Sensitivity Analysis of Tubular Packed-Bed Reactor by Pseudohomogeneous 2-D Model

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The sensitivity behavior of the fixed-bed catalytic reactors is examined using the pseudohomogeneous two-dimensional model with radial dispersion for the first-order irreversible reaction. The sensitivity criteria developed are tested. The relations between self-similarity and thermal runaway are studied. The pseudoadiabatic type of operation is taken into consideration. The boundaries of the sensitivity region in the space $Da-Pe$ are compared with those predicted by the standard one-dimensional model and the criterion of Hagan et al. The sensitivity behavior of the system in the space $\alpha - Bi$ is also discussed.

Introduction

The goal of sensitivity analysis is to determine the effect of uncertainties in parameters and initial conditions on the system's behavior. In the chemical reactor theory parametric sensitivity or runaway (Bilous and Amundson, 1956) indicates a particular condition of the reactor operation where, for any given small variation in the reactor input parameters, the steady-state reactor behavior undergoes large changes. In practice, chemical reactors usually are designed to avoid the region of parametric sensitivity. Therefore, the main task of the research in this area is to define *a priori* the region of parametric sensitivity and/or the formulation of the runaway criterion.

Earlier criteria are of a geometric nature and are based on some characteristic behavior of the temperature-conversion or temperature-axial coordinate trajectories. The most widely accepted is that first proposed by Adler and Emig (1964) and further developed by Hlavacek et al. (1969), van Welsenaere and Froment (1970), McGreavy and Adderley (1973), Rajadhyaksha et al. (1975), Soria Lopez et al. (1981), Henning and Perez (1986), and Hosten and Froment (1986). Another geometric method, the isocline method (Chambre, 1956; Oroskar and Stern, 1979), was used by Morbidelli and Varma (1982) to calculate the exact values of the critical parameters bounding the region of parametric sensitivity.

The sensitivity concept was reintroduced into the runaway theory by Boddington et al. (1983). In their formulation the sensitivity of the maximum temperature with respect to the Semenov number takes its maximum at a specific value of the Semenov number named critical value. This condition was generalized by Morbidelli and Varma (1988), who noticed that all sensitivities have their maximum at the same point. This criterion, originally proposed for the explosion model has been extended to further systems (Morbidelli and Varma, 1986a,b; Bauman et al., 1990). The relations between thermal runaway and self-similarity is analyzed by Vajda and Rabitz (1992). The sensitivity functions are shown to satisfy self-similarity relations if and only if the system exhibits critical or supercritical behavior. The condition for criticality reduces to the analysis of the eigenvalues of the Jacobian matrix. The critical values of the parameters estimated by Vajda and Rabitz (1992) are compared with those earlier computed by Morbidelli and Varma (1988) and Adler and Enig (1964) for the thermal explosion model. Also, Vajda and Rabitz (1992) consider their criterion as the most clear result concerning the parametric sensitivity.

In all the cases mentioned previously only the one-dimensional plug flow (pseudohomogeneous or heterogeneous) models of the packed-bed chemical reactor were considered. A model similar to the axial-dispersion model (premixed laminar flame) is analyzed using the rigorous concepts of the local sensitivity by Reuven et al. (1986), but without any reference to thermal runaway.

The limits of the one-dimensional models and the importance of the radial dispersion are thoroughly discussed by Froment and Bischoff (1990). A runaway criterion for the two-dimensional models is made by Hagan et al. (1988a,b). However, the analysis of Hagan et al. (1988a,b) is restricted to the case when $t_{dif}/t_{reac} \ll 1$, where t_{dif} is the timescale on which heat escapes the reactor by diffusing radially to the cooled reactor walls and t_{reac} is the timescale on which the reaction occurs ($t_{dif}/t_{reac} = Pe_h/\kappa \cdot Da$ in our notation). In such situations the two-dimensional model is well-approxi-

mated by the modified one-dimensional model. The runaway criterion, derived using geometric considerations, is obtained on the modified one-dimensional model. The two-dimensional model is used only to verify this criterion.

