Bounding Chemical Reactor Transients by Estimation of Growth or Decay Rates

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If the transient equations of a plug flow tubular reactor are transformed into a set of corresponding ordinary differential equations, stability information for the former may be obtained graphically from knowledge about the transients of the latter. The analysis presented in this paper combines this simplification with the definitions and theorems of Weiss and Infante to propose a method of direct computation whereby transient bounds may be found for this important class of distributed-parameter chemical reactor systems.

We have shown elsewhere (*7*) how if the transient equations of a plug flow tubular reactor (PFTR):

$$\partial C/\partial\theta = -v(\partial C/\partial x) - R \quad (1a)$$

$$\rho C_p\, \partial T/\partial\theta = -\rho C_p\, v(\partial T/\partial x) + \Delta HR - KA_r\,(T - T_w) \quad (1b)$$

are transformed into the set of corresponding ordinary differential equations:

$$D\hat{C}/D\tau = -\hat{R} \quad (2a)$$

$$D\hat{\eta}/D\tau = \hat{R} - G\hat{\eta} \quad (2b)$$

stability information for the former may be obtained graphically from knowledge about the transients of the latter.

The analysis presented here combines this simplification with the definitions and theorems of Weiss and Infante (*9*) to propose a method of direct computation, whereby transient bounds may be found for an important class of distributed-parameter chemical reactor systems. The arguments are based on the following vector form of Equations (*2*):

$$D\mathbf{U}/D\tau = \mathbf{F}(\mathbf{U}, \tau);\ 0 \leq \tau \leq \theta_L \quad (3)$$

for which it may be noted that the relationships are defined only over a finite time interval.

The finite residence time of the plug flow tubular reactor arises from the fact that the reactor length is finite and the velocity of the fluid is not zero. With this in mind, it is only meaningful to estimate the bounds on the transients of any fluid section while it remains in the reactor and it is rather immaterial whether the original steady state profiles are stable or unstable for all time.

Following Weiss and Infante, and Kalman and Bertram (*1*), a positive-definite *V*-function and a real $\xi(\tau)$ are proposed, such that

$$\dot{V} = \frac{DV}{D\tau} \leq \xi(\tau)\ V(\tau, \mathbf{U}) \quad (4)$$

and

$$\xi(\tau) = \text{Max}\,[\dot{V}(\tau, \mathbf{U})/V(\tau, \mathbf{U})] \quad (5)$$

in the region of state space of interest and over the relevant finite interval of time. Kalman and Bertram used ξ as an estimate of the transient of a dynamic system. Letov (*3*) called it a measure of *system quality*. Ling (*4*) referred to it as the *estimation of decaying time*.

The significance of this function for the problem of interest here can be seen by separating three subcases, according to the sign of $\xi(\tau)$:

1. If $\xi(\tau) < 0$, *V* will decay with time over the finite interval, $0 < \tau < \theta_L$. Then, if a trajectory of Equation (*3*) is initially within the region $V \leq \alpha$, it will always remain within that region, and will end up at reactor exit bounded by some smaller region $V \leq \beta$. Such a system is called contractively stable with respect to $(\alpha, \beta, \theta_L, V)$ by Weiss and Infante.
2. If $\xi > 0$, *V* may grow with time over the range from zero to θ_L. However, since this growth occurs for only a finite time, it is still possible for the trajectory to be bounded by $V \leq \beta$ at θ_L. If this is in fact the case, the system is stable according to the Weiss-Infante definition, but not contractively stable.
3. If $\xi = 0$, *V* will decay or remain constant. In either case, the test of stability with respect to $(\alpha, \beta, \theta_L, V)$ remains the same.

The formulations of Weiss and Infante are broad enough to include other norms, but for the purposes of this research, it was convenient to use as the *V*-function the distance measure in the state space. It is important to emphasize that the *V*-function proposed above may have positive as well as negative time derivative. Hence it is not a Liapunov function according to the definition given by LaSalle and Lefschetz (*2*). Furthermore, it is not a tracking function as used by Paradis and Perlmutter (*5*), for the latter is not necessarily positive definite in the state space.

Because of the sign indefiniteness of $\dot{V}$, transients of system (*1*) may approach or diverge from the steady state during the finite time interval. $\xi(\tau)$ is simply the bound governing the growth (when $\dot{V} > 0$) or decay rate (when $\dot{V} < 0$) of the proposed positive definite function. Because of this feature, many *V*-functions which cannot guarantee stability of a given system defined for all time, may be used to establish the practical stability of the same system defined over a finite time interval. In this respect less restrictive *V*-functions are required than for a stability analysis which relies on Liapunov functions. Whenever the choice of α and β takes into account the region in the state space which is physically feasible and practically allowable for a particular system, it may be called *Practically Stable* (*2, 5*).

