense of S. Further increases in temperature ultimately excite reaction 4 which reduces the yield of R. At sufficiently high temperatures, only A is produced.

Figure 3 shows the effect of residence time on the concentrations, at the typical temperature $u = 0.9$. Since τ can range from zero to large positive values, it is convenient to plot it as a redefined residence time

$$\theta = \frac{\tau}{1 + \tau} \tag{32}$$

The variable θ ranges conveniently from zero to unity. The behavior on Figure 3 is typical for such systems, showing a peak in the yield of the desired intermediate product, R.

One notes directly from Figures 2 and 3 the possibility for multiple steady-states in single-loop control. At the particular residence time chosen, as many as four different temperatures can yield certain values of c_R, while at the chosen temperature two different residence times can yield identical c_R values. However, it is not possible to detect from such single-loop plots alone whether there will be multiple steady-state possibilities for the multi-variable control system. We will instead use Eq. 20, together with the stability and plausibility results, to study the existence and stability of such multiple steady states. The physical implications of the results of these studies will then be demonstrated through illustrative transient responses.

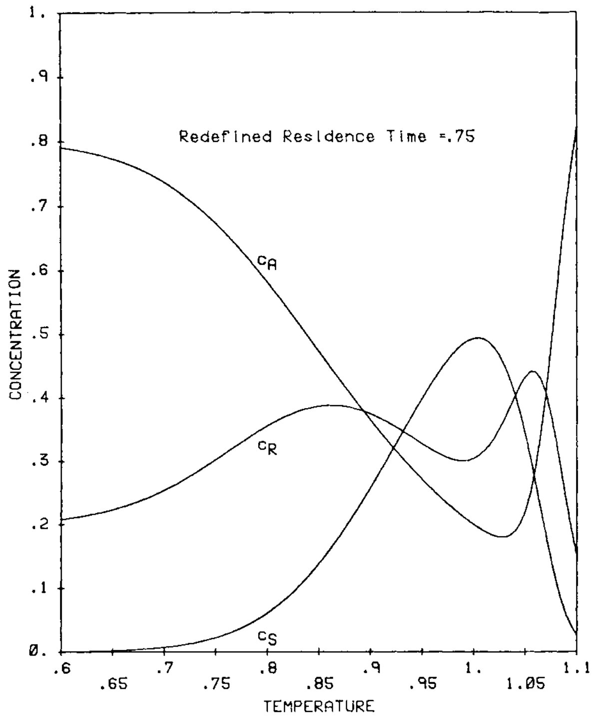

Figure 2. Variation of steady-state product concentrations with temperature at constant throughput.

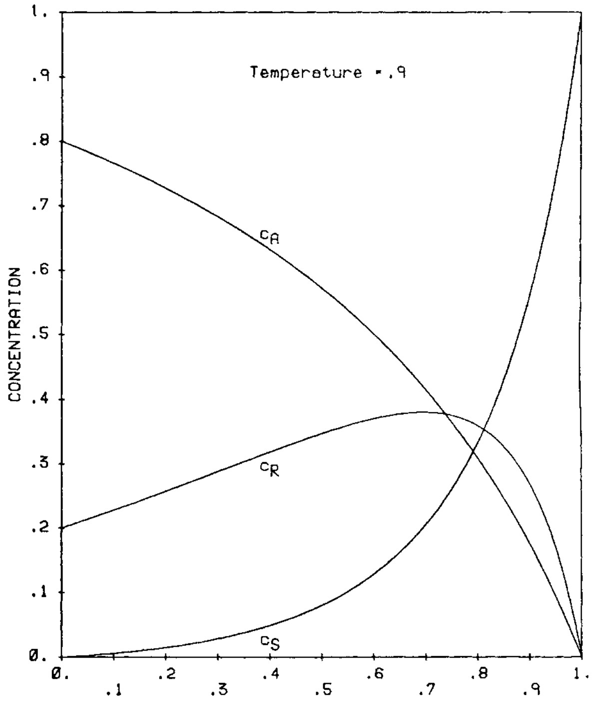

Figure 3. Variation of steady-state product concentrations with throughput at constant temperature.

