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APPENDIX 1: DEFINITION OF THE MEAN DIAMETER OF A UNIFORM MIXTURE

The friction forces on the total surface (ΣA_i), exposed by the particles in a mixture, equilibrate with the gravity forces, acting on the total volume (ΣV_i) of all the particles of the same density.

$$F_A \Sigma A_i = (\rho_d - \rho_c) g \Sigma V_i \tag{1A}$$

The number of particles of any size i per unit volume is

$$n_i = \frac{1 - \epsilon_i}{\frac{\pi}{6} d_i^3} \tag{2A}$$

while

$$A_i = n_i \cdot \frac{\pi}{4} d_i^2 \tag{3A}$$

and

$$V_i = n_i \cdot \frac{\pi}{6} d_i^3 \tag{4A}$$

Substitution of Equations (2A), (3A), and (4A) into Equation (1A) yields

$$\frac{3}{2} \frac{F_A}{(\rho_d - \rho_c)} = \frac{\Sigma(1 - \epsilon_i)}{\Sigma \frac{1 - \epsilon_i}{d_i}} \tag{5A}$$

The definition of the mean diameter d_m of a mixture assumes that the active forces are the same.

$$\frac{\Pi}{4} d_m^2 \cdot F_A = \frac{\Pi}{6} d_m^3 (\rho_d - \rho_c) g \tag{6A}$$

$$d_m = \frac{3}{2} \frac{F_A}{(\rho_d - \rho_c) g} \tag{7A}$$

Comparison of Equations (5A) and (7A) yields the definition of the mean diameter d_m as expressed in Equation (7).

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Stability of Nonlinear Systems Containing Time Delays and/or Sampling Operations

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In recent years the stability of nonlinear systems has been a topic of considerable interest. Relatively little attention, however, has been directed toward nonlinear time-delay systems, that is, systems whose dynamic behavior is described by a set of differential-difference equations. Although the fundamental stability theorems of Liapunov's second method have been extended to include time-delay systems (*3, 6, 7, 10*), difficulties in implementation have severely limited applications. Most applications have been concerned with the local stability of nonlinear systems (*8, 10, 16*), linear systems (*10, 16, 18, 19*), or linear systems containing simple nonlinear elements (*9, 23*). Quantitative estimates of the region of stability (or asymptotic stability) have not previously been reported for nonlinear time-delay systems. Such estimates would provide useful information concerning the range of disturbances for which a stable

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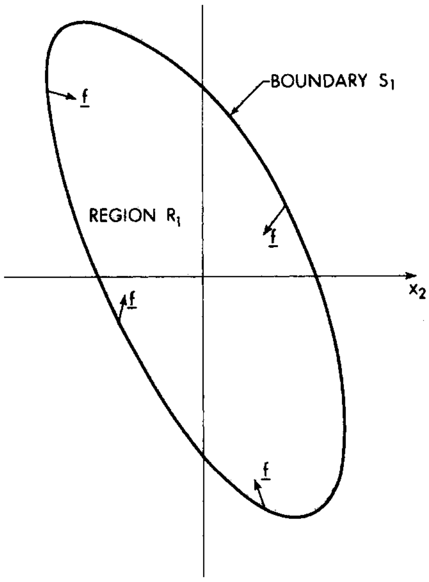

Fig. 1. Geometric criterion for a region of stability.

system can be guaranteed.

Previous applications of Liapunov's second method to reactor stability problems have assumed that time delays and sample-and-hold elements are not present (5). However, these phenomena are not uncommon in the process industries on account of the transportation lag associated with the flow of fluids and the sampling operations that are often required for composition measurement or computer control. The detrimental effects of time delays and sampling operations on reactor stability and control are well known (14, 24).

In this paper a general method is presented for constructing a region of stability (RS) for nonlinear lumped-parameter systems which contain time delays and/or sample-and-hold elements. The construction method, based on modified Liapunov stability theorems, is applicable to both higher order systems and systems containing several time delays. The new method provides a systematic approach for constructing a region of stability if a RS has previously been located for the system without time delays.

SYSTEMS WITHOUT TIME DELAYS

To illustrate the motivation for the new method, consider the following second-order system:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}); \quad \mathbf{x}(0) = \mathbf{x}_0 \tag{1}$$

where $\mathbf{x}$ and $\mathbf{f}$ are two-dimensional column vectors, and the origin is the steady state of interest; that is, $\mathbf{f}(\mathbf{0}) = \mathbf{0}$. The following stability concept will be of interest.

Definition: Let S_1 denote the boundary of a closed and bounded region R_1 in the (x_1, x_2) phase plane. Assume that R_1 contains the origin. Then R_1 is said to be a region of stability (RS) for the system in Equation (1), if for all $\mathbf{x}_0 \epsilon R_1$, then $\mathbf{x}(t) \epsilon R_1$ for $t > 0$.

According to this definition, if a region is a RS, then every trajectory initially in the region never leaves it. If, in addition, the trajectory eventually reaches the origin, the region is referred to as a region of asymptotic stability (RAS). The construction of RAS has been the objective of many applications of Liapunov's second method. Clearly, a RS may also be a RAS if limit cycles or additional steady states are not present within the region. The weaker but

In the following discussion a simple sufficient condition for a RS will be developed for the system in Equation (1). Suppose that at each point on S_1, the derivative vector $\mathbf{f}$ is directed into the interior of region R_1 as shown in Figure 1. Then R_1 must be a RS since any trajectory originating within R_1 can never leave R_1. Assume that region R_1 is defined by $V(\mathbf{x}) \leqq k$, where $V(\mathbf{x})$ is a scalar function which is positive definite in R_1. Then the geometric condition that $\mathbf{f}(\mathbf{x})$ is directed into R_1 for all $\mathbf{x} \epsilon S_1$ is equivalent to the algebraic condition that $\dot{V} < 0$ along S_1. This follows since $\dot{V} = \nabla V \cdot \mathbf{f}$ and ∇V is directed out of R_1 at each point on S_1. Thus a sufficient condition for R_1 to be a RS is that $\dot{V} < 0$ on S_1. A formal proof of this sufficient condition has been presented elsewhere (21, 22).