One other matter of nomenclature is nöteworthy. A region of finite-time stability can also be thought of as an estimate of initial-condition sensitivity, since it provides a bound on the worse changes (in the sense of *V*) that may be anticipated following an instantaneous system upset. It should be remembered, however, that the responses of

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interest are time-dependent and not a comparison of several steady states. Accordingly, if sensitivity considerations are to be raised at all, they must involve dynamic sensitivity as in Tomovic (6).

In the course of establishing a suitable α, β pair numerically, it is usually simplest to find a series of β_k at intermediate τ_k's $(0 < \tau_k < \theta_L)$, such that the transients of any fluid section will not exceed these regions at appropriate τ_k's. The ensemble of such a series, $V \leq \beta_k$, constitutes a region Ψ_τ in the product space of state space and τ. Since for the plug flow tubular reactor the time variable, τ, has a unique correspondence to the reactor length variable, x, the bounding region, Ψ_τ, is essentially a region Ψ_x in the space $(\hat{C}, \hat{\eta}, x)$, where x is between 0 and L, the total length of the reactor.

Although the discussion that follows is devoted specifically to a two state–variable reactor analysis, it should be noted that no restriction on the dimensionality of U is related to the ξ-bound method *per se*. Rather, it is the relative ease of computation and graphical display that recommends the relatively simpler case, considerations that arise in any and all dynamic analyses. When on the other hand this method is combined with an earlier graphical approach, as it is in the last section of this paper, the dimension restrictions of the more limiting part apply to the whole.

APPLICATION TO A PLUG FLOW TUBULAR REACTOR

To illustrate the application to the analysis of a plug flow tubular reactor, a simple circular V-function is proposed as follows:

$$V = \hat{C}^2 + \hat{\eta}^2 \tag{6}$$

Then $(DV/D\tau)$ should be

$$\dot{V} = 2\left(\hat{C}\frac{D\hat{C}}{D\tau} + \hat{\eta}\frac{D\hat{\eta}}{D\tau}\right) \tag{7}$$

Substituting Equations (2) into Equation (7), we have

$$\dot{V} = 2\,[(\hat{\eta} - \hat{C})\,\hat{R} - G\hat{\eta}^2] \tag{8}$$

From Equation (8) $\dot{V}$ is not sign definite, for the first term on the right hand side can be either positive or negative depending on the values of $\hat{C}$ and $\hat{\eta}$; it is nevertheless useful in the present method, for in this case, bounds on the transients of the system are only needed within a finite time interval. In this light the ξ-bound method requires less restrictive V-functions, and it may be expected that as a result many V-functions which fail to specify a region of stability for an ordinary lumped parameter system are still good for this method.

When Equation (8) and (6) are substituted into (5) one obtains:

$$\xi = \max\left[\frac{2(\hat{\eta} - \hat{C})\,\hat{R} - 2G\hat{\eta}^2}{(\hat{C}^2 + \hat{\eta}^2)}\right] \tag{9}$$

The dependence of ξ on τ comes from the fact that $\hat{R}$ in Equation (9) depends on C_s and η_s which in turn are functions of τ. After a region $V \leq \beta$ is specified consistent with practical limitations on the state variables of the reaction system, a region $V \leq \alpha$ is found from Equation (4):

$$\alpha \geqq \beta/\exp\left(\int_{\tau_o}^{\tau_b} \xi d\,\tau\right) \tag{10}$$

provided ξ is known. The region over which ξ is sought needs only to include all possible transients between $V = \alpha$ and $V = \beta$. Other values of $(\dot{V}/V)$ outside this annular region can be ignored, because either the trajectory of the system can never reach that point with $\tau_o < \tau < \tau_b$, or the transients have been sufficiently covered by the relation in Equation (10). Since α depends on both β and ξ, the search for ξ in (10) requires an iterative calculation.

Region $V \leq \alpha$ corresponds to the set of disturbances in a section, which a given steady state can tolerate at $\tau = \tau_o$ such that the transients of this fluid section will be confined in region $V \leq \beta$ when $\tau = \tau_b$ (sufficient condition). Since τ_o and τ_b can be any two points along the τ-axis such that $0 \leq \tau_o < \tau_b \leq \theta_L$, the tubular reactor can be divided into n equal sections, assigning $\tau_o = 0$ and $\tau_b = \theta_n$, the residence time of each small section. By letting the transients at the exit end of the reactor set the bounds on the transients of the entire system, the calculations indicated by Equation (10) can be carried out sequentially from the exit end to the inlet end one small section at a time. Starting at the exit end with given β_e, α_1 is found through (10) by adopting the equality relation. α_1 is then considered as β_2 for the second section and α_2 can be found in a similar manner. Such calculations are repeated for each reactor section from the exit end toward the inlet of the reactor. Eventually this results in a region $V \leq \alpha_0$, which specifies a set of inlet disturbances that will not cause the transients to exceed the region $V \leq \beta_e$ at the exit end. Finally, if the intermediate regions are all connected along the reactor, then the bounding region, Ψ_τ, is obtained, and the region of stability, Ψ_x, for the plug flow tubular reactor system follows directly.