Contour Plot

A preliminary search for the existence of multiple steady states can be made, in two-dimensional cases such as the one under consideration, by examining a contour plot. Figure 4 shows the steady-state behavior plotted as contours of constant c_R and of

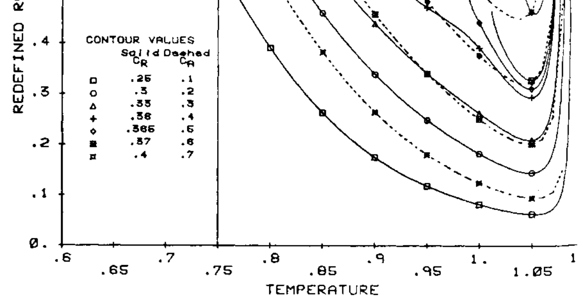

Figure 4. Contour plot of reactor steady-states.

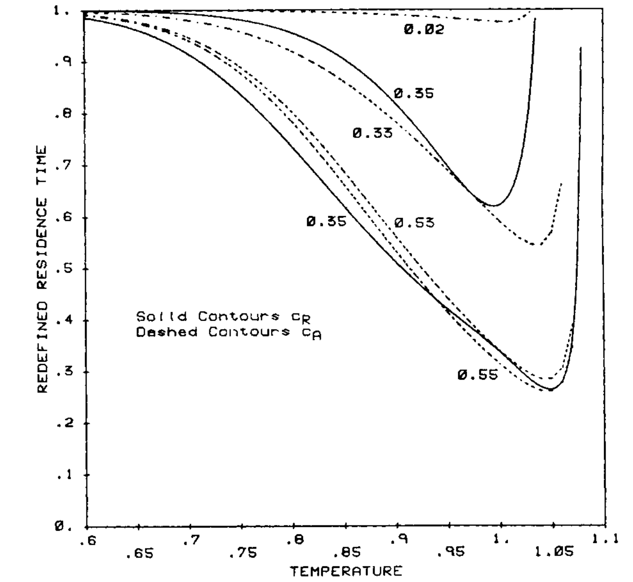

Figure 5. Detail showing multiple steady-state possibility.

constant c_A, on coordinate axes corresponding to the manipulated variables, temperature and residence time. If a pair of c_R and c_A contours intersect at more than one point, this corresponds to input multiplicity. Figure 5 illustrates this for one particular c_R contour at value 0.35, and four c_A contours at values 0.02, 0.33, 0.53, and 0.55. These c_A contours are each tangent to the chosen c_R contour. The tangencies in three cases are plain on the figure. For the contour $c_A = 0.02$, the tangency occurs at low temperature and high residence time, and cannot be easily shown on this plot. Clearly, contours with values of c_A between 0.53 and 0.55 will have multiple intersections with the $c_R = 0.35$ contour. In fact, as will be seen later, three intersections occur. Contours with values of c_A between 0.02 and 0.33 will have two intersections with the $c_R = 0.35$ contour. Therefore, the existence of input multiplicities for this system is evident from the contour plot.

It must be emphasized that contour plots are not readily drawn for more than two dimensions. Further, even for two dimensions preparing contour plots is not a straightforward calculation. For example, to plot a c_R contour, one must first fix the value of c_R in Eq. 29. Then, for each temperature one must find the correct residence time(s) by apparently implicit solution of Eq. 29, and enter the corresponding point(s) on Figure 5. In actual fact, Eq. 29 can be rearranged to a quadratic in residence time, thereby allowing explicit solution, but this would not be true in the general case. The point is that use of a contour plot to detect input multiplicities is not a recommended technique. The contour plot is presented here only as an aid in illustrating the phenomena under discussion.

In the subsequent sections we will use the ideas developed above to study input multiplicities and loop pairings. It will be notationally convenient to assume arbitrarily one of the two possible pairings; the results obtained will still be applicable to analysis of the opposite pairing. We will assume c_A is paired with temperature, and c_R with residence time. The partial derivatives in the process gain matrix $(\partial c/\partial m)$ will then be abbreviated as follows:

$$\frac{\partial c_A}{\partial u} = a_{11} \qquad \frac{\partial c_A}{\partial \tau} = a_{12} \qquad \frac{\partial c_R}{\partial u} = a_{21} \qquad \frac{\partial c_R}{\partial \tau} = a_{22} \tag{33}$$

and the value of the Jacobian determinant in the catastrophe condition, Eq. 20, will be abbreviated as

