STRUCTURAL STABILITY OF NONLINEAR CONVECTION-REACTION MODELS

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The design and simulation of chemical reactors involves mathematical modeling of the various transport and reaction phenomena occurring in them. Since these processes are often complex, simplifying assumptions are made in developing a model. Detailed models, which include most of the effects, contain a large number of parameters and may be unyielding to analysis or computation, while simplified models having fewer parameters make the task easier. A natural question that arises is whether or not the simplified models retain the qualitative features of the system under investigation. Generally speaking, a model is said to be structurally stable if its qualitative features do not change when it is subjected to small perturbations. Most linear models that remain linear after the perturbation may be shown to be structurally stable. This may not be the case with nonlinear models. The purpose of this article is to illustrate the structural stability of a widely used nonlinear convection-reaction model, namely, the pseudohomogeneous adiabatic plug flow (tubular) reactor model.

This model is based on the assumptions of flat velocity profile, negligible axial dispersion of heat, mass, inter-phase gradients, and no heat loss from the reactor. The model is described by the initial value problem

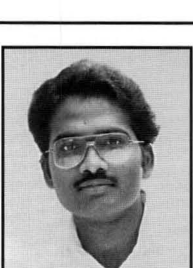
$$\frac{dx}{d\xi} = \mathrm{Da}(1-x)\exp\left(\frac{Bx}{1+Bx/\gamma}\right) \tag{1a}$$

$$\theta = Bx \tag{1b}$$

$$x = 0 \quad \text{at} \quad \xi = 0 \tag{1c}$$

Here, x, θ, and ξ represent the dimensionless conversion, temperature, and distance along the tube, respectively. This model contains three parameters: the dimensionless activation energy (γ), the dimensionless adiabatic temperature rise (B), and the dimensionless residence time or Damköhler number (Da). It reduces to a linear model when one of the reaction parameters (γ or B) is zero. Since it is described by an initial value problem (and the function appearing on the righthand side of Eq. (1a) satisfies the Lipschitz condition), it has a unique solution for all values of the parameters. Equivalently, the bifurcation diagram (or a plot) of exit conversion or temperature versus Da is single valued for all values of the reaction parameters B and γ. When this model is perturbed by including effects such as axial dispersion, recycle, or interphase gradients, the initial value problem becomes a boundary value problem that may have multiple solutions. When the magnitude of the perturbation is small and the boundary value problem has a unique solution, we expect this solution to be close to that of the initial value problem of the plug flow model. But when the boundary value problem has multiple solutions, the qualitative features of the solution are different. In this case, the simplified model does not retain the correct qualitative features. Here, we determine the magnitude of the perturbation at which the qualitative features (*i.e.,* the number of solutions) of the perturbed problem begin to differ from those of the unperturbed problem.

In this paper we will examine four different perturbations of the plug flow model, each containing one extra parameter and reducing to the plug flow model in the limit that the additional parameter (and hence the perturbation) becomes vanishingly small. We will consider the effects of axial dispersion, recycle, discretization (cell model), and



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inter-phase gradients. We place emphasis here on the results and their interpretation and omit the algebraic and computational details.

ANALYSIS OF PERTURBED CONVECTION-REACTION MODELS

Axial Disperson Model

When axial dispersion of heat and mass are included, the adiabatic plug flow model is perturbed to the adiabatic axial dispersion model given by the following two-point boundary value problem:

$$\frac{1}{Pe_m}\frac{d^2x}{d\xi^2}-\frac{dx}{d\xi}+Da(1-x)\exp\left(\frac{\theta}{1+\theta/\gamma}\right)=0 \tag{2a}$$

$$\frac{1}{Pe_h}\frac{d^2\theta}{d\xi^2}-\frac{d\theta}{d\xi}+B\,Da(1-x)\exp\left(\frac{\theta}{1+\theta/\gamma}\right)=0 \tag{2b}$$

$$\frac{1}{Pe_m}\frac{dx}{d\xi}-x=0 \quad \text{at} \quad \xi=0; \qquad \frac{dx}{d\xi}=0 \quad \text{at} \quad \xi=1 \tag{2c}$$

$$\frac{1}{Pe_h}\frac{d\theta}{d\xi}-\theta=0 \quad \text{at} \quad \xi=0; \qquad \frac{d\theta}{d\xi}=0 \quad \text{at} \quad \xi=1 \tag{2d}$$