When each section is small enough, the following arrangement can be made to simplify the numerical work, and always put the ξ estimation on the conservative side (the conclusion is always sufficient). Define

$$\xi^* = \max\,(\xi_j) \quad j = 1, 2, 3, \ldots n \tag{11}$$

where j represents the j^{th} reactor section from the exit end. Then, Equation (10) can be combined with (11) to give

$$\alpha\ \exp\,(\theta_n \xi^*) \geqq \alpha\ \exp\left(\int_0^{\theta_n} \xi d\tau\right) \geqq \beta$$

or

$$\alpha \geqq \beta/\exp\,(\theta_n \xi^*) \tag{12}$$

In the event that the transients at some part other than the exit end of a reactor are important in setting up the limiting V-contour in state space, a combination of two working formulas should be used to find Ψ_τ. Suppose, for example, that the k^{th} reactor section from the exit end is to be used as a basis in searching for the region of stability of this reactor system. Working from the k^{th} section back to the inlet, the above working formula can be used with β_k given and the index j increasing from k to n.

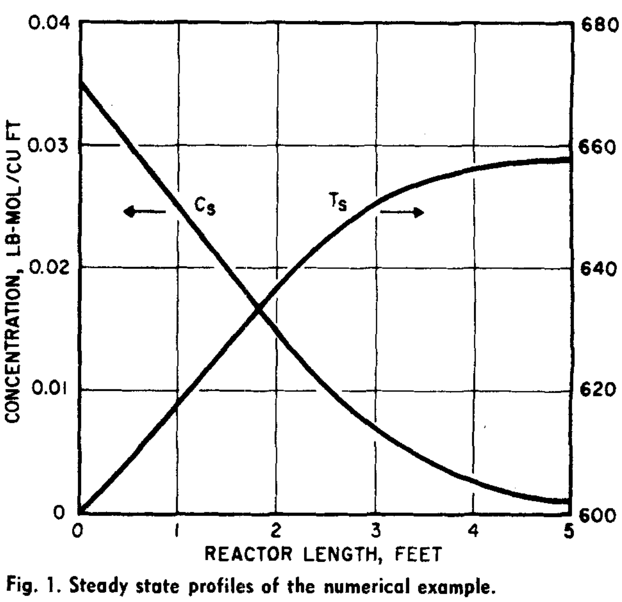

Fig. 1. Steady state profiles of the numerical example.

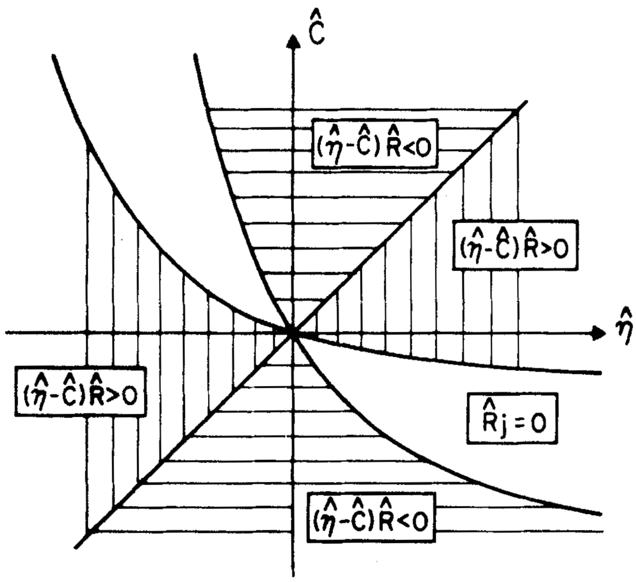

Fig. 2. Regions in CPP showing the signs of $(\hat{\eta}-\hat{C})\hat{R}$.

NUMERICAL EXAMPLE

A hypothetical plug flow tubular reactor system with concentration and temperature as state variables is treated in this section to illustrate the application of the ξ-bound method. The reactor system together with all necessary assumptions is that described by Equations (1), and the following set of physical constants are used:

A	$= 1.2 \times 10^{10}$	1/hr.	
Q	$= .94 \times 10^{4}$	B.t.u./°R.	
ΔH	$= 1 \times 10^{5}$	B.t.u./lb.-mol.	
v	$= 7{,}200$	ft./hr.	
L	$= 5$	ft.	
G	$= 1.4 \times 10^{2}$	1/hr.-lb.-mol.	
ρ	$= 50$	lb./cu.ft.	
C_p	$= 1$	B.t.u./lb.-mol. °F.	
T_w	$= 530$	°R.	
T_i	$= 600$	°R.	
C_i	$= 0.035$	lb.-mol./cu.ft.	
$\overline{C}$	$= 0.25$	lb.-mol./cu.ft.	
$\overline{T}$	$= 1{,}000$	°R.	