This sufficiency condition is also implicit in the major Liapunov stability theorems. For example, a well-known theorem due to LaSalle (11, 12) states that a region defined by $V(\mathbf{x}) < k$ is a RAS if within the region, $V(\mathbf{x})$ is positive definite and $\dot{V}$ is negative definite.

TIME-DELAY SYSTEMS

These same ideas provide the motivation for a RS criterion for time-delay systems. Consider the following second-order system containing a single time delay:

$$\dot{\mathbf{x}} = \mathbf{f}[\mathbf{x}(t), \mathbf{x}(t-\tau)] \tag{2}$$

and the initial condition

$$\mathbf{x}(t) = \mathbf{g}(t) \quad \text{for} \quad -\tau \leqq t \leqq 0$$

Again let S_1 denote the boundary of a closed and bounded region R_1 that contains the origin. If on S_1, $\mathbf{f}$ is always directed into R_1 (or equivalently, if $\dot{V} < 0$), then R_1 is a RS. However, for time-delay systems it is difficult to determine if these RS criteria are satisfied; at each point on S_1, $\mathbf{f}$ and $\dot{V}$ depend on the past state $\mathbf{x}(t-\tau)$, in addition to the current state $\mathbf{x}(t)$. Furthermore, the past state is in general not known, since the current state on the boundary S_1 could have been reached by more than one trajectory originating within R_1. Thus for time-delay systems the RS criterion must be modified to require that at each point on S_1, $\dot{V} < 0$ for all possible $\mathbf{x}(t-\tau)$.

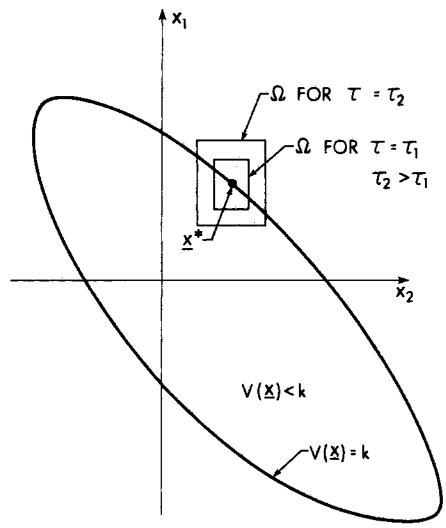

Fig. 2. Region Ω: $\Omega \equiv \{\mathbf{x}: |x_j - x_j^*| \leqq f_{j\max}\,\tau, j = 1, 2\}$.

In the following section, a simple method is presented for determining regions about the current state in which the past state must reside. The calculation of such regions is an essential feature of a new method of constructing RS for time-delay systems.

REGION OF POSSIBLE PAST STATES

Suppose that bounds on the rates of change of the state variables are known or can be estimated. Then these bounds can be used to restrict the past state to a specific region about the current state. For the system described by Equation (2), if

$$|\dot{x}_1| \leq f_{1\,\max} \tag{3}$$

and

$$|\dot{x}_2| \leq f_{2\,\max} \tag{4}$$

then for any $t > 0$ and $\tau > 0$, it follows that

$$|x_1(t) - x_1(t-\tau)| \leq f_{1\,\max}\,\tau \tag{5}$$

and

$$|x_2(t) - x_2(t-\tau)| \leq f_{2\,\max}\,\tau \tag{6}$$

Equations (5) and (6) restrict the past state to a rectangular region Ω about any current state, as shown in Figure 2. If the current state is on S_1 and is denoted by $\mathbf{x}^*$, then region Ω about $\mathbf{x}^*$ is defined by

$$\Omega \equiv \{\mathbf{x}:\ |x_i - x^*_i| < f_{i\,\max}\,\tau,\ i = 1,2\} \tag{7}$$

Although the past state of the system must be located in Ω, the converse is not necessarily true; it is possible that from some points in Ω, the trajectory cannot reach $\mathbf{x}^*$ during a time interval of τ units. Consequently, Ω will be referred to as a region of possible past states (RPPS).

SUFFICIENT CONDITION FOR A RS

The concept of a RPPS forms the basis for a RS criterion for the system in Equation (2). Again consider a closed region R_1 with boundary S_1. If at each $\mathbf{x}^* \epsilon S_1$, $\dot{V} < 0$ for all $\mathbf{x}(t-\tau)\epsilon\Omega$, then R_1 is a region of stability. If $\dot{V}_M$ is defined as

$$\dot{V}_M(\mathbf{x}^*) \equiv \max_{\substack{\mathbf{x}=\mathbf{x}^*,\ \mathbf{x}^*\epsilon S_1 \\ \mathbf{x}(t-\tau)\epsilon\Omega}} \dot{V}(\mathbf{x}) \tag{8}$$

then this sufficient condition for R_1 to be a RS can be stated as $\dot{V}_M(\mathbf{x}^*) < 0$ for all $\mathbf{x}^*\epsilon S_1$.