The purpose of this article is to apply the sensitivity analysis in the manner of Morbidelli and Varma (1988) and Vajda and Rabitz (1992), and to find the relations between sensitivity and self-similarity for the pseudohomogeneous two-dimensional reactor model. The preceding criteria were deduced on lumped-parameter models. The model used in this article is a distributed-parameter model. These statements make it possible for the point of this article to be viewed as a test of applying relations established for lumped-parameter models to a distributed-parameter model.

Model and Sensitivity Equations

The mass and energy balances, in dimensionless form, for the pseudohomogeneous two-dimensional model with cocurrent external cooling and a single irreversible reaction are represented by the following equations (Puszynski et al., 1981):

$$\frac{\partial x}{\partial z} = \frac{\kappa}{Pe_x^r}\left(\frac{\partial^2 x}{\partial r^2} + \frac{1}{r}\frac{\partial x}{\partial r}\right) + Da\cdot(1-x)\cdot\exp\left(\frac{\theta}{1+\mu\theta}\right) \quad (1)$$

$$\frac{\partial \theta}{\partial z} = \frac{\kappa}{Pe_\theta^r}\left(\frac{\partial^2 \theta}{\partial r^2} + \frac{1}{r}\frac{\partial \theta}{\partial r}\right) + B\cdot Da\cdot(1-x)\cdot\exp\left(\frac{\theta}{1+\mu\theta}\right) \quad (2)$$

$$\frac{d\theta_c}{dz} = \alpha\cdot Bi\cdot\frac{\kappa}{Pe_\theta^r}\cdot(\theta|_{r=1} - \theta_c), \quad (3)$$

with the initial and boundary conditions:

$$z = 0.0; \quad x = \theta = \theta_c = 0.0 \quad (4)$$

$$r = 0; \quad \partial x/\partial r = \partial\theta/\partial r = 0 \quad (5)$$

$$r = 1; \quad \partial x/\partial r = 0; \; -\partial\theta/\partial r = Bi\cdot(\theta - \theta_c) \quad (6)$$

The sensitivity criteria applied in this article are well-presented by their authors, Morbidelli and Varma (1988) and Vajda and Rabitz (1992), and it is not necessary to be reproduced in detail.

The criterion of Morbidelli and Varma (1988) is based on the local sensitivity analysis (Tilden et al., 1981). In the local sensitivity analysis, the sensitivity information is embodied in the so-called sensitivity coefficients. Indicating any of the reactor parameters as ϕ, the local sensitivity of Y (Y being x, θ and θ_c), that is, the first-order sensitivity coefficient is defined as

$$s(Y,\phi) = s_{Y,\phi} = \partial Y/\partial\phi. \quad (7)$$

There are two ways to compute the sensitivity coefficients, the direct method (Tilden et al., 1981) and the variational method (Tilden et al., 1981). The direct method is used here due to the fact that the pseudoadiabatic behavior is taken into account. Also, in the generic parameter ϕ, the Pe numbers are not included.

In the direct method the sensitivity coefficients are governed by the sensitivity equations

$$\frac{\partial s_{x,\phi}}{\partial z} = \frac{\kappa}{Pe_x^r}\left(\frac{\partial^2 s_{x,\phi}}{\partial r^2} + \frac{1}{r}\frac{\partial s_{x,\phi}}{\partial r}\right) + \frac{\partial R}{\partial x}s_{x,\phi} + \frac{\partial R}{\partial\theta}s_{\theta,\phi} + \frac{\partial R}{\partial\phi} \quad (8)$$

$$\frac{\partial s_{\theta,\phi}}{\partial z} = \frac{\kappa}{Pe_\theta^r}\left(\frac{\partial^2 s_{\theta,\phi}}{\partial r^2} + \frac{1}{r}\frac{\partial s_{\theta,\phi}}{\partial r}\right) + \frac{\partial R'}{\partial\theta}s_{\theta,\phi} + \frac{\partial R'}{\partial x}s_{x,\phi} + \frac{\partial R'}{\partial\phi} \quad (9)$$