The nonlinear reaction rate is chosen as $R = CA \exp(-Q/R)$. The steady state profiles are shown in Figure 1.

Assume that $V \leq \beta_e$ has been given as a circular region about the steady state at the exit end of the reactor. It is required to find a region at the inlet such that disturbances initially within it will have transients at the exit within $V \leq \beta_e$. From a distributed parameter point of view, a bounding region Ψ_x with a given exit-end cross section is to be sought, such that any transient profile that is initially within Ψ_x will never get out. Since it is practical stability (2, 5) that is most important in this analysis, it is assumed that the region furnished by the designer has already been constrained by the practical limitations of the reactor system.

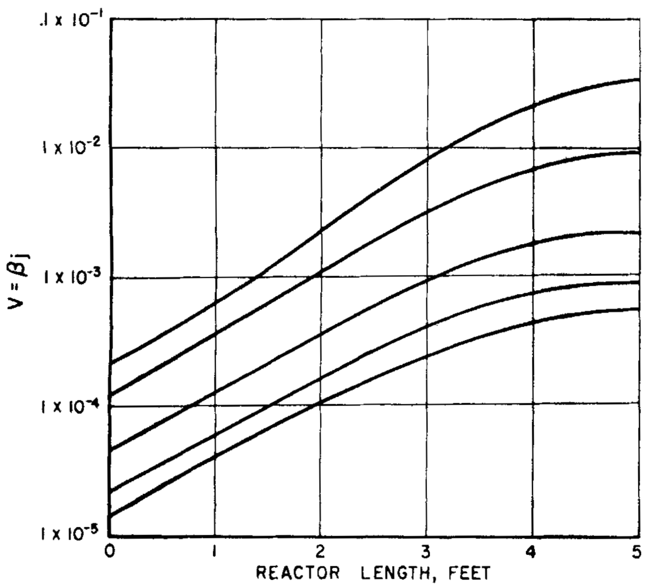

Fig. 3. The profiles of $V = \beta_j$ along the reactor.

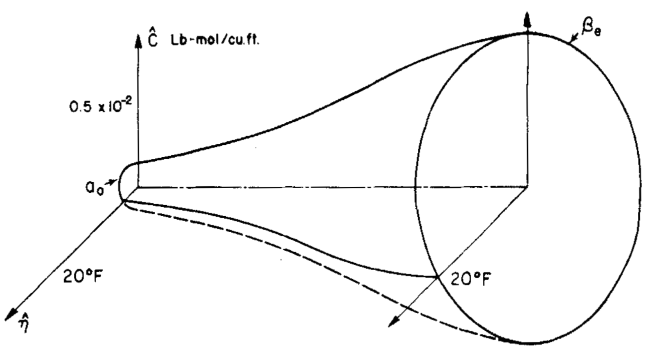

Fig. 4. An isometric view of a typical bounding region.

With the simple circular V-function of Equation (6), the backward formula (12) can be used to find α_o for the inlet end. This entails a numerical search for ξ^*, which may be simplified by the observation from Equation (9), that $(\hat{\eta} - \hat{C})\,\hat{R} > 0$ is a necessary condition for a Max $(\dot{V}/V)$. One should then search for ξ^* only in regions where $(\hat{\eta} - \hat{C})$ and $\hat{R}$ are of the same sign. These regions are shown in the composite phase plane (CPP) of Figure 2 [computational details on $\hat{R}$ may be found elsewhere (7)]. Numerical search for ξ^* may be further simplified by showing that the Max $(\dot{V}/V)$ is always on the boundary of a region where $\hat{\eta} > 0$ (8).

The profiles of $V = \beta_j$ along the reactor with different β_e are plotted on a semilog scale in Figure 3, where the β_e's given correspond to a range from ± 120 to ± 20°F. in temperature disturbances. The calculated α_o's correspond to a range in temperature disturbances from ± 9.7 to ± 3°F. It may be noted that the relative magnitudes of β_e and α_o are not proportional to each other, a result of the exponential nonlinearity in $\hat{R}$. A simple isometric illustration of $V = \beta_j$ along the reactor is shown in Figure 4 for the case of temperature disturbance not to exceed ± 20°F. at exit. The approximate conical region in this figure is Ψ_T or Ψ_x, the region of stability of the plug flow tubular reactor system studied: the boundary surface of