This model contains two extra parameters, namely the mass and heat Peclet numbers. In order to reduce the number of parameters to one we shall assume that the Peclet numbers are equal (Pe_m=Pe_h). A similar analysis can be done by assuming $Pe_m=\infty$ and Pe_h finite or any fixed ratio of Peclet numbers, but the dispersion (conduction) term in the energy balance must be retained since the nonlinearity of the model is in the temperature. With equal Peclet numbers, the invariant given by Eq. (1b) is valid, and we obtain the perturbed model containing a single extra parameter, namely the Peclet number, Pe:

$$\frac{1}{Pe}\frac{d^2x}{d\xi^2}-\frac{dx}{d\xi}+Da(1-x)\exp\left(\frac{Bx}{1+Bx/\gamma}\right)=0 \tag{3a}$$

$$\frac{1}{Pe}\frac{dx}{d\xi}-x=0 \quad \text{at} \quad \xi=0; \qquad \frac{dx}{d\xi}=0 \quad \text{at} \quad \xi=1 \tag{3b}$$

This form of the axial dispersion model was first analyzed by Hlavacek and Hoffmann[1] in 1970 and many others since then. It reduces to the plug flow model in the limit $Pe\to\infty$. Although our interest is mainly for large Pe values, it should also be pointed out that in the limiting case of Pe approaching zero, x (and θ) becomes independent of ξ, and Eqs. (3a,b) can be integrated to give the CSTR model

$$x-Da(1-x)\exp\left(\frac{Bx}{1+Bx/\gamma}\right)=0 \tag{4}$$

The bifurcation diagram of x versus Da given by Eq. (4) has a hysteresis point at

$$x=\frac{1}{2}\frac{\gamma-4}{\gamma-2}; \qquad \theta=\frac{2}{1-2/\gamma} \tag{5a}$$

$$Da=(1-4/\gamma)e^{-2}; \qquad B=\frac{4}{1-4/\gamma}\equiv B_h \tag{5b}$$

For any fixed $\gamma>4$ and $B<B_h$, the bifurcation diagram of x versus Da is single valued, while for $B>B_h$ it is S-shaped with an ignition and extinction point. For $\gamma\to\infty$ (positive exponential approximation), the hysteresis point coordinates approach the limit $B_h=4, Da=e^{-2}$, and $x=0.5\ (\theta=2)$, while for $B\to\infty$ (negligible reactant consumption or zeroth order reaction) they approach the limit $\gamma=4, Da^*(=BDa)=e^{-2}$, and $\theta=4$.

We now examine how the hysteresis point coordinates change as the Peclet number is increased from zero to infinity. For any finite Pe, the hysteresis point can be calculated using the procedure outlined by Subramanian and Balakotaiah.[2] Figures 1 and 2 show the dependence of the hysteresis point on the Peclet number for three cases ($\gamma\to\infty$, $\gamma=B$, and $B\to\infty$). We will discuss the results

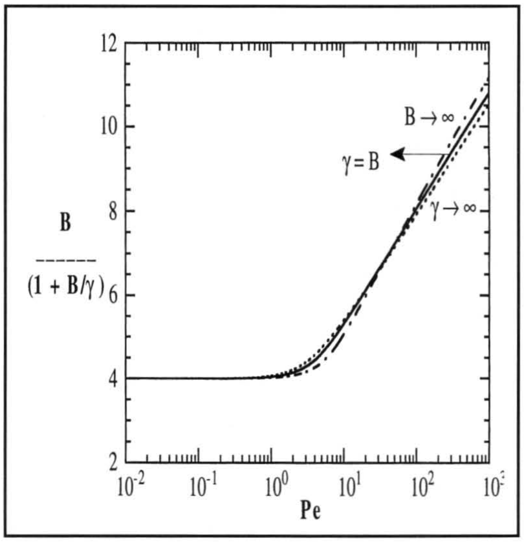

***Figure 1.** Hysteresis locus of the axial disperson model (boundary separating the regions of unique and multiple solutions of Eq. (3)).*