$$\frac{ds_{\theta_c,\phi}}{dz} = \frac{d}{d\phi}\left(\alpha\cdot Bi\cdot\frac{\kappa}{Pe_\theta^r}\right)\cdot(\theta|_{r=1} - \theta_c) + \alpha\cdot Bi\cdot\frac{\kappa}{Pe_\theta^r}\cdot(s_{\theta,\phi}|_{r=1} - s_{\theta_c,\phi}) \quad (10)$$

where ϕ stands for any of the parameters α, B, Bi, Da, and μ, and R is the reaction rate expressions ($R = Da\exp(\theta/(1.0 + \mu\theta))$, $R' = B\cdot R$). The initial and boundary conditions are

$$z = 0.0; \quad s_{x,\phi} = s_{\theta,\phi} = s_{\theta_c,\phi} = 0.0 \quad (11)$$

$$r = 0; \quad \partial s_{x,\phi}/\partial r = \partial s_{\theta,\phi}/\partial r = 0.0 \quad (12)$$

$$r = 1; \quad \partial s_{x,\phi}/\partial r = 0; \; -\partial s_{\theta,\phi}/\partial r = d/d\phi(Bi)(\theta - \theta_c) + Bi(s_{\theta,\phi} - s_{\theta_c,\phi}). \quad (13)$$

Equations 8–13 are obtained by differentiating the model Eqs. 1–6 with respect to ϕ. The direct approach consists of solving 1–6 together with 8–13 to obtain the sensitivity coefficients.

Previous analysis dedicated to the numerical solution of the two-dimensional model (Finlayson, 1972; Mihail and Iordache, 1976) indicate as the most performant method the reduction of the partial differential equations to ordinary differential equations by discretizing the radial derivatives with the orthogonal collocation method and the integration of the resultant ODE system with an adequate method. The same way is followed in this article. The radial derivatives were discretized with the orthogonal collocation method (Finlayson, 1972). Eight internal collocation points were used. The resulting ODE system was solved using the Deuflhard (1983) semi-implicit method. The Vajda and Rabitz (1992) criterion needs the evaluation of the spectrum of the Jacobi matrix of the righthand side of the system 1–3. The Jacobian eigenvalues are computed using MATHLAB.

Results

Two problems are the main subjects of this section. The first refers to the specific ways in which the sensitivity criterion of Morbidelli and Varma (1988) and Vajda and Rabitz (1992) can be applied to the two-dimensional model. The second concerns the influence of the Pe/κ parameters on the system sensitivity behavior.

The parameters' values are considered according to the recommendation made in Froment and Bischoff (1990), Young and Finlayson (1973), and Puszynski et al. (1981). Of

course, when the definitions of these parameters differ from those used here the necessary transformations are made. Concerning the choice of the ratio between the mass and heat *Pe* numbers (the Lewis number *Le*), Froment and Bischoff (1990), for the *o*-xylene oxidation reactor, obtained $Le \approx 2$. For the CO oxidation reactor, in Puszynski et al. (1981), $Le \approx 10.0$. The value found by Young and Finlayson (1973) for the SO_2 oxidation reactor is composed between the above values. The values 2.0 and 10.0 are considered limit values of the *Le* number in this article.

As usual in the sensitivity analysis, the results are reported in terms of normalized sensitivity, defined as

$$S_{Y,\phi} = \phi/Y \cdot s_{Y,\phi}. \tag{14}$$

To alleviate the agglomeration in figures, no more than three or four curves are depicted.

To present in detail the sensitivity of the system, two parameter sets, which lead to typical behaviors, are selected. In the first case the hot spot is presented. The second corresponds to the pseudoadiabatic operation.