So far, methods of calculating values of $f_{1\,\max}$ and $f_{2\,\max}$ have not been discussed. This matter is of considerable importance since conservative estimates of $f_{1\,\max}$ and $f_{2\,\max}$ will increase the size of Ω and thus reduce the possibility that $\dot{V} < 0$ for all $\mathbf{x}(t-\tau)\epsilon\Omega$. Suppose that R_1 is a region of stability. Then if the system is initially in R_1 [that is, $\mathbf{g}(t)\epsilon R_1$], it follows that the system must remain in R_1 and that $f_{1\,\max}$ and $f_{2\,\max}$ can be estimated from

$$f_{1\,\max} = \max |f_1| \quad \text{for} \quad \mathbf{x}(t),\ \mathbf{x}(t-\tau)\epsilon R_1 \tag{9}$$

$$f_{2\,\max} = \max |f_2| \quad \text{for} \quad \mathbf{x}(t),\ \mathbf{x}(t-\tau)\epsilon R_1 \tag{10}$$

In the following theorem it will be shown that the converse situation is also true; that if $f_{1\,\max}$ and $f_{2\,\max}$ are evaluated according to Equations (9) and (10) and if $\dot{V}_M < 0$ on S_1, then R_1 is indeed a region of stability. Since the proof of this theorem is quite lengthy and has appeared elsewhere (*21, 22*), it will not be presented here.

Theorem

Consider the following n^{th}-order system containing two time delays:

$$\dot{\mathbf{x}} = \mathbf{f}[\mathbf{x}(t),\ \mathbf{x}(t-\tau_1),\ \mathbf{x}(t-\tau_2)] \tag{11}$$

where

1. $\mathbf{x} = \text{col}\,[x_1 \ldots x_n]$, $\mathbf{f} = \text{col}\,[f_1 \ldots f_n]$
2. $\mathbf{f}(0, 0, 0) = \mathbf{0}$
3. τ_1 and τ_2 are constants, $\tau_2 > \tau_1$
4. The initial conditions are

$$\mathbf{x}(t) = \mathbf{g}(t) \quad \text{for} \quad -\tau_2 \leq t \leq 0$$

Assume that $\mathbf{g}(t)$ is continuous and bounded in the interval of definition. Also assume that $\mathbf{f}$ is sufficiently well-behaved in a region R_0 defined by

$$R_0 \equiv \{\mathbf{x}:\ ||\mathbf{x}|| < r\} \quad \text{for some } r > 0$$

so that the solution to Equation (11) is continuous, unique, and also continuous with respect to the initial function $\mathbf{g}(t)$.

It is also assumed that in R_0, $V(\mathbf{x})$ is positive definite and $V(\mathbf{x}) = k$ defines a closed surface. Denote this surface as S_1 and the closed and bounded region, $V(\mathbf{x}) \leq k$, as R_1. Assume that $R_1 \subset R_0$ and that $V(\mathbf{x})$ has continuous first partial derivatives on S_1. Then R_1 is a region of stability, provided that

$$\dot{V}_M(\mathbf{x}^*) < 0 \quad \text{for all} \quad \mathbf{x}^*\epsilon S_1 \tag{12}$$

where

$$\dot{V}_M(\mathbf{x}^*) = \max_{\substack{\mathbf{x}=\mathbf{x}^* \\ \mathbf{x}(t-\tau_1)\epsilon\Omega_1 \\ \mathbf{x}(t-\tau_2)\epsilon\Omega_2}} \dot{V}(\mathbf{x}) \tag{13}$$

and

$$\Omega_k \equiv \{\mathbf{x}:\ |x_j - x_j^*| \leq f_{j\,\max}\,\tau_k,\ j = 1, \ldots n\} \quad \text{for} \quad k = 1, 2 \tag{14}$$

$$\left.\begin{array}{l} f_{1\,\max} \equiv \max |f_1| \\ \quad\vdots \\ f_{n\,\max} \equiv \max |f_n| \end{array}\right\} \quad \text{for} \quad \mathbf{x}(t),\ \mathbf{x}(t-\tau_1),\ \mathbf{x}(t-\tau_2)\epsilon R_1 \tag{15}$$

SINGLE CONTINUOUS STIRRED-TANK REACTOR

Consider the now classic problem of a single first-order reaction occurring in a continuous stirred tank reactor (CSTR). Applications of Liapunov's second method to this and other reactor stability problems have been reviewed by Gurel and Lapidus (*5*). Recent studies concerned with higher order systems (*1, 20*) and utilization of state constraints (*13*) have also been reported. It should be emphasized that in all previous applications of Liapunov's second method to reactor stability problems, neither time delays nor sampling operations were considered. The only extensive treatment of the effects of time delays and sampling operations on reactor stability is due to Min and Williams (*14, 24*). They used an analog computer simulation of a second-order reaction occurring in a CSTR to illustrate the detrimental effects of time delays and sampling operations on reactor stability.

The energy and material balances for this hypothetical reactor are

$$\rho v C_p \frac{dT}{dt} = \Delta H v r - U A_r (T - T_c) - \rho q C_p (T - T_0) \tag{16}$$

$$v \frac{dc}{dt} = -vr - q(c - c_0) \tag{17}$$

where the rate expression is given by $r = k_0 c e^{-E/T}$. A simple control scheme for this reactor consists of two feedback control loops. In the temperature loop, the coolant temperature is manipulated on the basis of the measured reactor temperature. In the concentration loop the reactor composition is measured and used to manipulate the feed composition. It is assumed that both loops contain time delays due to measurement or other causes. If proportional controllers are used, the equations relating controlled and manipulated variables are

$$T_c(t) = \overline{T}_c - K_1 [T(t-\tau_1) - \overline{T}] \quad (18)$$

$$c_0(t) = \overline{c}_0 - K_2 [c(t-\tau_2) - \overline{c}] \quad (19)$$

where K_1 and K_2 are controller gains, τ_1 and τ_2 are time delays, and the bar denotes a steady-state value.

The following parameter values were originally proposed by Berger and Perlmutter (*2*):

k_0	$= 10^8$ hr.$^{-1}$	ρ	= 50 lb./cu.ft.
E	$= 10^4$ °R.	$\overline{T}_0$	= 530°R.
U	= 5 B.t.u./(hr.)(sq.ft.)(°F.)	$\overline{T}_c$	= 530°R.
A_r	= 100 sq.ft.		
v	= 100 cu.ft.	ΔH	$= 10^4$ B.t.u./lb.-mole
C_p	= 1.0 B.t.u./(lb.)(°F.)	q	= 200 cu.ft./hr.
		$\overline{c}_0$	= 0.2704 lb.-mole/cu.ft.