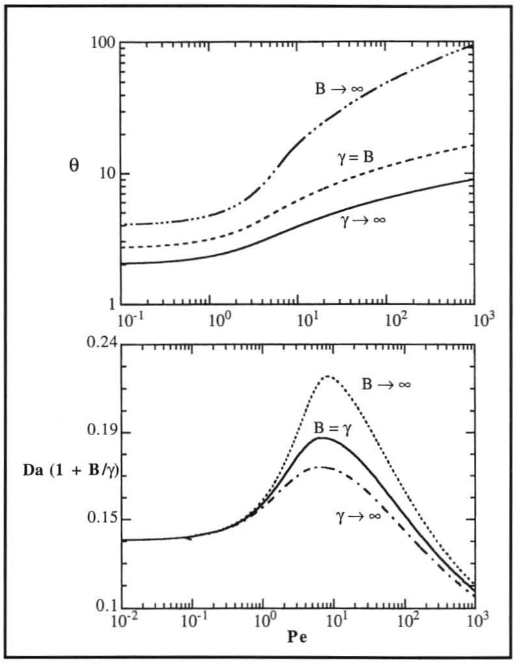

***Figure 2.** Variation of the exit temperature (θ_1) and the residence time (Da) at the hysteresis point with the Peclet number.*

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for the first case only ($\gamma \to \infty$) since the results and their interpretation for the other two cases are similar.

As expected, the coordinates of the hysteresis point approach the CSTR limit for $Pe \to 0$ (Figure 1). For large Pe values, however, B_h is a logarithmic function of Pe. Equivalently, the magnitude of the perturbation (1/Pe value) at which multiple solutions appear is an exponentially small function of B. The results in Figure 2 show that the exit temperature $\theta_1 (= \theta(1))$ and the Damköhler number at the hysteresis point also vary logarithmically with Pe. These results may be anticipated by examining the bifurcation diagram of the plug flow model (for $\gamma \to \infty$) given by the algebraic equation

$$Da = \int_0^{\theta_1} \frac{d\theta}{(B-\theta)\exp(\theta)} \tag{6}$$

Differentiation of Eq. (6) gives

$$\frac{dDa}{d\theta_1} = \frac{\exp(-\theta_1)}{(B-\theta_1)} \tag{7a}$$

$$\frac{d^2Da}{d\theta_1^2} = \frac{(1+\theta_1 - B)\exp(-\theta_1)}{(B-\theta_1)^2} \tag{7b}$$

It follows from Eqs. (7b) and (6) that the bifurcation diagram of the plug flow model has an inflexion point (defined by $d^2Da/d\theta_1^2 = 0$) at $\theta_1 = B-1$, $Da \approx 1/B$, and at which the first derivative is exponentially small ($Da/d\theta_1 = \exp(1-B)$). We also note that the inflexion point nearly satisfies the conditions of a hysteresis point (defined by $dDa/d\theta_1 = 0$, $d^2Da/d\theta_1^2 = 0$). Thus, only an exponentially small perturbation is sufficient to make the first derivative $dDa/d\theta_1$ also zero. By examining the numerical results shown in Figures 1 and 2, it can be verified that an excellent approximation to the hysteresis locus for large B values is given by

$$\frac{2}{Pe} \approx B\exp(2-B) \tag{8a}$$

$$\theta_1 \approx B-1 \tag{8b}$$

$$Da\,B \approx 1 + \frac{1}{B} \tag{8c}$$

In summary, it may be concluded that the plug flow model is structurally unstable to the axial dispersion type perturbation in the sense that the magnitude of the perturbation (1/Pe value) at which multiple solutions appear is an exponentially small function of B. In contrast, the CSTR model is structurally stable since the qualitative features (number of solutions) for Pe = 0 and any small but finite Pe value are the same.

Recycle Model

With the addition of recycle, the plug flow model is perturbed to the boundary value problem

$$\frac{d\theta}{d\xi} = \frac{Da}{1+R}(B-\theta)\exp\left(\frac{\theta}{1+\theta/\gamma}\right) \tag{9a}$$

$$\theta(0) = \frac{R}{1+R}\theta(1) \tag{9b}$$

where R is the recycle ratio. (Again, θ and x are related by the invariant $\theta = Bx$, and we use them interchangeably for convenience.) Integration of Eqs. (9a) and (9b) gives the following relationship between the exit temperature θ_1 and the Damköhler number:

$$Da = (1+R)\int_{\frac{R}{1+R}\theta_1}^{\theta_1} \frac{d\theta}{(B-\theta)\exp\left(\frac{\theta}{1+\theta/\gamma}\right)} \tag{9c}$$