$$\left|\frac{\partial c}{\partial m}\right| = d \tag{34}$$

Clearly, with the nomenclature chosen above,

$$d = a_{11}a_{22} - a_{12}a_{21} \tag{35}$$

The Catastrophe Locus

We must next evaluate the determinant d by differentiating Eqs. 29 and 30 at various points, and search for changes in sign. In the present case, analytical differentiation is feasible, but offers little computational advantage. In any case we fix, say, the residence time and vary temperature over its relevant range, approximately 0.6 to 1.1 in the present example. At each temperature we evaluate d and note the temperatures, if any, at which d changes sign. For example, at $\tau/(1+\tau) = 0.8$, d is negative at low temperatures, becomes positive at a temperature just above 0.95, then becomes and remains negative at a temperature just above 1.06. Repeating this series of calculations, at residence times chosen at reasonably uniform spacings of $\tau/(1+\tau)$ values between zero and unity, will produce a $d = 0$ locus. This is shown on Figure 6, together with other loci to be discussed later.

In this two-dimensional case, it is easy to demonstrate that at any point where $d = 0$, the c_A and c_R contours must be tangent. Indeed, if $d = 0$ then Eq. 35 may be rearranged to

$$\frac{a_{11}}{a_{21}} = \frac{a_{12}}{a_{22}} \tag{36}$$

which states that the gradient vectors to the c_A and c_R contours are collinear, thus demonstrating tangency. The $d = 0$ locus connects all points at which c_A and c_R contours are tangent. Comparison of Figures 4 and 6 will emphasize this point.

In cases of more than two dimensions, the locus becomes a surface and will require considerably more effort to construct, represent, and interpret. The remaining discussion here of the two-dimensional case will capitalize on the relative ease of geometric representation, and will thereby reach conclusions not likely to be so readily accessible in cases of more than two interacting loops. However, the example is chosen primarily to illustrate what can happen in a process control system when the catastrophe condition $d = 0$ is satisfied at some steady-state points. In cases of more than two loops, of primary concern must be simply the detection of whether d changes sign anywhere in the vicinity of likely operating

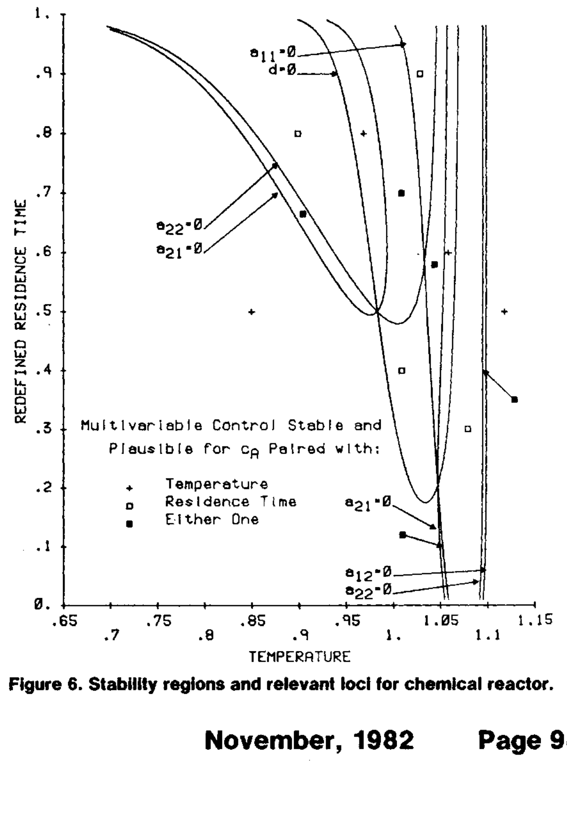

Figure 6. Stability regions and relevant loci for chemical reactor.

conditions. Such detection may be by brute force numerical computations on the process model. Intuitively, one would search in earnest primarily in cases where cross-plots such as Figures 2 and 3, or corresponding physical arguments, indicate the existence of maxima or minima. However, it is possible to construct situations involving multiplicities in which there are no minima or maxima in the crossplots.

It should also be emphasized that the two-dimensional case is one which will occur with some frequency in applications. Therefore, the techniques illustrated for this example may be of some modest generality.

The Catastrophe Set

At each point on the $d = 0$ catastrophe locus, we may use the values of temperature and residence time to calculate the corresponding values of c_A and c_R from Eqs. 29 and 30. The locus of these points may be plotted on c_A, c_R coordinates, as in Figure 7. The region inside this locus is called the catastrophe set (Chang and Calo, 1979). Pairs of c_A and c_R values lying inside this region have the distinguishing feature that they can be produced by more than one set of values of temperature and residence time manipulations.

