STEADY STATE PROFILES AND STABILITY OF ADIABATIC PACKED BED REACTORS

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ABSTRACT

A few catalytic reactions carried out on the industrial scale are characterized by a large energy-transport parameter and low Thiele parameter. As a consequence a part of the reactor operation resides in a regime of kinetic control where the adiabatic effectiveness factor may go through a maximum. Therefore the effectiveness factor has been used explicitly in the reactor analysis based on the cell model. A modified graphical marching technique for the computation of the steady state profiles is used and the equations on which this is based have been analysed for deriving a uniqueness criterion for the steady state :

$$\bar{J} \geqslant \frac{4e^{-A}}{\gamma^2} e^{(\gamma-2)} \cdot \frac{M}{(H+1)}$$

A linearized stability analysis has resulted in the formulation of the following necessary and sufficient conditions for local stability:

$$\frac{dQ^-}{dT_p} > \frac{(H+1)}{H} \frac{dQ^+}{dT_p}$$

$$\frac{\delta_o R T_{ps}}{E} \left(\frac{T_{po}}{T_{ps}}\right)^2 > \frac{h_{Fs}}{4} \left(\frac{\delta \eta}{\delta h_F}\right)_s$$

Key Words: Adiabatic packed bed reactors; Stability; Cell Model,

INTRODUCTION

The necessary and sufficient conditions of local stability of a packed bed reactor, modelled as a sequence of well stirred cells, have been obtained by Vanderveen and co-workers [1] by examining the characteristic polynomial of the set of linearized dynamic conservation equations written for each of the cells. These conditions are stronger than those obtained when only the local perturbation of the catalyst particle is considered. Based on the cell model, Berty and others [2] have recently analysed the transient adiabatic behavior of a pilot plant for the oxidation process of a hydrocarbon. Their investigations have shown the strong influence of radiative heat transfer in the propagation of the high temperature reaction zone. Narasimhan [3] in his analysis of the analogous case of gas-soild non-catalytic reatctions has obtained a condition of sectional stability and has indicated an inequality criterion based on the system properties and inlet conditions that guarantees stable operation for the whole reactor. A modified graphical marching technique has also been indicated for the computation of steady state profiles that has resulted in significant economy in computational effort. This technique bears some strong elements of similarity with those adopted for the steady state graphical analysis of conventional staged processes.

Carberry [4] has investigated the effect of transport processes in catalytic reactor design in some detail and for the system of competing and consecutive reactions in naphthalene oxidation has shown that under the usual operating conditions the ratio of adiabatic and isothermal effectivene s factor is close to unity. Consequently the characterization of the effectivene factor as isothermal at the particle surface temperature has been justified One can therefore conclude that the system operates wholly in a regime of pore diffusion control with high Thiele parameter and low δ, lhe energy-transport parameter (lower than critical δ equal to $0 \cdot 3$ obtained by Petersen) at which non-isothermal effects may be ignored. In a recent critical review concerning the dynamics and control of fixed bed reactors Ray [5] has referred to a table of pertinent parameters of representative industrial catalytic exothermic reactions compiled by Halvacek and co-workers (6). In such a table one can pick out several systems characterized by low Thiele parameter h and high δ values. As such it could be inferred that the processes operate, at least a significant part, in a regims of kinetic control where the adiabatic effectiveness factor goes through a maximum. It may so happen that with a feeble catalyst (large E) and a high heat of reaction, the system may start off in the kinetic regime and as the temperature rises along the reactor, the sets of concurrent values of (h, δ) would be such that η, the adiabatic effectiveness factor may rise beyond unity and go through a maximum in the kinetic regime itself and then fall off in the high temperature regime governed primarily by pore diffusion. The presence of a kinetic regime in the early section of the adiabatic reactor is desirable from the point of higher conversion rates but this advantage has to be reconciled with the problem of instabity that may arise as a consequence. Therefore for a generalized treatment of reactor analysiss, it is useful to include the effectiveness factor explicitly in the dynamic conservation equations and compute its numerical value at any particle temperature appropriate to the corresponding values of δ and h_p from the chart. As a consequence when the problem of local stability is considered, the linearization procedure for the energy and mass conservation equations for the particulate phase would involve two partial derivatives

$$\left(\frac{\delta\eta}{\delta\delta}\right)_s \quad \text{and} \quad \left(\frac{\delta\eta}{\delta h_p}\right)_s .$$

(δ) is the energy-transport parameter. Of these derivatives, the sign of

$$\left(\frac{\delta\eta}{\delta h_p}\right)$$

would depend on whether it is evaluated after or ahead of the maximum in the η correlation and this may prove crucial in the stability analysis.