For these conditions the uncontrolled system has the single steady state of $\overline{T}$ = 550°R. and $\overline{c}$ = 0.165 lb.-mole/cu.ft.

It will be convenient to define dimensionless perturbation variables such that the steady state is translated to the origin. Let

$$x_1 = \frac{\rho C_p (T - \overline{T})}{\Delta H \overline{c}_0} \qquad x_2 = \frac{c - \overline{c}}{\overline{c}_0}$$

$$\alpha = \frac{q}{v} \qquad \beta = \frac{UA_r}{\rho C_p v} \qquad R = \frac{r - \overline{r}}{\overline{c}_0} \quad (20)$$

Substitution of these values into Equations (16) and (17) gives the following nonlinear differential-difference equations:

$$\frac{dx_1}{dt} = f_1[x_1, x_2, x_1(t-\tau_1)] = R - (\alpha + \beta)x_1 - \beta K_1 x_1(t-\tau_1) \quad (21)$$

$$\frac{dx_2}{dt} = f_2[x_1, x_2, x_2(t-\tau_2)] = -R - \alpha x_2 - \alpha K_2 x_2(t-\tau_2) \quad (22)$$

or in vector form

$$\dot{\mathbf{x}} = \mathbf{f}[\mathbf{x}(t), \mathbf{x}(t-\tau_1), \mathbf{x}(t-\tau_2)]; \quad \mathbf{f}(0,0,0) = \mathbf{0} \quad (23)$$

For future reference, the vector equation for the corresponding system without delays (that is, $\tau_1 = \tau_2 = 0$) is written as

$$\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}); \quad \mathbf{F}(0) = \mathbf{0} \quad (24)$$

The following calculational procedure was used to construct regions of stability:

1. Select a Liapunov function $V(\mathbf{x})$ and an initial value for the contour parameter k.
2. Calculate $f_{1\,\max}$ and $f_{2\,\max}$.
3. Evaluate $\dot{V}_M(\mathbf{x})$ along the closed curve $V(\mathbf{x}) = k$.
4. Increase the value of k and repeat steps 2 and 3 until the maximum RS is obtained.

A popular Liapunov function (LF) for many stability problems has been the Krasovskii type, $V(\mathbf{x}) = \mathbf{F}^T\mathbf{A}\ \mathbf{F}$, where $\mathbf{F}^T$ is the transpose of the derivative vector $\mathbf{F}$ and $\mathbf{A}$ is a positive definite matrix. In this investigation, as in several earlier studies (*1, 2, 13*), the $\mathbf{A}$ matrix was arbitrarily set equal to the identity matrix. Thus for the time-delay system in Equation (23), the following LF was used to define potential RS:

$$V(\mathbf{x}) = \mathbf{F}^T\mathbf{F} \quad (25)$$

In step 2 of the RS calculations, $f_{1\,\max}$ and $f_{2\,\max}$ must be calculated. In general the maximization required by Equation (15) is a difficult nonlinear programming problem. In this example, however, each system equation is monotonic in a state variable; consequently the maximum values of $|\dot{x}_1|$ and $|\dot{x}_2|$ occur at points on the boundary of region R_1 rather than at interior points. Thus $f_{1\,\max}$ and $f_{2\,\max}$ could easily be determined by evaluating $|\dot{x}_1|$ and $|\dot{x}_2|$ at a grid of points on the boundary of R_1. One hundred points proved to be adequate for their determination.

Equations (21) and (22) indicate that the evaluation of $|\dot{x}_1|$ and $|\dot{x}_2|$ at a grid point $\mathbf{x}\epsilon S_1$ requires values of $x_1(t-\tau_1)$ and $x_2(t-\tau_2)$. Furthermore, the definitions of $f_{1\,\max}$ and $f_{2\,\max}$ in Equation (15) require that the values of $x_1(t-\tau_1)$ and $x_2(t-\tau_2)$ in region R_1 which maximize $|\dot{x}_1|$ and $|\dot{x}_2|$ should be used. Since Equation (21) is first order with respect to $x_1(t-\tau_1)$, the maximum of $|\dot{x}_1|$ at a grid point will occur when $x_1(t-\tau_1)$ is at either an upper or lower limit. Similarly, in order to maximize $|\dot{x}_2|$ at a grid point, $x_2(t-\tau_2)$ should be set equal to its upper or lower limit. Since the conditions of the theorem restrict the delay terms to region R_1, the extreme values of

TABLE 1. EFFECT OF K_2 ON THE MAXIMUM RAS FOR THE CSTR WITHOUT TIME DELAYS

K_1	K_2	$k_{\max}$	$T_{\max}$, °R.
0	0	0.38	580
0	2	0.07	569
0	6	0.03	567
0	10	0.02	565
16	0	7.8	613
16	10	1.3	589
16	20	1.0	586

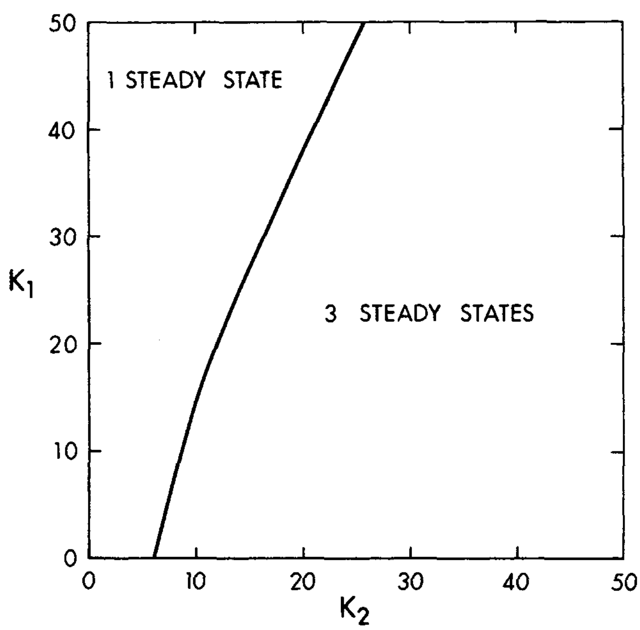

Fig. 3. Number of steady states for various controller settings.