To illustrate this catastrophe set, consider the particular value $c_R = 0.35$. It will be seen that the locus on Figure 7 passes through this value of c_R at four different values of c_A: 0.02, 0.33, 0.53, and 0.55. This corresponds to the tangency values and the conclusions already illustrated in Figure 5.

Stability Analysis at a Particular Steady State

We next choose a particular steady state

$$\begin{aligned} c_A &= 0.49 \\ c_R &= 0.37 \end{aligned} \tag{37}$$

and analyze the prospect of controlling the system at this steady state. The intended manipulated variable set which will produce this steady state is

$$\begin{aligned} u_1 &= 0.915 \\ \tau_1 &= 1.38\ (\theta_1 = 0.580) \end{aligned} \tag{38}$$

However, the c point chosen falls inside the catastrophe set on Figure 7. There are two other sets of manipulations which will produce this steady-state:

$$\begin{aligned} u_2 &= 1.042 \\ \tau_2 &= 0.504\ (\theta_2 = 0.335) \end{aligned} \tag{39}$$

and

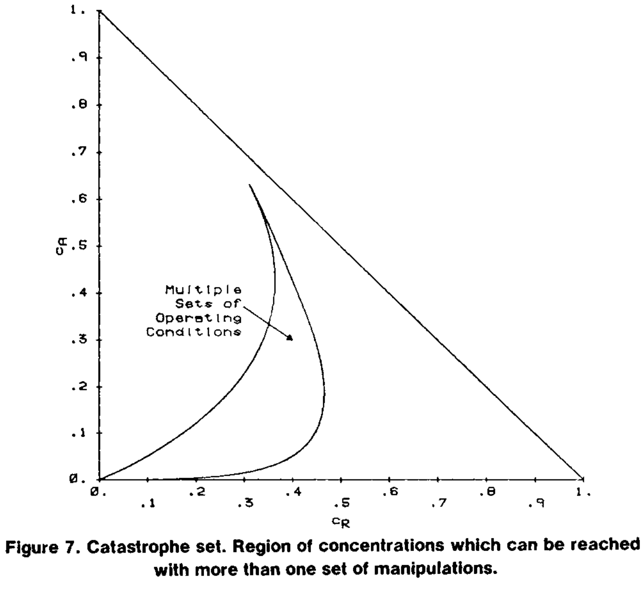

Figure 7. Catastrophe set. Region of concentrations which can be reached with more than one set of manipulations.

$$\begin{aligned} u_3 &= 1.074 \\ \tau_3 &= 2.00\ (\theta_3 = 0.667) \end{aligned} \tag{40}$$

At the intended steady state, $(u_1, \tau_1,)$, the partial derivatives have values

$$\begin{aligned} a_{11} &= -1.892 \\ a_{12} &= -0.1378 \\ a_{21} &= 0.1587 \\ a_{22} &= 0.0259 \end{aligned} \tag{41}$$

which yield

$$d = -0.027$$

We next use Eq. 18 to test whether the tended pairing satisfies the necessary conditions for stability and plausibility at the intended steady state. Since

$$\left(\frac{\partial c}{\partial m}\right) = \begin{pmatrix} -1.892 & -0.1378 \\ 0.1587 & 0.0259 \end{pmatrix}$$

$$\left(\frac{\partial c}{\partial m}\right)_+ = \begin{pmatrix} 1.892 & -0.1378 \\ -0.1587 & 0.0259 \end{pmatrix}$$

$$\left|\left(\frac{\partial c}{\partial m}\right)_+\right| = 0.027$$

the answer is affirmative.

The necessary condition in Eq. 18 only guarantees that there exist values of the reset gains g_1 and g_2 for which both the necessary conditions for stability and the plausibility condition will be satisfied. We next consider the problem of finding appropriate values of the gains g_1 and g_2. This will lead us to Figure 8 which shows, for a specific choice of gains, the regions in m space at which the proposed control system satisfies the necessary conditions for stability. However, it will also show the significance of the other loci on Figure 6, which divide the space into regions of differing stability and plausibility properties.