The parameter values of the first case are $B = 20.0$, $Bi = 10.0$, $Pe_h/\kappa = 0.30$, $Pe_m/\kappa = 0.60$, $\mu = 0.06250$. The *Da* number is the varying parameter. In Figure 1 the values of the normalized sensitivities of the maximum temperature (for $r = 0.0$) are shown as functions of the *Da* number for various selections of the generic parameter ϕ. It can be observed that *S* exhibits an extreme value at a specific value of *Da*, which is substantially independent from the parameter ϕ. The same behavior can be viewed for the wall temperature in Figure 2. The differences of the parameter critical values predicted by the two temperatures is very small. The critical *Da* number, Da_c, is equal to $Da_c = 0.4381$ in Figure 1 and $Da_c = 0.4383$ in Figure 2. A similar behavior was observed for the sensitivity conversion coefficients. Differences between the critical values predicted by the usual sensitivities *s* and the normal-

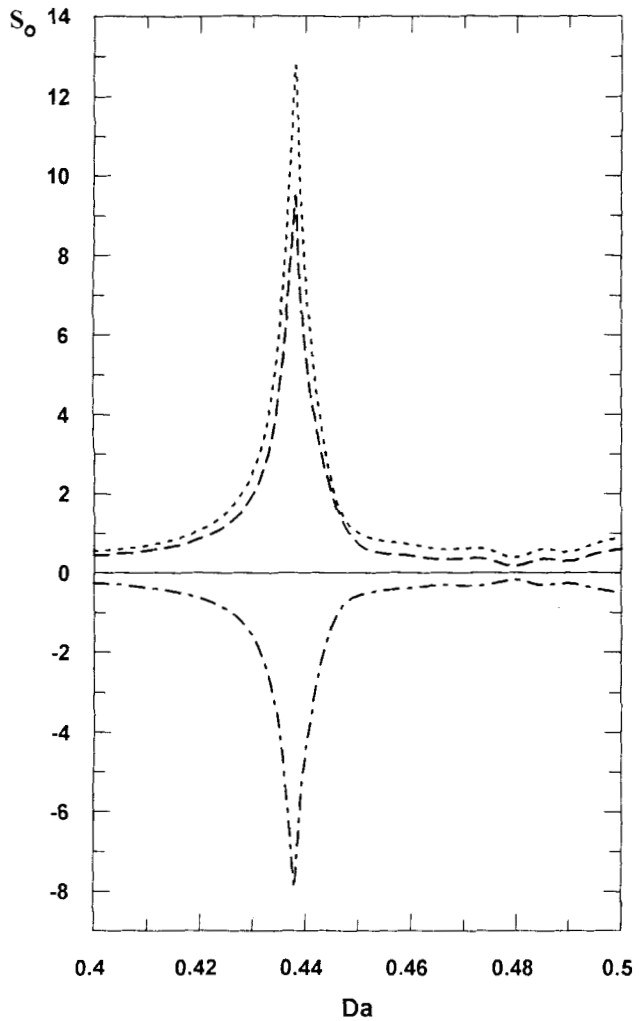

Figure 1. Normalized sensitivity S_ϕ of the maximum reactor dimensionless temperature at $r = 0.0$ as a function of the Damköhler number, *Da*, for various input parameters ϕ and $B = 20.0$, $Bi = 10.0$, $Pe_h/\kappa = 0.30$, $Pe_m/\kappa = 0.60$, $\alpha = 0.0$ and $\mu = 0.06250$: -- ($\times 10^{-1}$) $\phi = Da$, ...($\times 10^{-1}$) $\phi = B$, -·- $\phi = \mu$.