For R=0, Eq. (9c) reduces to the plug flow model, while for $R = \infty$ it reduces to the CSTR model given by Eq. (4)

The hysteresis locus of Eq. (9c) can be determined analytically in a parametric form for any finite γ or B. Since the expressions for the general case are lengthy, we present the results here only for the two limiting cases of $\gamma \to \infty$ and $B \to \infty$. For the first case, the locus is given by

$$\theta_1 = (1+z)\ell n\left(\frac{1+z}{z}\right)\left[1 + z\,\ell n\left(\frac{1+z}{z}\right)\right]$$

$$R = z + z(1+z)\ell n\left(\frac{1+z}{z}\right)$$

$$B = \left[1 + z\,\ell n\left(\frac{1+z}{z}\right)\right]\left[1 + z\,\ell n\left(\frac{1+z}{z}\right) + \ell n\left(\frac{1+z}{z}\right)\right]$$

$$Da = (1+R)\int_{\frac{R}{1+R}\theta_1}^{\theta_1} \frac{\exp(-\theta)}{(B-\theta)}d\theta; \quad 0 < z < \infty \tag{10}$$

and is shown in Figure 3. Again, as expected, the hysteresis point coordinates approach the CSTR limit for $z \to \infty$ ($R = 2z, \theta_1 = 2, B = 4, Da = \exp(-2)$). For $z \to 0$, the parametric representation given by Eq. (10) may be simplified to

$$\theta_1 \approx \ell n\left(\frac{1}{z}\right); \quad R \approx z\left[1 + \ell n\left(\frac{1}{z}\right)\right]; \quad B \approx 1 + \theta_1; \quad B\,Da = 1 + \frac{1}{B} \tag{11}$$

Eliminating z and θ_1 from Eq. (11) gives

$$R = B\exp(1-B) \tag{12}$$

This is a key analytical result showing that the magnitude of the perturbation (recycle ratio) at which multiple solutions appear is an exponentially small function of B. The analytical results given by Eq. (11) for the exit temperature and Da at the hysteresis point are in agreement with Eq. (6).

For the second limiting case of $B \to \infty$ (zeroth order reaction), the hysteresis locus may be calculated explicitly as

$$\gamma_h = \left[\sqrt{R} + \sqrt{1+R}\right]^2 \ell n\left(\frac{1+R}{R}\right) \tag{13a}$$

$$\theta_1 = \gamma_h \sqrt{\frac{1+R}{R}} \tag{13b}$$

$$Da^* = \gamma_c (1+R) \int_{\sqrt{\frac{R}{1+R}}}^{\sqrt{\frac{1+R}{R}}} \exp\left(\frac{-\gamma_h y}{1+y}\right) dy \tag{13c}$$

As expected, Eq. (13a) reduces to the CSTR limit ($\gamma_h = 4$) for $R \to \infty$, while for $R \to 0$ we have

$$\gamma_h \approx \ell n\left(\frac{1}{R}\right)$$

or

$$R \approx \exp(-\gamma_h) \tag{14}$$

Thus, for the case of a zeroth order reaction, the recycle ratio needed to obtain multiple solutions is an exponentially small function of the activation energy. Again, we conclude that the plug flow model is structurally unstable to the recycle-type perturbation.