For the specific case of a 2×2 system, the conditions of stability in Eq. 14 become

$$\begin{aligned} g_1 g_2 (a_{11}a_{22} - a_{12}a_{21}) &> 0 \\ g_1 a_{11} + g_2 a_{22} &> 0 \end{aligned} \tag{42}$$

Let us first ask what is necessary for stability but not necessarily plausibility. We may divide the first condition of Eq. 42 by g_1^2 without changing the sense of the inequality. Adopting the abbreviations

$$\begin{aligned} g &= \frac{g_2}{g_1} \\ G &= a_{11} + g a_{22} \end{aligned} \tag{43}$$

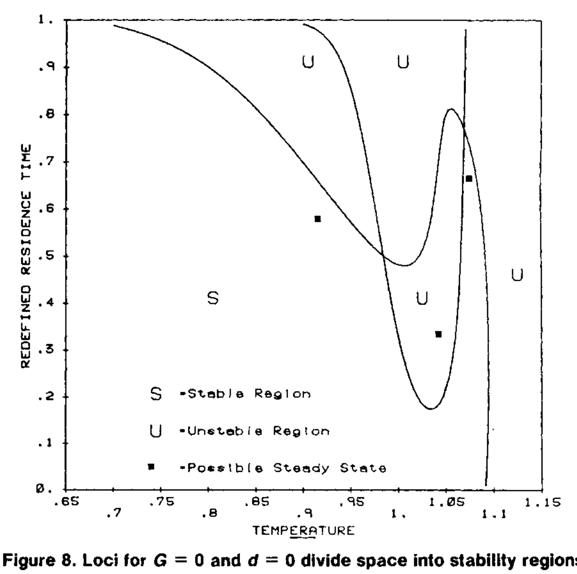

Figure 8. Loci for $G = 0$ and $d = 0$ divide space into stability regions.

The stability conditions become

$$g \cdot \left|\frac{\partial c}{\partial m}\right| > 0$$

$$g_1 G > 0 \tag{44}$$

Once gains g_1 and g_2 have been chosen, Eqs. 44 express the stability conditions in terms of the signs of the quantities $|\partial c/\partial m|$ and G. These equations show that the influence of the gain values g_1 and g_2 on the stability test is only through their ratio, and the sign of one of them.

Now, we add plausibility as a further restriction; this will result in a condition independent of the gains g_1 and g_2. The second stability condition is automatically satisfied for a plausible system. We divide the first condition of Eq. 42 by the product $a_{11}a_{22}$ to obtain

$$g_1 a_{11} g_2 a_{22}\left(1 - \frac{a_{12}a_{21}}{a_{11}a_{22}}\right) > 0 \tag{45}$$

Plausibility enables cancellation of the guaranteed positive factor $g_1 a_{11} g_2 a_{22}$ without changing the sense of the inequality. Abbreviating

$$D = \left(1 - \frac{a_{12}a_{21}}{a_{11}a_{22}}\right) \tag{46}$$

the condition for stability *and* plausibility in a two-dimensional system is then simply

$$D > 0 \tag{47}$$

We note that for plausibility we need not be concerned about $a_{11} = 0$ or $a_{22} = 0$, which would invalidate Eq. 45. If either condition prevails, the system cannot be made plausible by any choice of gains g_1 and g_2, as shown by Eq. 11.

Equation 47 was used with the process model in Eqs. 29 and 30 to plot the stability/plausibility regions for the reactor control system. Figure 6 shows the results.

Each element a_{ij} of $\partial c/\partial m$ is a candidate for a diagonal gain, depending on which pairing is chosen. Figure 6 is intended to show the results for each pairing. Therefore, each locus $a_{ij} = 0$ is plotted. These loci actually show where the individual loop gains g_i must change sign to satisfy plausibility, depending on the pairing chosen. Therefore, these loci pass through the points where satisfaction of the plausibility condition may change for a particular pairing. Comparison of Figures 4 and 6 will confirm that these loci merely connect points of horizontal or vertical tangencies of the c_A and c_R contours.

Within each region, each pairing is considered for satisfaction of Eq. 47. If the $c_A - u$ and $c_R - \tau$ pairing is considered, D is obtained directly from Eq. 46, while for the opposite pairing the ratio of the a_{ij}'s is inverted. The results are as shown. At least one pairing can be made stable and plausible in each region, and both pairings in some regions. The computational inconvenience of calculating such loci must be emphasized for the general case. Figure 6 is intended primarily to illustrate the highly varied stability/plausibility behavior which can be exhibited by a relatively simple system.

If we ask only for stability, and not plausibility, the necessary conditions are those in Eq. 44. It is clear that the loci $G = 0$ and $|\partial c/\partial m| = 0$ will form the stability boundaries. The latter locus can be plotted immediately, but the $G = 0$ locus requires specification of gains.