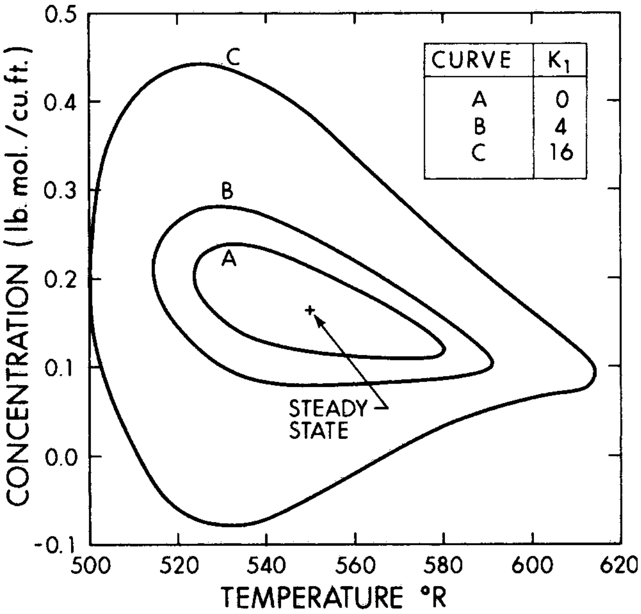

Fig. 4. Effect of K_1 on the region of stability, $V(\mathbf{x}) \leqq k_{max}$ ($K_2 = 0, \tau_1 = 0$).

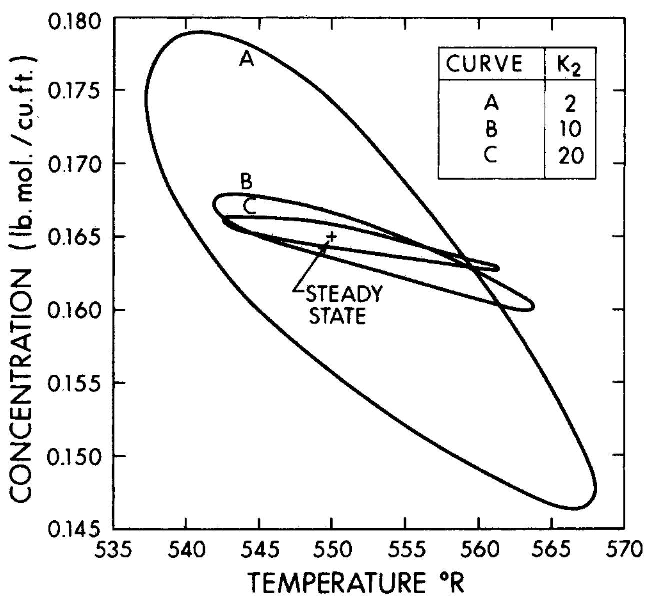

Fig. 5. Effect of K_2 on the region of stability, $V(\mathbf{x}) \leqq k_{max}$ ($K_1 = 0, \tau_2 = 0$).

x_1 and x_2 in region R_1 provide convenient estimates of the limits on $x_1(t - \tau_1)$ and $x_2(t - \tau_2)$. A simple iterative method based on initial estimates of $f_{1\,max}$ and $f_{2\,max}$ has also been used to calculate these limits (*21*).

In step 3 of the RS calculations $\dot{V}_M$ is evaluated at a series of points on the closed curve $V(\mathbf{x}) = k$. If $\dot{V}_M < 0$ at each point, then region R_1 is a RS. Since $\dot{V}$ can be expressed as

$$\dot{V} = \nabla V \cdot \dot{\mathbf{x}} \tag{26}$$

then for the reactor system in Equations (16) and (17)

$$\dot{V} = -\frac{\partial V}{\partial x_1}\,\beta K_1 x_1(t - \tau_1) - \frac{\partial V}{\partial x_2}\,\alpha K_2 x_2(t - \tau_2) + \text{terms without delays} \tag{27}$$

ly definition, the evaluation of $\dot{V}_M$ at a point on S_1 reuires maximizing $\dot{V}$ for all $x_1(t - \tau_1)\epsilon\Omega_1$ and $x_2(t - \tau_2)\epsilon\Omega_2$. However, since Equation (27) is first order in each f the delay terms, a bang-bang situation exists. That is, r $\dot{V}$ to be a maximum, each delay term must be at either maximum or minimum value, depending on the values $\partial V/\partial x_1$ and $\partial V/\partial x_2$. Bounds on the delay terms are known to exist since $x_1(t - \tau_1)$ and $x_2(t - \tau_2)$ are restricted to the rectangular regions Ω_1 and Ω_2, respectively. Thus in this example the evaluation of $\dot{V}_M$ at each grid point on boundary S_1 requires only a single evaluation of $\dot{V}$ for specified values of $x_1(t - \tau_1)$ and $x_2(t - \tau_2)$ rather than a search over all possible values.

Regions of stability were calculated for several combinations of controller constants and time delays. Figure 3 indicates that three steady states existed for many controller settings. The number of steady states was determined from the familiar plot of heat generation and heat removal rates versus temperature.