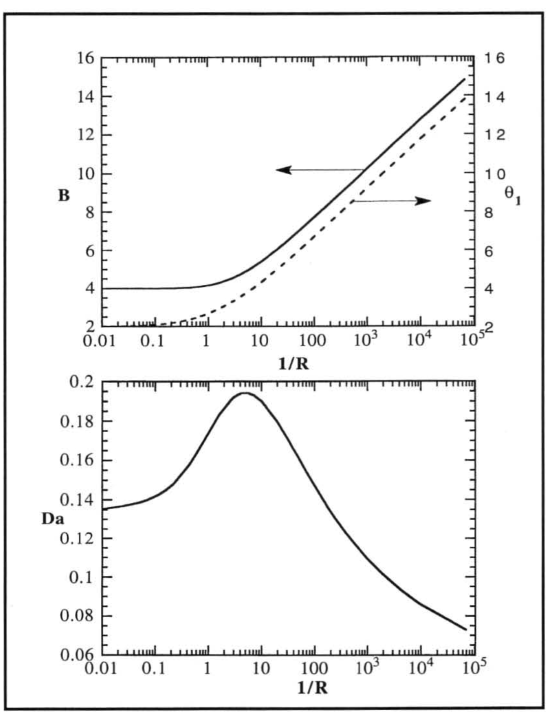

Figure 3. *Hysteresis locus of the recycle model.*

Tanks in Series or Cell Model

The third perturbation we consider to the plug flow model is that of discretization, *i.e.*, replacing the tube by a cascade of well-mixed tank reactors of the same total volume. This model may be obtained by using the following discretization of Eq. (1a):

$$\frac{d\theta}{d\xi} \approx \frac{\Delta\theta}{\Delta\xi} = \frac{(\theta_i - \theta_{i-1})}{\frac{1}{N}}$$

This gives the perturbed model

$$\theta_i - \theta_{i-1} = \frac{Da}{N}(B - \theta_i)\exp\left(\frac{\theta_i}{1+\theta_i/\gamma}\right); \quad i = 1,2,\ldots,N \tag{15a}$$

$$\theta_0 = 0 \tag{15b}$$

with a single extra parameter N, the number of cells. By analyzing Eq. (15a) for each i, it may be reasoned that for any fixed N, hysteresis first appears in the model equation corresponding to tank N. Using this result, we can determine the locus of parameter values at which the cell model begins to exhibit multiplicity behavior.

We consider here only the case of $\gamma \to \infty$. For this case, the hysteresis locus may be calculated using the recursive relations

$$\alpha_N = 2 \qquad \delta_N = 1$$

$$\alpha_{i-1} = \alpha_i(1+\delta_i) \qquad \delta_{i-1} = \delta_i \exp(-\alpha_i \delta_i); \qquad i = N,\ldots,2$$

$$\theta_N = \sum_{i=1}^{N} \alpha_i \delta_i \qquad B = 2 + \theta_N$$

$$Da = N \exp(-\theta_N) \tag{16}$$

The results of the calculation are summarized in Table 1(next page). Again, the value of B at the hysteresis point is a logarithmic function of N and for large N, and the locus may be approximated by the equations

$$\frac{1}{N} \approx B \exp(2-B) \tag{17a}$$

$$\theta_N = B - 2 \tag{17b}$$

$$B\,Da \approx 1 + \frac{1}{B} \tag{17c}$$

It follows from Eq. (17a) that the cell size at which multiple solutions appear is an exponentially small function of the reaction parameter B.

Two-Phase Model

As a fourth and final type of perturbation to the plug flow model, we introduce the interphase heat and mass transfer resistances into the species and energy balances. This gives the two-phase model given by the following set of differential-algebraic equations:

$$\frac{d\theta}{d\xi}=\frac{Da}{Da_{ph}}(\theta_s-\theta); \qquad \theta=0 \ \text{at} \ \xi=0 \tag{18a}$$

$$\theta_s-\theta=\frac{(B-\theta)Da_{ph}\exp\left(\frac{\theta_s}{1+\theta_s/\gamma}\right)}{1+Da_{ph}\exp\left(\frac{\theta_s}{1+\theta_s/\gamma}\right)} \tag{18b}$$

Here, θ_s is the solid phase temperature, while Da_{pm} (Da_{ph}) is the particle mass (heat) Damköhler number. The solid and fluid phase conversions are related to θ_s and θ by

$$x=\frac{\theta}{B} \quad \text{and} \quad x_s=x+\frac{\theta_s-\theta}{B}\frac{Da_{pm}}{Da_{ph}} \tag{18c}$$

As in the case of the axial dispersion model, this perturbed model contains two extra parameters but reduces to the plug flow model when the interphase gradients are negligible ($Da_{pm}\to 0$, $Da_{ph}\to 0$). In order to reduce the number of extra parameters to one, we shall assume that $Da_{pm} = Da_{ph} = Da_p$. Again, a similar analysis can be done by assuming $Da_{pm} = 0$ and a finite Da_{ph} or any fixed ratio of the particle Damköhler numbers, but the interphase heat transfer resistance must be retained since the nonlinearity of the model is in the temperature. With this simplification, the two-phase model may be written as