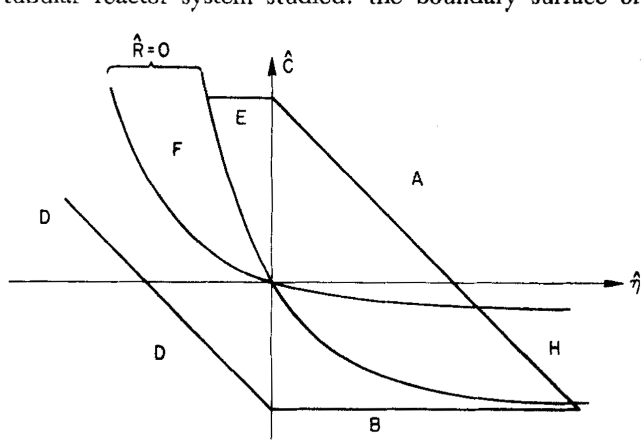

Fig. 5. A composite phase plane diagram (7).

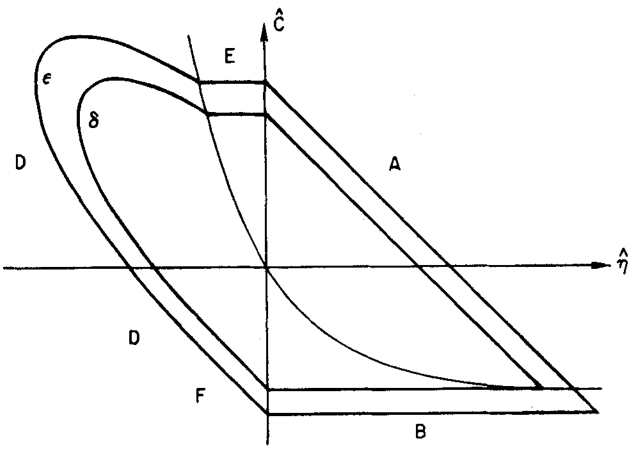

Fig. 6. A typical ε and δ pair for a nonadiabatic PFTR.

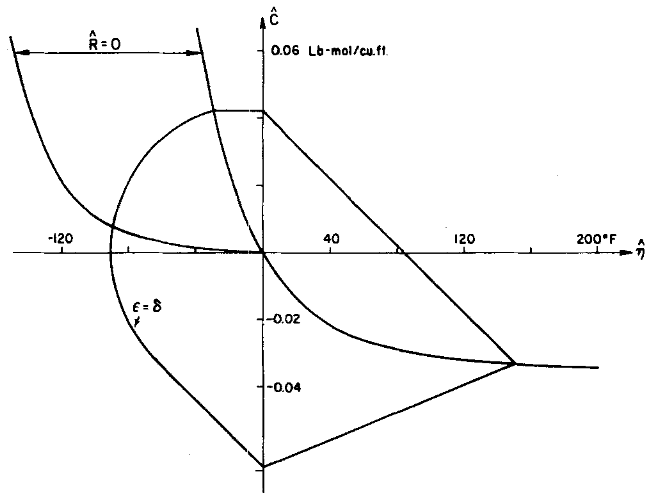

Fig. 8. The ε = δ region of the example: circular V-function.

Ψ_x limits all possible transients of this dynamic system.

The inlet cross section of the regions of stability calculated for this particular example are quite small. Such conservative α_o's are partly due to the exponential dependence of V on the temperature of the system and partly due to the inherent nature of the ξ-bound method. To remedy this shortcoming, this method is combined in the next section with a less conservative technique.

COMBINED ANALYSIS

In an earlier work on plug flow tubular reactor stability (7), it was shown that almost closed regions were attainable with relative ease. The results were less conservative than those just obtained, but were weak to a greater or lesser extent because the regions were not entirely closed. It is clear in comparison that a combination of both approaches can produce results with the best features of each, less conservative, easily computed, closed-regions.

Referring to the composite phase plane (CPP) diagram (from reference 7) in Figure 5, it is evident that the gap in regions D and F is the one previously left open. Because it is open, no assurance can yet be given that transients in the region can be bounded. In order to close this open gap, the ξ-bound method cited before may be adopted just in regions D and F to utilize part of a closed V-contour. In this way it is possible to find a pair of closed V-contours, (α_o, β_e), which bound the transients at inlet and exit, respectively. Such a V-contour can be used to close a gap and as a result, an ε and δ pair may be obtained. Since the open gap is always in regions D and F, only that part of a V-contour that lies in these regions need be considered. In other words, the range in which max $(\dot{V}/V)$ is sought can be restricted within regions D and F, consequently reducing considerably the necessary computations. Recalling from the first example that the largest $(\dot{V}/V)$ in regions D and F is smaller than that in region A, the estimation of δ from ε should be less conservative than would be found by the ξ-bound method alone.