Considering again our previous example, let us choose the $c_A - u$ and $c_R - \tau$ pairing, and design a system which will be both stable and plausible at the first steady-state, described by Eq. 38. From Eq. 41 it follows that g_1 must be negative for plausibility, because a_{11} is negative. By similar reasoning, g_2 must be positive, and therefore we know that the ratio g must be negative. If we impose these sign conditions on g_1 and g_2, the stability-only necessary conditions in Eq. 44 become

$$\left|\frac{\partial c}{\partial m}\right| < 0$$

$$G < 0 \tag{48}$$

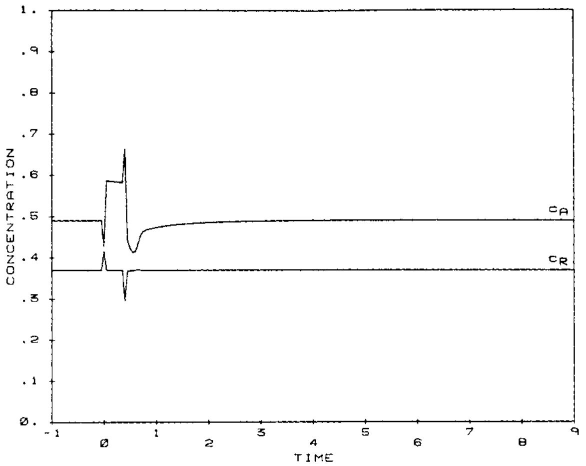

Figure 9. Concentration transients resulting from feed concentration deficit of duration 0.5

With a particular purpose in mind, we will choose the numerical value $g = -2500$ for the ratio of gains. We can then plot the $G = 0$ locus for this value. The results are shown in Figure 8, and the resulting regions are marked according to whether or not the control system will satisfy the necessary conditions in Eq. 48 for stability. Also located on Figure 8 are the three possible steady-state m values, described by Eqs. 38, 39, and 40, which will produce the desired steady-state c value in Eq. 37.

Figure 8 shows that the first and third steady states satisfy the stability condition, but the second does not. The first also satisfies the plausibility condition, by design. Comparison of Figures 8 and 6 will show that neither the second nor the third steady states will be plausibly controlled by this specification of gains. In other words, one of the individual loops will be unstable, if the other loop is opened, because its gain has the wrong sign. The motivation for the choice of $g = -2500$ can be understood from Figure 8. It causes the third steady state to be stable, enabling illustration of transients under the existence of two stable steady states.

This illustration of transients is presented in Figures 9 through 12. The time scale is arbitrary since only the ratio of the reset gains has been specified. Figures 9 and 10 present the c_A and c_R responses resulting from two different disturbances in feed concentration c_{A_0}. These plots of the output variables are all that would normally be available in a plant situation. However, in Figures 11 and 12 are presented the corresponding responses of the manipulated variables and the record of the disturbance variable. In each case, the disturbance is a square pulse. The difference is the duration of the pulses, which is 0.5 time units for Figures 9 and 11, and 1.5 time units for Figures 10 and 12. Inspection of Figures 9 and 10 suggests

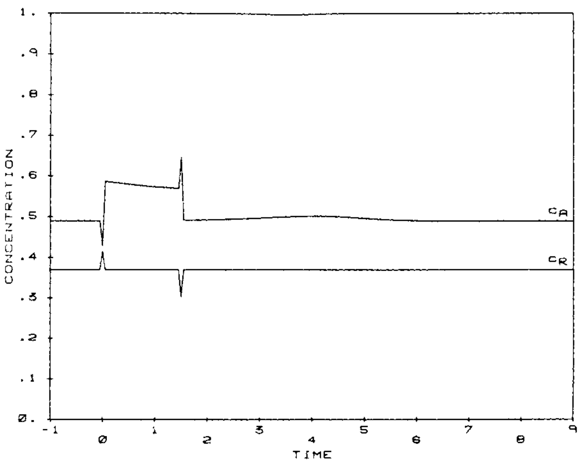

Figure 10. Concentration transients resulting from, feed concentration deficit of duration 1.5.