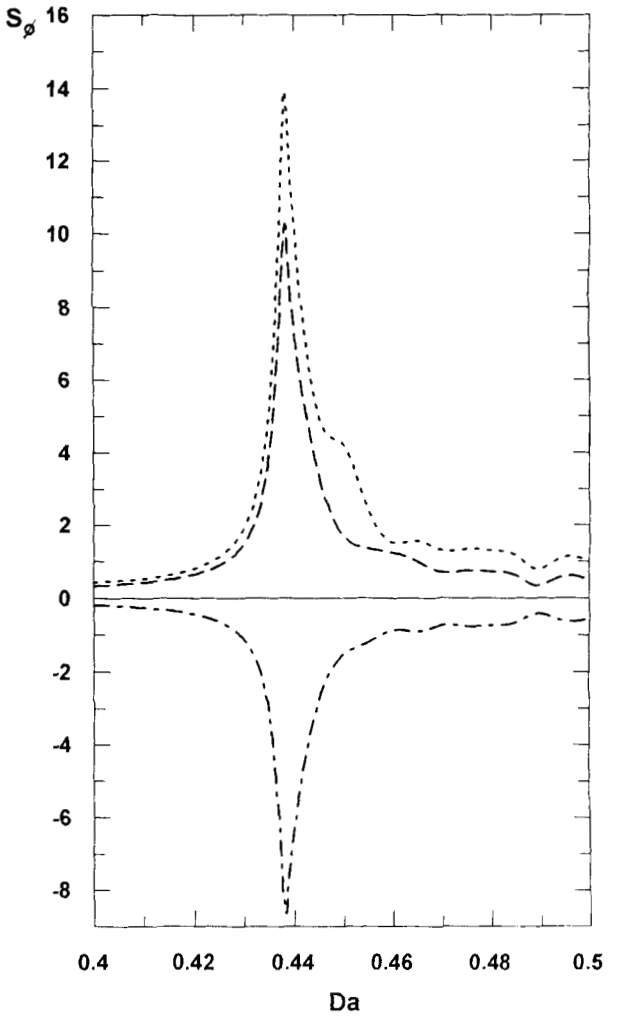

Figure 2. Normalized sensitivity $S\phi$ of the maximum reactor dimensionless temperature at $r = 1.0$ as a function of the Damköhler number, *Da*, for various input parameters ϕ and $B = 20.0$, $Bi = 10.0$, $Pe_h/\kappa = 0.30$, $Pe_m/\kappa = 0.60$, $\alpha = 0.0$, and $\mu = 0.06250$: --($\times 10^{-1}$) $\phi = Da$, ..., ($\times 10^{-1}$) $\phi = B$, -· · · -$\phi = \mu$.

ized sensitivities S were not observed. So, it can be concluded that both the generalized criterion of Morbidelli and Varma (1988) and the self-similarity principle apply. Figure 3 shows the variation of the larger real part of the Jacobian matrix eigenvalues function of the Da number. The two curves correspond to the maximum central reactor temperature and the maximum wall temperature, respectively. First, it must be said that the system exhibits, in the depicted domain, one positive eigenvalue, the other being negative. Figure 3 shows that the eigenvalue computed to the reactor central hot spot exhibits, after the first local maximum, other local extremum points. Significant changes in the system behavior at these extremum points were not observed. The first local maximum at $Da = 0.4368$ seems to be important and this Da value can be adopted as the critical value. To insist on the spectrum computation is not too fair because the eigenvalues are calculated on a discrete approximation, which is not unique, and not on the continuous system. The variation of the wall eigenvalue provided a smaller critical value for the Da number ($Da_c = 0.43530$).

The differences in the critical parameter values, provided by the criteria considered, are very small (less than 1%) and probably are due more to the numerical approximation used.