$$\frac{d\theta}{d\xi}=\frac{\theta_s-\theta}{P}; \qquad \theta=0 \ \text{at} \ \xi=0 \tag{19a}$$

$$\frac{(\theta_s-\theta)}{P}=\frac{Da(B-\theta)\exp\left(\frac{\theta_s}{1+\theta_s/\gamma}\right)}{1+P\,Da\exp\left(\frac{\theta_s}{1+\theta_s/\gamma}\right)} \tag{19b}$$

where we have substituted

$$Da_p=P\,Da; \qquad P=\frac{1}{a_v k_c \tau} \tag{19c}$$

The parameter P, which is the ratio of interphase transfer time ($1/a_v k_c$) to the residence time (τ), plays the same role as that of 1/Pe, R, and 1/N of the previous models.

It may be reasoned that the differential algebraic system defined by Eqs. (19a,b) has a unique solution whenever the particle equation (Eq. 19b) has a unique solution for θ_s for any fixed θ. Equivalently, multiple solutions start to appear in this model whenever the particle equation evaluated at the exit fluid conditions begins to have multiple solutions. Using this observation, the hysteresis locus of the two-phase model for the case of $\gamma\to\infty$ may be determined analytically in a parametric form:

$$\theta_1=(4-u)\exp(u-2)-u; \qquad -\infty<u<2 \tag{20a}$$

$$\theta_s(1)=2+\theta_1; \quad B=4+\theta_1; \quad Da_p=P\,Da=\exp(2-B) \tag{20b}$$

$$Da=\int_{u+\theta_1}^{2+\theta_1}\frac{\left[\exp(-y)-(3+\theta_1-y)\exp(-2-\theta_1)\right]}{(4+\theta_1-y)}dy \tag{20c}$$

This locus is shown in Figure 4. For small values of P, Eqs. (20) may be simplified to

$$\theta_1=B-4; \qquad \theta_s(1)=B-2 \tag{21a}$$

$$B\,Da\approx 1+\frac{1}{B}; \qquad P\approx(B-1)\exp(2-B) \tag{21b}$$

We note that while the two-phase model reduces to the

TABLE 1
Values of the Parameters
at the Hysteresis Point for the Cell Model

N	θ_N	B	Da
1.0000	2.0000	4.0000	0.13534
2.0000	2.5413	4.5413	0.15752
5.0000	3.3862	5.3862	0.16918
10.0000	4.0977	6.0977	0.16611
20.0000	4.8476	6.8476	0.15695
50.0000	5.8685	7.8685	0.14136
100.0000	6.6486	8.6486	0.12958
150.0000	7.1051	9.1051	0.12314
200.0000	7.4284	9.4284	0.11882
400.0000	8.2049	10.205	0.10932
500.0000	8.4539	10.454	0.10653
700.0000	8.8284	10.828	0.10255
1000.0000	9.2242	11.224	0.098628
2000.0000	9.9894	11.989	0.091768
4000.0000	10.750	12.750	0.085790
5000.0000	10.994	12.994	0.084029
10000.0000	11.749	13.749	0.079000

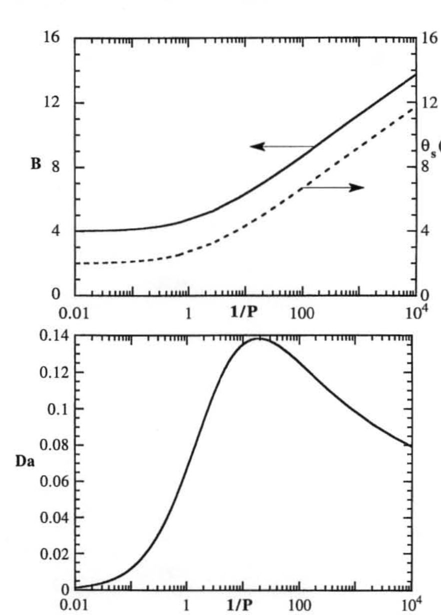

Figure 4. Hysteresis lows of the two-phase model.

plug flow model in the limit of $P \to 0$, it does not approach the CSTR limit for any finite P. But, as for other models, Eq. (21b) shows that the critical value at which multiple solutions appear is an exponentially small function of B.