Since the slopes of transients in region D and possibly in region F are between 0 and 135 deg. and their tendencies are toward increasing $\hat{C}$, an elliptical V-contour is proposed in order to cover most of the transients in these regions. As shown in Figure 6, the elliptical V-contour about the origin is inclined at 45 deg. The mathematical expression is

$$V = (a^2 + b^2)(\hat{\eta}^2 + \hat{C}^2) + 2(b^2 - a^2)\hat{C}\hat{\eta} \quad (13)$$

where a and b are the minor and major axes of the ellipse. By differentiating with respect to τ, and substituting Equations (2), yields $DV/D\tau$ along the trajectory of the system as

$$\dot{V} = 4a^2(\hat{\eta} - \hat{C})\hat{R} - 2G\hat{\eta}[a^2(\hat{\eta} - \hat{C}) + b^2(\hat{\eta} + \hat{C})] \quad (14)$$

which may be rearranged to give:

$$\frac{\dot{V}}{V} = -G - \frac{G}{V}(a^2 + b^2)(\hat{\eta}^2 - \hat{C}^2) + \frac{4a^2}{V}(\hat{\eta} - \hat{C})\hat{R} \quad (15)$$

Equation (15) may now be substituted into the recurrence formula (12). The search for ξ^* is along that part of the ellipse that is in regions D and F and above the 45 deg. line. Although elliptical V-contours are used to show the resulting ε and δ in Figure 6, other shapes of V-contour may also be used to close the region.

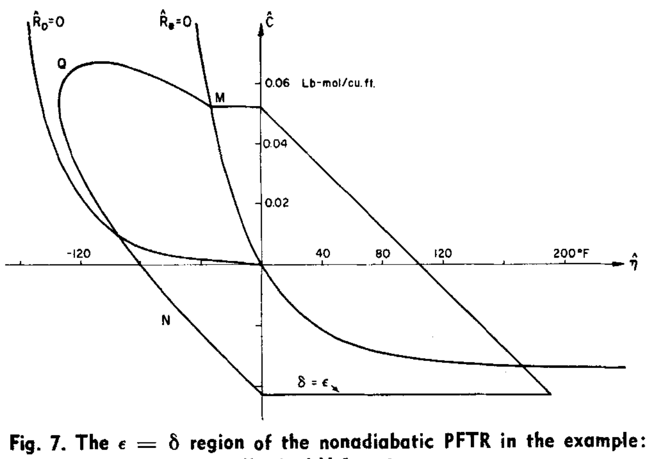

Fig. 7. The ε = δ region of the nonadiabatic PFTR in the example: elliptical V-function.

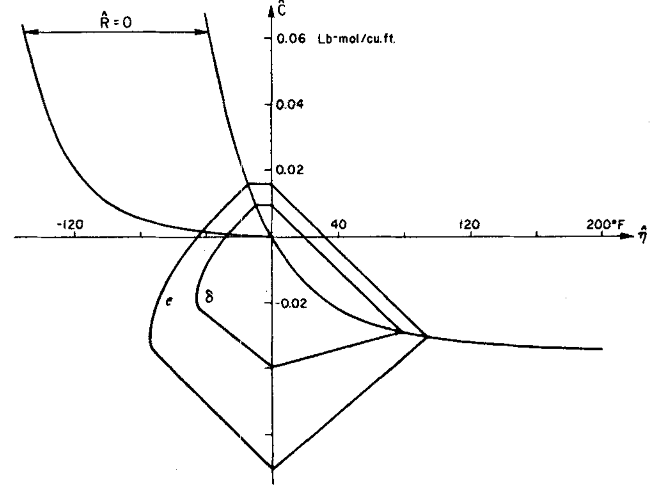

Fig. 9. The ε and δ pair of the example: different elliptical V-function.

One caution must be observed in combining regions from the two techniques. If a V-contour at the inlet is larger than that at the exit ($\alpha_o > \beta_e$), there is no guarantee that all possible disturbances within δ will lead to transients within a smaller ϵ as $\tau \to \theta_L$, because the boundary of δ is based on isoclines and tracking functions which give only limits in slopes and directions of the transients rather than a bound on their rate of growth or decay. For such cases a compromise is reached such that practical stability of the original system is always sufficiently guaranteed, by considering δ as ϵ. A pair of ϵ and δ obtained in this way without considering any physical constraints of the system is shown in Figure 6, establishing a region of practical stability for a nonadiabatic plug flow tubular reactor. The contours labeled ϵ, δ and the area between them are the projection of Ψ_τ.