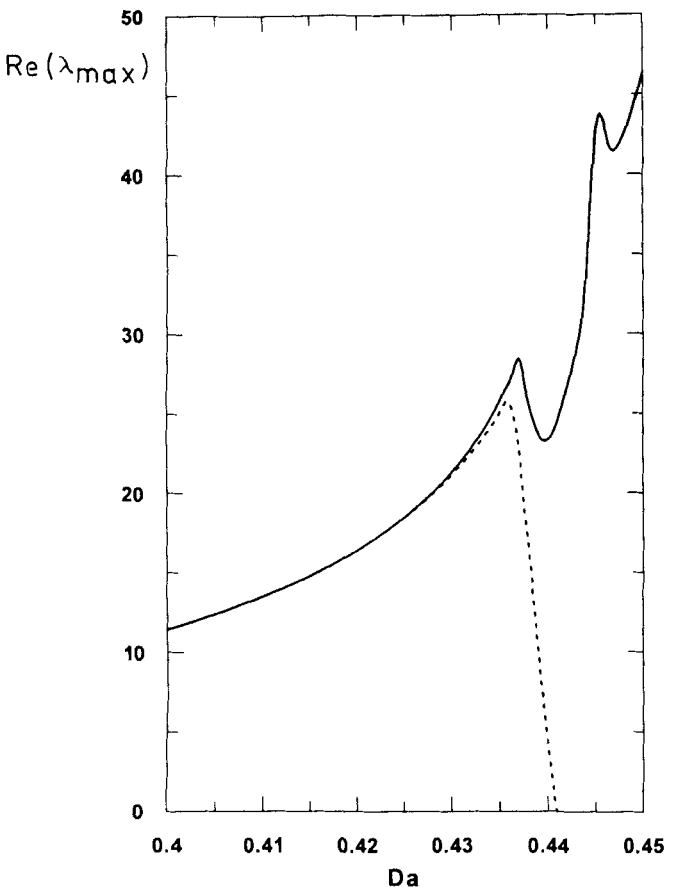

Figure 3. Larger real part of the maximum dimensionless temperature Jacobian eigenvalues as function of the Da number at $B = 20.0$, $Bi = 10.0$, $Pe_h/\kappa = 0.30$, $Pe_m/\kappa = 0.60$, $\alpha = 0.0$, and $\mu = 0.06250$: — $r = 0.0$, ..., $r = 1.0$.

So, it can be concluded that these computations confirm the validity and the coincidence of these criteria.

The parameter values of the second chosen case are $B = 20.0$, $Bi = 10.0$, $Pe_h/\kappa = 1.0$, $Pe_m/\kappa = 10.0$, $\alpha = 0.0$, $\mu = 0.06250$. The behavior of the system for this parameter set can be synthesized by the following statements:

- The thermal runaway is present;
- In the critical domain the temperature reaches its maximum at $z = 1$ for all radial positions;
- Both the criteria of Morbidelli–Varma and Vajda–Rabitz can be applied;
- The self-similarity principle is valid;
- The critical Da number values are $Da_c = 0.1453$ ($r = 0.0$) and $Da_c = 0.1489$ ($r = 1.0$) (Morbidelli–Varma criterion); $Da_c = 0.1453$ (Vajda–Rabitz criterion).

Because any new or spectacular result was not detected in the analysis of this parameter set, no more details seem to be necessary.

The usual result of the runaway analysis is the trace of the sensitivity domain boundaries in the parameter space. Even though the model used in this article is for the first time sensitivity analyzed, the effect of the reaction parameters (B, Da, γ) or the heat-transfer parameters (α and Bi) is previsible. For this reason the analysis is focused on the effect of the parameter Pe/κ on the sensitivity behavior.

The critical curves in the space $Pe_h/\kappa - Da$ are shown in Figure 4. The values of the other parameters are $B = 20.0$, $Bi = 10.0$, $\alpha = 0.0$, and $\mu = 0.06250$. The sensitivity domain is situated above the curves. For any value of Le between 2 and 10, the resultant critical curves belong to the space delimitated by the curves depicted in Figure 4. The sensitivity criterion used to trace these curves is that of Morbidelli and Varma (1988) applied to the reactor central temperature. For the standard one-dimensional model (SODM), the Morbidelli–Varma criterion is used.

In the previous studies the usual comparison made is between the runaway geometrical criteria and the runaway criteria based on the mathematical sensitivity theory. The limits of the geometrical runaway criteria are well-established on the SODM, and it is not necessary to reproduce them here. The Hagan et al. (1988a,b) criterion was derived on a modified one-dimensional model and was not taken into consideration too much until now. For this reason the comparison is made here with the SODM and Hagan et al. criterion.