The effects of K_1 and K_2 on the calculated *RS* for the system without time delays are presented in Table 1 and Figures 4 and 5. k_{max} denotes the largest value of k for which the region $V(\mathbf{x}) \leqq k$ is a region of stability. T_{max} refers to the maximum temperature on the Liapunov contour $V(\mathbf{x}) = k_{max}$. The Krasovskii type of LF given by Equation (25) was used in all of the RS calculations. The results in Figure 4 support the previously reported conclusion (*2, 13*) that increasing K_1 increases the size of the RS. Table 1 and Figure 5 indicate that increasing K_2 decreases the size of the region of stability. These results are in contrast to an assertion by Berger and Perlmutter (*2*) that increasing K_2 increases the size of the RAS. However, their qualitative assertion was based on a more conservative method of determining regions where $\dot{V} < 0$.

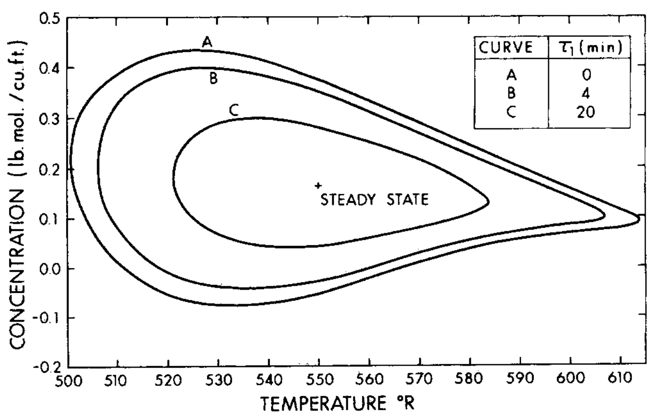

Fig. 6. Effect of τ_1 on the region of stability, $V(\mathbf{x}) \leqq k_{max}$ ($K_1 = 16, K_2 = 0$).

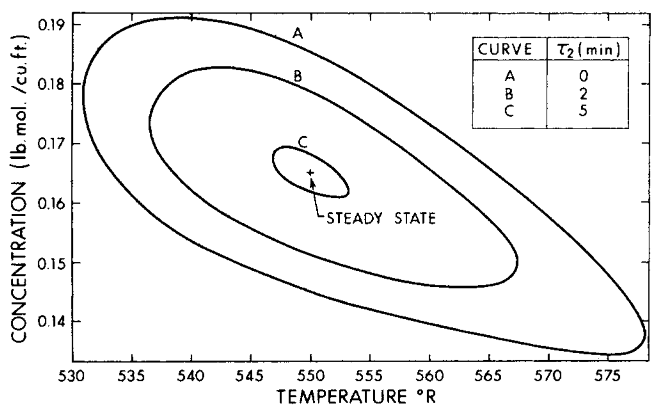

Fig. 7. Effect of τ_2 on the region of stability, $V(\mathbf{x}) \leqq k_{max}$ ($K_1 = 4, K_2 = 2, \tau_1 = 0$).

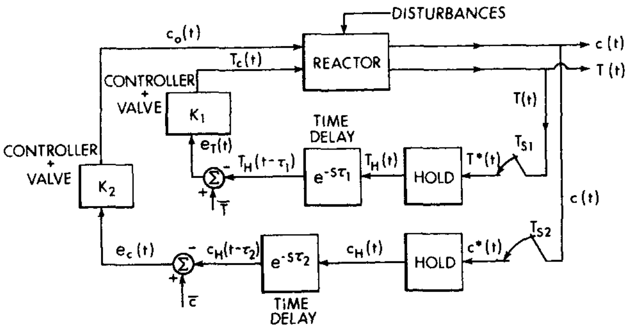

Fig. 8. Block diagram for the controlled CSTR.

The detrimental effect of time delays on the region of stability is indicated by the results presented in Tables 2 and 3 and Figures 6 and 7. Increasing τ_1 or τ_2 tends to decrease the size of the RS, as would be expected since time delays are a well-known destabilizing influence. Perhaps the most surprising aspect of these results is that the reactor remains stable for values of τ_1 as large as 10 to 30 min. Numerical integration of the system equations confirmed these results. Time delays of 10 to 30 min. are certainly much larger than those normally encountered in temperature control loops. For several combinations of K_1 and K_2, RS were obtained despite the complications introduced by the presence of three steady states (*21, 22*).

The calculated regions of stability, although large enough to be of practical significance, could probably be increased by utilizing a more general **A** matrix or other types of Liapunov functions. Attempts were made to determine the actual regions of stability by numerical integration of Equations (21) and (22). These calculations were made for several combinations of K_1, K_2, τ_1, and τ_2 that appear in Tables 2 and 3. In each case the reactor displayed asymptotic stability for a wide variety of initial states. Although inconclusive, these results imply that when a single steady state exists, the reactor is asymptotically stable for all physically meaningful initial states (that is, $T > 0$, $c > 0$). Thus these results and those from previous investigations indicate that the Berger and Perlmutter CSTR example exhibits a high degree of stability, both with and without time delays in the control loops.

The computational requirements for the RS calculations were quite moderate. For example, the calculation of $\dot{V}$ on 25 Liapunov contours required about 40 sec. of execution time on an IBM 7094 computer. This time estimate is for a grid of 100 points on each contour.

CSTR WITH TIME DELAYS AND SAMPLING OPERATIONS IN THE CONTROL LOOPS

In many practical situations an important process variable cannot be measured on a continuous basis. Composition measurement, for example, often requires intermittent sampling followed by on-line or laboratory analysis. In some circumstances, process variables are sampled even when continuous measurement is possible. This situation occurs when an analytical instrument is multiplexed (shared) among several process streams in order to reduce instrumentation costs. Also, computer control requires sampling since a digital computer inherently is a discrete-acting device. Time delays are often associated with sampling operations, particularly in composition measurement where the time required to analyze a sample is often a significant time delay.