CONCLUSIONS

The four perturbations we have examined show that the classical plug flow (convection-reaction) model is structurally unstable. We have examined other perturbations such as the inclusion of radial gradients (characterized by the radial Peclet number, Pe_r), heat exchange between the effluent and inlet stream, *i.e.,* autothermal operation (characterized by the Stanton number), and found similar results, *i.e.,* the critical values of these parameters at which multiple solutions appear are exponentially small functions of the reaction parameters (γ or B). We have also examined other types of kinetics and found similar results. For example, for the case of an isothermal Langmuir-Hinshelwood kinetics (which leads to an algebraic nonlinearity), we found that the magnitude of the perturbation at which multiple solutions appear is algebraically small.

The above results can be unified and interpreted better using residence time distribution theory and the homotopy concept.[3] We consider a general convection-reaction model of the form

$$\frac{dc}{d\xi} = \mathrm{Da}\, f(c); \quad c = 1 \text{ at } \xi = 0 \tag{22}$$

where c is the dimensionless concentration (or temperature) and f(c) is the normalized reaction rate (f(1)=1 and f(c)>0 for c>0). Applying each of the four perturbations to Eq. (22), the exit concentration for small values of Da may be expressed as

$$c_e = 1 - \mathrm{Da} + \frac{\mathrm{Da}^2}{2!} f'(1)\left(1+\sigma^2\right) + O\left(\mathrm{Da}^3\right) \tag{23}$$

where

$$\begin{aligned}
\sigma^2 &= \frac{2}{Pe} - \frac{2}{Pe^2}\left(1 - e^{-Pe}\right) && \text{(axial dispersion model)} \\
&= 1/N && \text{(cell model)} \\
&= R/(1+R) && \text{(recycle model)} \\
&= 2P && \text{(two-phase model)}
\end{aligned} \tag{24}$$

is the (normalized) variance of the residence time distribution function. We note that for the first three models, σ^2 lies between zero and unity, with $\sigma^2 = 0$ for the plug flow limit and $\sigma^2 = 1$ for the CSTR limit. The structural stability of the plug flow model can now be stated in a more general form (independent of the specific type of perturbation) as follows: The (plug flow) convection-reaction model defined by Eq. (1) is structurally unstable in the sense that the magnitude of the perturbation (σ^2 value) at which multiple solutions appear is an exponentially small function of the reaction parameters.

DISCUSSION

It is the author's opinion that although the structural stability result illustrated here is quite profound, its implications are not known to most chemical engineers involved in the modeling and simulation of reacting systems. For example, based on the analysis of linear models, it is often stated in the reaction engineering literature (and textbooks) that "axial disperson effects are negligible if the tube is sufficiently long." Another often-used assumption is "interphase gradients are negligible if the mass transfer (heat transfer) coefficient is sufficiently large." These are, at best, misleading statements since we have shown that for an exothermic reaction, the tube length (value of mass transfer coefficient, k_c, or heat transfer coefficient, h) at which axial dispersion (interphase resistance) becomes negligible increases exponentially (and not linearly) with the reaction parameters!

Convection-dominated nonlinear problems are often solved numerically on the computer. Again, intuition derived from the solution of linear models does not apply to nonlinear models. For example, when the linear convective diffusion equation is solved using finite differences, the mesh size is often selected based only on the value of the Peclet number. Our analysis of the cell model, however, showed that the mesh size (needed to retain the features of the formulated model) is an exponentially small function of the reaction parameters.

It is the author's experience that the problem of structural stability is not limited to convection-dominated systems. It also appears in nonlinear diffusion-reaction problems as well as in more complex problems involving fluid flow, heat and mass transfer, and chemical reactions. It is hoped that the results presented here for the simple convection-reaction model serve as a guide in the understanding of these more complex nonlinear problems.

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REFERENCES

1. Hlavacek, V., and H. Hofmann, "Modeling of Chemical Reactors-XVI: Steady-State Axial Heat and Mass Transfer in Tubular Reactors: An Analysis of Uniqueness of Solutions," *Chem. Eng. Sci.,* **25**, 173 (1970)
2. Subramanian, S., and V. Balakotaiah, "Classification of Steady-State and Dynamic Behavior of Distributed Reactor Models," *Chem. Eng. Sci.,* **51**, 401 (1996)
3. Aris, R., "Ends and Beginnings in the Mathematical Modeling of Chemical Engineering Systems," *Chem. Eng. Sci.,* **48**, 2507 (1993) ❒