The features of the combination method may be further illustrated by example. Based on the steady state profiles in Figure 1, the $\hat{R} = 0$ family is represented by the two extreme curves among the family in Figure 7. Inequality constraints on concentration and temperature are assumed as $\overline{\hat{C}}$, $\underline{\hat{C}}$, $\overline{\hat{\eta}}$, and $\underline{\hat{\eta}}$, all being constant. A tilted ellipse is given to replace one of the corners of a parallelogram in the CPP and this closed region shown in Figure 7 is taken as ϵ. The major and minor axes of the ellipse correspond to a temperature disturbance of 130 and 40°F. respectively. The ellipse and the parallelogram are connected at point M where the ellipse crosses one of the extreme curves of the $\hat{R} = 0$ family and at point N where the ellipse is tangent to the 45 deg. line in the third quardrant. The max $(\dot{V}/V)$ is sought according to Equation (15) along MQN on the ellipse. With this max $(\dot{V}/V)$, recurrence formula (12) is used to find α_j sequentially. In the present example, max $(\dot{V}/V)$ along MQN of this particular ellipse ($a{:}b = 1{:}3$) is very small but always negative. The ellipse at inlet is thus larger than the one given with ϵ; hence δ is set equal to ϵ according to the reasoning above. From the $\epsilon = \delta$ region in Figure 7, region Ψ_x is revealed to be a noncircular cylinder along the steady state curve.

To illustrate that different V-contours will give different types of ϵ and δ, two other V-functions were examined for this example. The circular V-contour leads to a similar $\epsilon = \delta$ region in the CPP, while a different elliptical V-contour ($a{:}b = 3{:}1$) gives a δ that is smaller than ϵ. These cases are shown in Figures 8 and 9.

A direct comparison between the combined analysis and the ξ-bound method alone is made in Figure 10 by superimposing one pair of α_o, β_e regions from the latter and ϵ and δ regions from the former on the same CPP It may be observed that the results of the ξ-bound method are quite conservative, for $V \leq \alpha_o$ is much smaller than δ when $V \leq \beta_e$ and ϵ are of comparable sizes. This can be explained by noting that the ξ-bound method always takes the largest $(\dot{V}/V)$ on each V-contour to estimate the next V-contour. In so doing, a fictitious trajectory is traced which represents the worst (most sufficient) trajectory that can be constructed without concern as to whether this trajectory can be one of the possible transients of the system. For instance, curve $PQRS$ in Figure 10 is the fictitious trajectory on which estimation of α_o from β_e is based. At each point on $PQRS$ the slope and tendency of this trajectory are in fact physically unrealizable, for the slope and tendencies of the transients in that region should be bounded by the —45 deg. lines according to the arguments presented earlier. Information on the slopes and tendencies of the transients serve to relax the conservative estimation of the ξ-bound method.

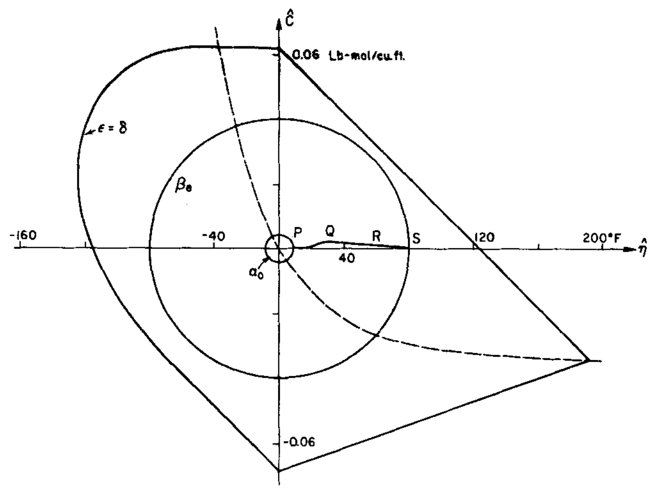

Fig. 10. Comparison of the results from the ξ-bound and combined methods.

ACKNOWLEDGMENT

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NOTATION

A = frequency factor
A_r = heat transfer area per unit volume of reactor
C = concentration of reactant
C_p = specific heat
G = normalized heat transfer coefficient
ΔH = molal heat of reaction
K = over heat transfer coefficient; constraint constant
L = length of a reactor
R = rate of chemical reaction
T = absolute temperature
$\mathbf{U}$ = the state vector $(\hat{C}, \hat{\eta})$
v = velocity of fluid or flow rate in the reactor
x = reactor length

Greek Letters

δ = positive number; region in the state space (or CPP) which corresponds to the inlet end of the reactor
ϵ = region in the state space (or CPP) which corresponds to the exit end of the reactor
η = normalized temperature, $(TC_p\rho/\Delta H)$
θ = time
ρ = density
τ = moving time variable
Ψ_τ = bounding region

Superscripts

$\wedge$ = disturbance variable

Subscripts

i = initial condition
o = inlet condition
s = steady state
L = at exit

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Dispersion in Developing Velocity Fields

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Convective diffusion in laminar flows which develop from rest and in the velocity entrance region of tubes, is studied. Criteria for the validity of the simple dispersion model are established by comparison of analytical results with numerical experiments.