TABLE 2. EFFECT OF TIME DELAYS ON THE MAXIMUM REGION OF STABILITY

Case A: $K_1 = 16$, $K_2 = 10$

τ_1, min.	τ_2, min.	k_{max}	T_{max}, °R.
0	0	1.3	588
10	0	1.3	588
20	0	1.1	582
30	0	0.50	568
0	1.0	0.44	567
10	1.0	0.29	563
20	1.0	0.09	557
0	0.5	0.96	578
0	1.5	0.08	556

TABLE 3. EFFECT OF TIME DELAYS ON THE MAXIMUM REGION OF STABILITY

Case B: $K_1 = 16, K_2 = 2$

τ_1, min.	τ_2, min.	k_{max}	T_{max}, °R.
0	0	3.5	600
0	1	2.9	594
0	4	1.6	581
0	8	0.55	567
10	0	2.9	594
10	4	1.1	575
10	8	0.23	560

For linear sampled-data systems the stability analysis is quite straightforward and can be carried out by classical methods (*17*). For nonlinear systems Liapunov's second method can, in principle, be used to construct regions of stability or asymptotic stability. However, applications of the Liapunov stability theorems for this purpose have not been reported. Consequently, stability analyses of nonlinear sampled-data systems of interest to chemical engineers have relied on linearized analysis or integration of differential equations (*14, 15, 24*).

Returning to the previous reactor example, it will now be assumed that both of the controlled variables, temperature and concentration, are measured on an intermittent rather than a continuous basis. Again the possibility of time delays in the feedback control loops will be allowed.

A schematic representation of the controlled reactor is shown in Figure 8. The open switches represent idealized samplers with sampling periods of T_{S1} and T_{S2}. The hold circuits following the samplers reconstruct continuous signals from the sampled signals. Hold circuits are necessary whenever a sampled signal is an input to a continuous acting (analog) device such as the proportional controllers in this example. It is assumed that a simple zero-order hold is used with each sampler. Figure 9 compares the output of the hold circuit with the variable being sampled.

The block diagram in Figure 8 indicates that the controller equations are

$$T_c(t) = \overline{T}_c - K_1\,[T_H(t-\tau_1) - \overline{T}] \qquad (28)$$

$$c_0(t) = \overline{c}_0 - K_2\,[c_H(t-\tau_2) - \overline{c}] \qquad (29)$$

It will be convenient to express T_H and c_H in terms of the reactor variables T and c. A relation between T_H and T will now be derived.

Assume that the temperature of the reactor is sampled at evenly spaced increments of time. The time between two successive samples is referred to as the *sampling period* T_{S1}. At each sampling instant t_k, the values of T_H and T

are identical since a new sample has just been taken. (Idealized sampling of zero duration is assumed.) Immediately prior to the next sampling instant t_{k+1}, a time delay equal to the sampling period is present. That is, at time t_{k+1} the output of the hold circuit is still clamped at the value of the last sample $T(t_k)$, although the temperature of the reactor is now $T(t_{k+1})$. Similarly, at a point midway between the two sampling instants, the time delay between T and T_H is half a sampling period. Thus between successive sampling instants the time delay varies linearly with time, reaching a maximum value of T_{S1}. Since periodic sampling is assumed, the time delay is also periodic. The relationship between T_H and T can be expressed as

$$T_H(t) = T[t - h_1(t)] \tag{30}$$

where $h_1(t)$ is the saw-tooth function shown in Figure 10. Thus the sample-and-hold operation is mathematically equivalent to a time delay which varies periodically with time. The analogous relation between c_H and c is

$$c_H(t) = c[t - h_2(t)] \tag{31}$$

where $h_2(t)$ is shown in Figure 10.

The block diagram in Figure 8 indicates that the signal sent to the temperature controller is $T_H(t - \tau_1)$. Use of Equation (30) gives

$$T_H(t - \tau_1) = T[t - h_1(t) - \tau_1] \tag{32}$$

Therefore the equation for the temperature controller can be written as

$$T_c(t) = \overline{T}_c - K_1 \{T[t - h_1(t) - \tau_1] - \overline{T}\} \tag{33}$$

The analogous equation for the concentration controller is

$$c_0(t) = \overline{c}_0 - K_2 \{c[t - h_2(t) - \tau_2] - \overline{c}\} \tag{34}$$

Next, it will be shown that by using the new method regions of stability can be constructed for nonlinear sampled-data systems. In the f_{max} and $\dot{V}$ calculations outlined in the theorem, the past states were restricted to certain regions about the current state. In the previous case of constant time delays, τ_1 and τ_2 were used in defining these regions. But from the above discussion, the sample-and-hold element can be represented as a time-varying delay whose maximum value is the sampling period. Thus when a control loop contains both a time delay and a sample-and-hold element, the maximum time delay is the sum of the constant time delay and the sampling period. Defining

$$\hat{\tau}_1 \equiv \tau_1 + T_{S1} \tag{35}$$

and

$$\hat{\tau}_2 \equiv \tau_2 + T_{S2} \tag{36}$$

then if $\hat{\tau}_1$ and $\hat{\tau}_2$ are used in place of τ_1 and τ_2 in the theorem, regions of stability can be constructed for the sampled-data system. The necessary generalization of the above theorem to the more general case of time-varying time delays has been presented elsewhere (*21*).