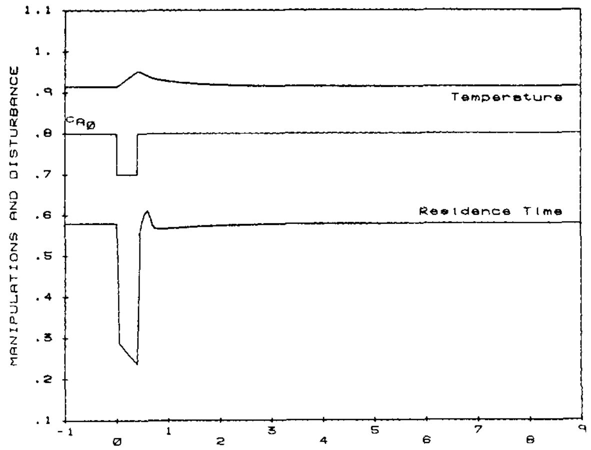

Figure 11. Manipulations and disturbance corresponding to Figure 9.

little difference, other than duration, between the two transients. However, Figures 11 and 12 show that much more has happened in the case of the longer disturbance. Initially of course, the manipulated variables are at the designed-for steady state described by Eq. 38. Following the longer disturbance, the manipulated variables first try to regain control at the second steady state, with values given by Eq. 39. This persists from approximately 1.5 to 2.5 units on the time scale. However, as shown by Figure 8, this steady-state is unstable, so the manipulated variables eventually leave, and finally come to rest at the third steady-state, described by Eq. 40. It is of interest that during the period from approximately $t = 3$ to $t = 6$, while the manipulated variables change significantly, the output variables barely move from their intended steady-state values.

It should again be emphasized that plots such as Figures 11 and 12 are not likely to be available in a plant situation. Even if such data were available, without a good process model there would be no apparent way to determine whether the observed changes in the manipulations were needed to hold the outputs at their desired values because of unmeasured load changes, or were due to the existence of input multiplicities.

It must also be emphasized that these transients are not intended to represent those of a well-designed control system. The control settings have been selected with the primary purpose of illustrating the possibility for control system transition between multiple steady states.

The process chosen here is indeed a simple one compared with typical plant situations. These will involve many more than 2 × 2 variables, and will often be mathematically and structurally much more complex. Typical mathematical complexities will be distributed-parameter models needed to describe spatial effects, complex kinetic and rate expressions, etc. Structural complexities such as recycle are the rule rather than the exception. It seems plausible that these more complex situations are even more likely to allow the existence of input multiplicities.

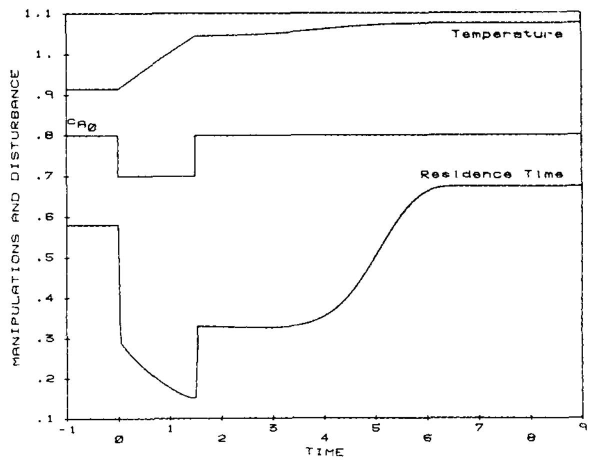

Figure 12. Manipulations and disturbance corresponding to Figure 10.

As discussed above, it would be difficult to argue the existence or non-existence of the phenomenon based on existing plant data. Instead, one might consider input multiplicity as one possible cause for observed deficiencies in the performance, economic or operational, of any plant. If warranted by such considerations, a mathematical model can be constructed and differentiated to detect any changes in the sign of the Jacobian determinant. A troublesome plant, for which such sign changes do occur, would seem to be a prime candidate for a search for the existence of input multiplicities as the cause of the troubles.

SIGNIFICANCE OF THE CATASTROPHE CONDITION FOR PROCESS CONTROL

The catastrophe condition is that of Eq. 20. Considered solely from the viewpoint of catastrophe theory, satisfaction of this criterion means that we should consider the possible existence of multiple steady states, in this case input multiplicities.

However, we have established additional physical interpretation for this condition in the process control framework. The relative gain array, a useful guide for pairing of manipulated and control variables, is not defined when the catastrophe condition is satisfied. In addition, the locus of points at which the catastrophe condition is satisfied will divide the operating space into regions in which alternate pairings can satisfy limiting stability and plausibility conditions.