It is found that the extent of dispersion is less in developing velocity fields than in those which are fully developed. This occurs because dispersion is enhanced by differences in the velocity of the fluid particles on a plane perpendicular to the main direction of flow. Such differences are greatest when the flow is fully developed.

Previous work on dispersion in well defined systems has been concerned exclusively with fully developed flows which are independent of the axial coordinate (*1* to *3*, *5*, *7* to *11*, *13*). This is so, even though the velocity entrance region is of considerable practical importance (*12*), primarily because of the apparent mathematical difficulty involved in analyzing such systems.

Another effect which may well influence dispersion experiments is the development of the velocity field from rest. It is easy to see that this is the case in the most easily conceived dispersion experiments with slug stimuli. Probably, the simplest possible way to introduce a slug of fluid into a stream in a well defined manner is to start the system from rest with the slug initially separated from the main body of fluid by partitions on both sides. Indeed it is quite difficult to introduce a well defined slug into a steadily flowing stream without disturbing the flow and distorting the slug. Consequently, it seems desirable to analyze carefully dispersion in flows which start from rest so that the results of such experiments may be interpreted in a completely rational manner. Here, the results of a recent study of dispersion in time variable flow (*8*) are generalized somewhat to provide the basis for performing such an analysis.

It will be shown that the dispersion coefficient is time dependent for time dependent flows and is given explicitly by Equation (22) when the flow develops from rest. Once the dispersion coefficient is known it enables one to predict the average concentration distribution in higher dimensional systems in terms of well known solutions to the one dimensional Equation (9). In so doing, the dispersion model markedly simplifies the theory of convective diffusion.

The purposes of our work in the present article are:

1. to examine analytically the dispersion model for velocity fields in which the components depend on the axial coordinate which is parallel to the main direction of flow as is the case in the velocity entrance region of a tube.
2. to establish approximate limits for the validity of the analytical theory by comparing the results with numerical experiments carried out as finite difference solutions of the convective diffusion equation for the important case of flow in the velocity entrance region of a tube.
3. to examine the effects on dispersion of having the velocity field develop from rest. For this type of time dependent flow we shall determine approximate limits of applicability of the analytical dispersion theory. This will be done also by comparing the analytical theory with finite difference calculations.

ANALYSIS

Consider the velocity field to be prescribed so that $u = u(t, x, r)$ and $v = v(t, x, r)$ are known, continuous functions of time and the spatial coordinates. Consequently the convective diffusion equation in cylindrical coordinates is

$$\frac{\partial c}{\partial t} + u(t, x, r)\frac{\partial c}{\partial x} + v(t, x, r)\frac{\partial c}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r} r\, D_r(t, r)\frac{\partial c}{\partial r} + \frac{\partial}{\partial x} D_x(t, r)\frac{\partial c}{\partial x} \quad (1)$$

Note that we have taken account of turbulence in a phenomenological way by allowing for eddy diffusion in $D_r(t, r)$ and $D_x(t, r)$.

In dimensionless form Equation (1) is

$$\frac{\partial \theta}{\partial \tau} + u_1\frac{\partial \theta}{\partial X} + N_{Pe}\, v_1\frac{\partial \theta}{\partial y} = \frac{1}{y}\frac{\partial}{\partial y} y\, D_1\frac{\partial \theta}{\partial y} + \frac{1}{N_{Pe}^2}\frac{\partial}{\partial X} D_2\frac{\partial \theta}{\partial X} \quad (2)$$

and we shall restrict our attention to boundary conditions of the kind

$$\frac{\partial \theta}{\partial y}(\tau, X, 0) = \frac{\partial \theta}{\partial y}(\tau, X, 1) = 0 \quad (3)$$

The solution of Equation (2) is now formulated as a series expansion in $\partial^k\theta_m/\partial X_1^k$ where X_1 is defined by

$$X_1 = X - \int_0^\tau U(\tau)d\tau$$

and

$$U(\tau) = 2\int_0^1 y u_1 dy \quad (4)$$

Then Equation (2) becomes

$$\frac{\partial \theta}{\partial \tau} + (u_1 - U)\frac{\partial \theta}{\partial X_1} + N_{Pe}\, v_1\frac{\partial \theta}{\partial y} = \frac{1}{y}\frac{\partial}{\partial y} y\, D_1\frac{\partial \theta}{\partial y} + \frac{1}{N_{Pe}^2}\frac{\partial}{\partial X_1} D_2\frac{\partial \theta}{\partial X_1} \quad (5)$$

Now let

$$\theta = \theta_m + \sum_{k=1}^{\infty} f_k(\tau, X_1, y)\frac{\partial^k \theta_m}{\partial X_1^k} \quad (6)$$

where

$$\theta_m = 2\int_0^1 y\theta dy$$