For a fair comparison between the SODM and the two-dimensional model, a correct correspondence between the different parameters of these models must be established. The reaction parameters Da, B, and μ are identical for the two models. To convert the Pe and Bi numbers of the two-dimensional model into the dimensionless heat-transfer coefficient β of the SODM, the relation developed by Finlayson (1972),

$$\beta = Bi(6\kappa/Pe_h)/(3.0 + Bi)$$

is used. The Hagan et al. (1988) criterion does not necessitate any transformation of the parameters model.

Figure 4 shows that the Pe_m number influences the sensitivity boundary domains only for values of the Pe_h/κ parameter smaller than 1.0 and not in a significant manner. The

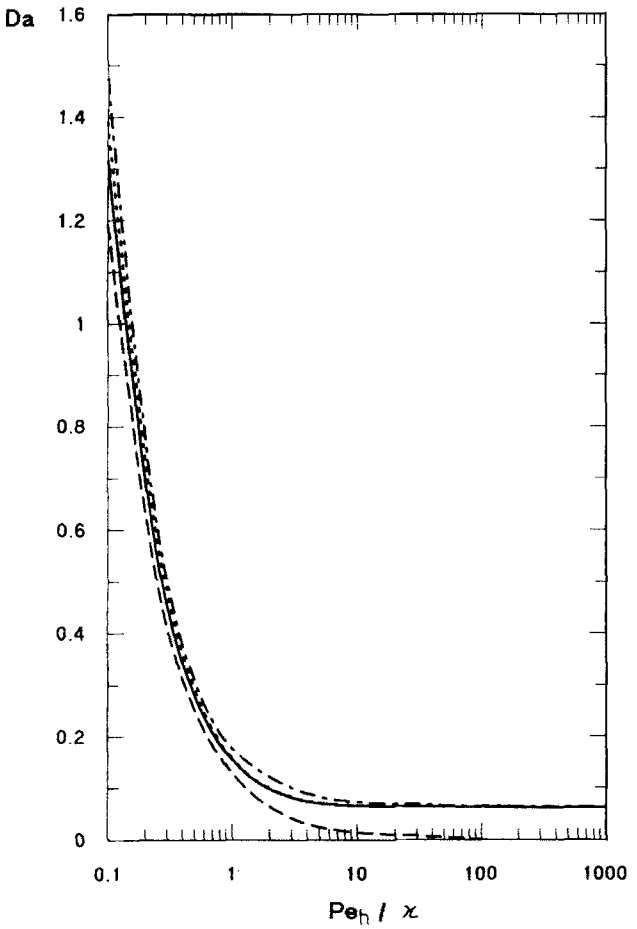

Figure 4. Parameteric sensitivity regions in the $Da-Pe_h/\kappa$ reactor parameter space at $B=20.0$, $Bi=10.0$, $\alpha=0.0$, $\mu=0.06250$: — $Le=2.0$, ... $Le=10.0$, –·– SODM; – – Hagan criterion.

maximum relative difference between the two curves is not greater than 8%. With the increase of the Pe_h/κ number the Da_c decreases, tending to an asymptotic value for $Pe_h/\kappa > 10.0$. From Figure 4, it can also be seen that the critical values predicted by the SODM are close to those predicted by the two-dimensional model. It is obvious that the SODM could not take into account the Pe_m number variation for a given Pe_h/κ value. The critical values predicted by the SODM are greater than those of the two-dimensional model. However, the maximum relative difference is 7% (in comparison the values obtained at $Le=10.0$ are used). Similar behavior was observed in other $\phi - Pe_h/\kappa$ spaces, ϕ being B, μ, or Bi. The Hagan criterion can be safely applied only for $Pe_h/\kappa \leq 1$. In this domain the critical values predicted are lower than those of the two-dimensional models (the maximum relative difference is 10% from the $Le=2$ curve). Note that Hagan et al. (1988) considered $Le \equiv 1$. At high values of the Pe_h/κ values, the main assumptions used by Hagan et al. (1988), that is, $Pe_h/\kappa \cdot Da \ll 1$ in our notations, implies $Da \rightarrow 0$ and the comparison becomes senseless.