Thus by approximating the time-varying delay due to sampling by a constant delay equal in magnitude to the sampling period, the new method can also be applied to sampled-data systems. However, this modification does not allow the new method to distinguish between the following problems:

1. Time delay $= \tau$ (no sampling)
2. Time delay $= \tau/2$, sampling period $= \tau/2$
3. Sampling period $= \tau$ (no time delay)

In general the stability characteristics of the three problems will be quite different. Usually one would expect increased stability in proceeding from 1 to 3, since a common approximation to a sample-and-hold element is a time delay equal to half the sampling period (*17*). The new method however will produce identical results for all three problems. Consequently, the results in Figures 6 and 7 and Tables 2 and 3 are also valid for the sampled-data system if the values of τ_1 and τ_2 are interpreted to be $\hat{\tau}_1$ and $\hat{\tau}_2$. For example, Table 3 implies that if controller constants of $K_1 = 16$ and $K_2 = 2$ are used and the sum of the time delay and sampling period in the concentration loop is less than 4 min., then a RS defined by $V(\mathbf{x}) \leq 1.6$ exists.

HIGHER ORDER SYSTEMS

It should not be inferred from the above example that the construction method is restricted to second-order systems. On the contrary, the new method is applicable to systems containing an arbitrary number of state variables, as indicated in the statement of the theorem.

For higher order systems, the f_{max} and $\dot{V}$ calculations require locating minima on the Liapunov surface defined by $V(\mathbf{x}) = k$. Berger and Lapidus (*1*) have demonstrated

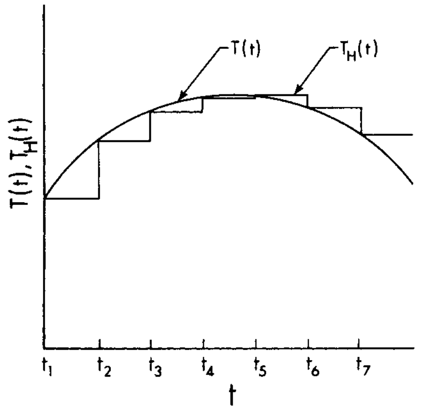

Fig. 9. Input and output for the sample-and-hold device.

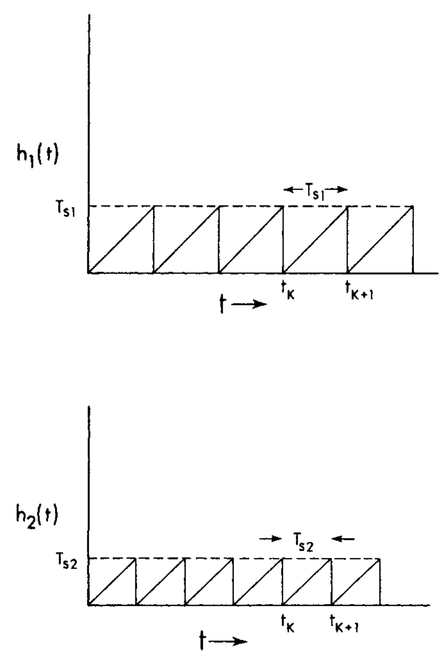

Fig. 10. $h_1(t)$ and $h_2(t)$ versus t.

that combining the Fletcher-Powell minimization technique with a penalty-function procedure provides an efficient computational algorithm. Seborg (*21*) has used this algorithm to construct RS for a four-variable reactor system containing two time delays.

CONCLUSIONS

A method has been developed for constructing regions of stability for nonlinear systems which contain time delays and/or sample-and-hold elements. The new method is applicable to a large class of problems, including higher order systems and systems containing multiple time delays or time-varying delays. The new method offers the advantage that it is not restricted to a particular type of a Liapunov function such as a quadratic form or a Krasovskii type of function. The new method provides a systematic procedure for constructing a region of stability for a time delay system if a RS has been determined for the same system without time delays.

The computational requirements for the new method are quite modest, particularly if the state equations are monotonic in each of the delay terms. This requirement is usually satisfied in control problems of interest to chemical engineers.

A major shortcoming of the new method is that it requires an already conservative method, Liapunov's second method, to be more conservative. Consequently, the calculated regions of stability may be quite small. However, alternative methods for constructing RS for nonlinear, time delay systems are not available.

ACKNOWLEDGMENT

Financial support from Princeton University in the form of an Esso Fellowship and research assistantships to D. E. Seborg is gratefully acknowledged.

NOTATION

$\mathbf{A}$ = constant matrix
A_r = area of cooling coil
C_p = specific heat
c = concentration
c_0 = feed concentration
E = activation energy divided by the gas constant
$\mathbf{F}$ = derivative vector for system without time delays
F_j = j^{th} component of $\mathbf{F}$
$\mathbf{f}, f_j$ = derivative vector and j^{th} component, respectively
$f_{j\,max}$ = max $|\dot{x}_j|$
$\mathbf{g}$ = initial condition vector
ΔH = heat of reaction
h_1, h_2 = time-varying time delays shown in Figure 10
K_1, K_2 = controller constants
k = contour parameter used to define a Liapunov surface, $V(\mathbf{x}) = k$
k_0 = frequency factor in Arrhenius type of rate expression
n = dimension of state vector = order of the system
q = volumetric flow rate
R = dimensionless reaction rate
R_0, R_1 = regions in state space
r = temperature
S_1 = rate of reaction per unit volume
T = boundary of region R_1
T_c = coolant temperature
T_0 = feed temperature
T_{S1}, T_{S2} = sampling periods
t = time
t_k = k^{th} sampling instant
U = overall heat transfer coefficient
$V(\mathbf{x})$ = Liapunov function
v = reactor volume
$\mathbf{x}, x_j$ = state of the system, j^{th} state variable
$\mathbf{x}_0$ = initial state

Greek Letters

α = q/v
β = $UA_r/\rho C_p v$
∇ = del operator
ρ = density
τ, τ_j = time delay, j^{th} time delay
$\hat{\tau}_1$ = $\tau_1 + T_{S1}$
$\hat{\tau}_2$ = $\tau_2 + T_{S2}$
Ω, Ω_j = regions of state space

Subscripts

— = vector
H = hold
M = maximum
max = maximum

Superscripts

$*$ = sampled function
— = steady state
$\cdot$ = time derivative
T = vector transpose

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