The necessary condition for limiting stability and plausibility is expressed by Eq. 18, in terms of the sign of the determinant $|(\partial c/\partial m)_+|$. However, since this determinant and $|(\partial c/\partial m)|$ can differ only in sign, it follows that the locus of catastrophe points is also a locus for change in the possibility for limiting stability and plausibility of any selected pairing. A pairing which can be stable and plausible on one side of the locus, cannot be so when the locus is crossed.

The limiting stability condition and the plausibility condition both have physical importance. Limiting stability rests on division of the stability question into two parts. The first part relates to short-term stability, and whether there exists a control without reset action which will operate the process in a dynamically stable manner. This part is not addressed by limiting stability. Analysis of this part would require a detailed dynamic model for the process. Limiting stability addresses only whether the process can be operated stably under very slow reset control. The rationale is that, if we obtain a negative indication regarding limiting stability, we usually have little interest in whether we can obtain short-term stability. If slow reset control cannot be made stable, it is doubtful that any control action containing reset can be made stable. The only process information required for analysis of slow reset control is the steady-state model. Thus, the necessary condition in Eq. 18, for stability and plausibility, gives generally useful information about multivariable pairings.

The condition of plausibility was added to the limiting stability analysis. This condition insists that each of the individual loops be stable under slow reset control. In other words, we are constrained to use the usual negative, rather than positive, feedback in each of the individual loops. When this physically based requirement of plausibility is added to limiting stability, one can judge the desirability of pairings by consideration of properties of the process only.

Thus there are physical relationships among catastrophe theory and aspects of multivariable control system design. When the catastrophe condition is satisfied, it divides the operating space into regions having different sets of c and m variables which can be paired to yield a potentially stable and plausible control system. It further alerts the designer to the possibility of input multiplicity.

We have seen that such multiplicity can have a significant impact on system performance. It thus appears desirable to study further how to detect such multiplicities, both from process models and from operating data, and to generalize as far as possible the characteristics of processes likely to lead to input multiplicities. The potential benefits include elimination of the possibility of transients such as those illustrated by Figures 10 and 12. In these transients, the existence of input multiplicities has allowed a transition of the process to an undesirable steady state. Such transitions may be very difficult to detect in practice, and may show up only in longer-term economics of the process operation.

NOTATION

A = general square matrix
a_{ij} = partial derivatives, defined by Eq. 33
C_A, C_R, C_S = concentrations of chemical species
c = general controlled variables
c^* = desired value of c; set-point values
c_A, c_R, c_S = normalized concentrations defined by Eq. 27
D = quantity defined by Eq. 46
d = determinant, defined by Eq. 35
E = activation energy
f = function symbol
G = quantity defined by Eq. 43
G_r = diagonal matrix of reset gains, Eq. 4
g = gain ratio, Eq. 43
g_i = reset gain used in ith control loop
k = reaction velocity constant, time units normalized to one typical residence time
k_o = reaction velocity constant at temperature T_o
M = deviation in manipulated variable, Eq. 9
m = general manipulated variables
p = defined by Eq. 28
R = gas law constant
T = absolute temperature
T_o = reference absolute temperature
t = time
tr = trace
u = normalized absolute temperature, T/T_o
$\partial c/\partial m$ = process gain matrix, Eq. 8
$(\partial c/\partial m)_+$ = transformed process gain matrix, Eq. 18
θ = redefined residence time. Eq. 32
μ = interaction matrix, relative gain array, Eq. 19
τ = residence time, normalized to be unity at typical throughout

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Photo-Assisted Heterogeneous Catalysis with Optical Fibers

Part III: Photoelectrodes

The concept of using optical fibers to distribute light within heterogeneous photo-assisted catalysts is extended to photo-electrochemical cells. The potential drop in a semiconductor photo-electrode is predicted for various types of ohmic electrical contacts, and the optimum contact location is determined. The variation of electrical conductivity with temperature in non-isothermal bundles of semiconductor-coated optical fibers is considered.

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SCOPE

Optical fibers coated with heterogeneous photo-assisted catalyst are a possible scale-up configuration for all such catalysts. Previous papers considered light transport from the fiber to the catalyst (Marinangeli and Ollis, 1977), and heat and mass transport in bundles of such fibers (Marinangeli and Ollis, 1980). In this paper the bundle of coated optical fibers is analyzed as a photo-electrode for photo-electrochemical cells. Appropriate expressions for the position-dependent conductivity and current density in the semiconducting photo-catalyst are developed.

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