The previous results show that the two-dimensional model sensitivity behavior, in the usual parameter spaces, can be anticipated relatively accurately from the predictions of the one-dimensional models. One can conclude that the SODM provides conservative results. In these conditions it is not necessary to insist on this way. Bauman et al. (1990) have shown, for the one-dimensional model, that in the parameter space $\alpha - \beta$ (β being the dimensionless heat-transfer coefficient that also contains reaction parameters) the sensitivity criterion of Morbidelli–Varma is no longer generalized for sufficiently high values of α. The last problem analyzed in this article is the sensitivity behavior of the two-dimensional model in the $\alpha - Bi$ parameter space. The reason is to verify if the same phenomenon occurs to the two-dimensional model.

As was mentioned by Bauman et al. (1990), the increase of α causes a strong decrease in the extreme values of the normalized sensitivity functions. The hot spot sensitivities defined for parameters α and B functions of the Bi number exhibit many local extreme values of the same magnitude. Also there exists a positive real eigenvalue of the Jacobian; the Bi variation of this eigenvalue is similar to that encountered at the normalized sensitivity functions. From these facts the conclusion can be drawn that the system in this region does not exhibit thermal runaway.

Conclusions

The sensitivity criteria previously proposed by Morbidelli and Varma (1988) and Vajda and Rabitz (1992) in the context of thermal explosion theory have been tested on the pseudohomogeneous two-dimensional model of the packed-bed tubular reactor. In both, the preceding criteria thermal runaway and self-similarity are defined in terms of parameter sensitivity functions but are independent from the choice of a particular parameter being perturbed. The analysis covers both cases when the hot spot is present and the pseudoadiabatic operation type.

The results show that both criteria previously mentioned can be applied to the pseudohomogeneous two-dimensional model, and the self-similarity principle is valid. The pseudoadiabatic regime exhibits both parametric sensitivity and self-similarity. The region of parametric sensitivity in the reactor parameter space $Da - Pe_h/\kappa$ is reported for various values of the ratio Pe_m/Pe_h. Comparison is made with the predictions of the SODM and the Hagan et al. (1988) criterion. An important result of the analysis is the closure between the sensitivity frontiers predicted by the one-dimensional and the two-dimensional models, respectively. The loss of the generality of the Morbidelli-Varma criterion in some parameter spaces—in this article the $\alpha - Bi$ parameter space—is explained as a lack of criticality in these spaces.

Notation

B = dimensionless adiabatic temperature rise, $-\Delta H_R C_o/\rho C_p T_o \mu$
Bi = Biot number, $h_w d/2\lambda_R$
C = concentration
C_p = heat capacity
d = reactor diameter
Da = Damköhler number for mass, $k_o e^{-1/\mu} L/v$
D_R = radial effective diffusivity
E = activation energy of the reaction
h_w = wall heat-transfer coefficient
ΔH_R = heat of reaction
k_o = preexponential factor

L = reactor length
Pe_x^r = radial Peclet number for mass, $vd/2D_R$
Pe_θ^r = radial Peclet number for heat, $\rho C_p v d/2\lambda_R$
r = dimensionless radial position, $2r'/d$
r' = radial position
R_g = gas constant
T = temperature
v = velocity of the gas phase
w = coolant flow rate
x = conversion $(C_o - C)/C_o$
y = axial position
z = dimensionless axial position, y/L

Greek letters

α = ratio of reactant to coolant heat capacity, $2\pi R_2 v \rho C_{p,g}/wC_{p,c}$
λ_R = radial effective thermal conductivity
μ = dimensionless activation energy, $R_G T_o/E$
ρ = density
θ = dimensionless temperature $(T - T_o)/\mu T_o$
$\kappa = 2L/d$

Subscripts

c = coolant
o = feed
g = reactant

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