In the present note, the graphical marching technique and the subsequent problem of local stability will be considered for the adiabatic operation of a catalytic packed bed reactor which starts off with low h_p and high δ values. In the analysis, slab geometry and first order, inversible and exothermic reaction would be assumed. The equivalent ($\eta - h_F$) chart as indicated by Narasimhan [7] (Fig. 1) would be used for the computation of point effectiveness factor. Of course, the cell model of Vanderveen is the basis of the analysis and some thoughts concerning the uniqueness criterion are developed.

Analysis

Consider the following system equations for the n-th cell, written for steady state conditions:

Fluid phase:

$$-(1+M)p_n + p_{pn} + Mp_{n-1} = 0 \tag{1}$$

$$-(1+H)T_n + T_{pn} + HT_{n-1} = 0 \tag{2}$$

Particulate phase:

$$p_n - (1 + K_R \cdot \eta) p_{pn} = 0 \tag{3}$$

$$-(T_{pn} - T_n) + \beta . K_R \cdot \eta \cdot p_{pn} = 0 \tag{4}$$

Given the conditions in cell $(n-1)$, appropriate solution of the energy balance equation (4) could provide the steady state vector for cell n. Since in the computational procedure, conditions other than the initial and entrance conditions, are not known, the graphical marching technique is applied, starting from the first cell. In order to apply this technique the following operations are indicated.

Equation (4) is rewritten as:

$$\frac{\beta . K_R . \eta}{(1 + K_R . \eta)} = (T_{pn} - T_n) \tag{5}$$

The overall energy balance for the fluid phase from entry upto the n-th cell is:

$$GC_p (T_n - T_o) = \frac{G . p_o}{p . M_m} \left(1 - \frac{p_n}{p_n}\right) (- \Delta H_r) \tag{6}$$

where G, p_0, T_o represent entrance conditions for the fluid. Setting $p_n = 0$, the maximum temperature rise $(T_{max} - T_o)$ may be obtained as:

$$(T_{max} - T_o) = J = \frac{p_o (- \triangle H_r)}{p . M_m C_p} \tag{7}$$

The partial pressure of reactant, p_n in the stream leaving the n-th cell is given by:

$$p_n = \frac{P . M_m . C_p}{(- \triangle H_r)} (T_{max} - T_n) \tag{8}$$

Substituting for p_n in equation (5) and rewriting:

$$\frac{(- \triangle H_r)}{\beta . P . M_m . C_p} \frac{(T_{pn} - T_n)}{(T_{max} - T_n)} = \frac{K_R . \eta}{(1 + K_R . \eta)} \tag{9}$$

and $$\frac{(- \triangle H_r)}{\beta . P . M_m . C_p} = \frac{M}{H}$$

In equation (9) one can recognize the heat abstraction term Q^- and generation term, (Q^+)

$$Q^- = \frac{M}{H} \frac{(T_{pn} - T_n)}{(T_{max} - T_n)} \tag{9 A}$$

$$(Q^+) = \frac{K_R \eta}{(1 + K_R \eta)}$$

A set of equations similar to (9A) but involving T_{n-1} may be written after suitable manipulation:

$$Q^- = \frac{M}{H} \frac{(T_{pn} - T_{n-1})}{(T_{max} - T_{n-1})} \tag{10}$$

$$(Q^+_*) = \frac{(H + 1)}{H} \frac{M . (Q^+)}{(M + (Q^+))}$$

It may be noted that $Q^-(T_p)$ has the same form in both (9A) and (10). (Q^+) and (Q_*^+) may be plotted as functions of temperature noting the exponential character of K_R and the temperature dependence of η. Since $\eta(T_p)$ is a function of both δ and h_F, the progressive variation of η with T_p may be computed, given the starting values of δ and h_F, namely, δ_0 and h_{F0}. The temperature dependence of δ and h_F may be given as:

$$\left[\frac{\delta}{\delta_o}\right] = \left[\frac{T_{po}}{T_p}\right]^2 \tag{11}$$

$$\frac{h_F}{h_{FO}} = \exp \frac{E}{2RT_{po}}\left[1 - \frac{T_{po}}{T_p}\right] \tag{12}$$

where the energy transport parameter δ is:

$$\delta = \left[\frac{- \triangle H_r . p_o}{RT_o\,(\rho C_p)_e}\left(\frac{D_s}{\lambda_e}\right)\right]\frac{E}{RT_p\,2} \tag{13}$$

where the Thiele parameter h_F for the slab is:

$$h_F = a\left[\frac{\rho_p\,(1-\epsilon)\;S_g.k_g}{D_s}\right]^{\frac{1}{2}} \exp\left[(-\,E/2RT_p) + \frac{A}{2}\right] \tag{14}$$

Let a hypothetical reacting system be characterized by the following parameters:

$K_R \quad = \exp\left(16 - \dfrac{10{,}000}{T_p}\right); \quad A = 16.$

$\delta_0 \quad = 3{\cdot}0$

$h_{F0} \quad = 0{\cdot}1$

$\dfrac{\lambda_e}{D_s} \quad = 4{\cdot}0$

$E/RT_0 \quad = 20{\cdot}0$

$T_0 = T_{p0} = 500°\,\mathrm{K}$

$(T_{max} - T_0) = 300°\,\mathrm{C}$

$\dfrac{M}{H} \quad = 1{\cdot}40.$

Figure 1 represents the modified version [7] of the variation of adiabatic catalyst effectiveness factor η with h_F and δ for slab geometry. The isothermal correlation ($\delta = 0$) is also indicated. Based on the starting values of δ and h_F, their variation with T_p is computed and shown in Fig. 2. Based on Figs. 1

and 2, Fig. 3 is drawn which shows the variation of η with T_p for the temperature range of interest. Based on Fig. 3, (Q^+) and (Q^+_*) are plotted as functions of T_p in Fig. 4. The graphical marching technique is then applied after erecting a pole equal to (M/H) at $T = T_{max}$. The variation in the particle and fluid temperature over a total of 10 cells is computed and shown in Fig. 7, as curves designated 1. Figure 5 represents the marching technique when η is assumed to be unity over the entire temperature range and Fig. 6 when η is computed as η under isothermal conditions corresponding to the particle temperature T_p. The appropriate curves for the above cases are shown in Fig. 7, designated as 2 and 3 respectively. The incidence of error in the prediction of temperature profiles as predicted by 2 or 3 is evident although the particle temperature at which the temperature jump occurs and the magnitude of the jump are just about the same, namely 550° K and 170° C respectively. However with correct prediction it is

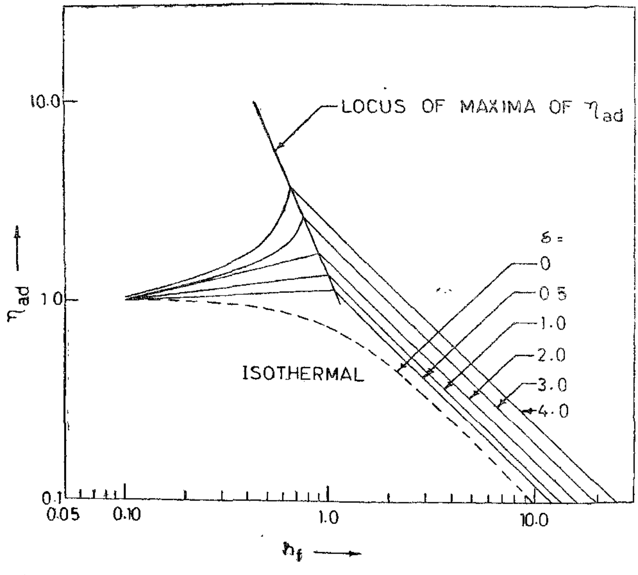

FIG. 1. Variation of adiabatic catalyst effectiveness factor with Thiele modulus for a flat plate (after Narsimhan[7]).

cell 4 that is subject to a condition of instability; whereas this condition is delayed until 6 or 7 for the other two cases.

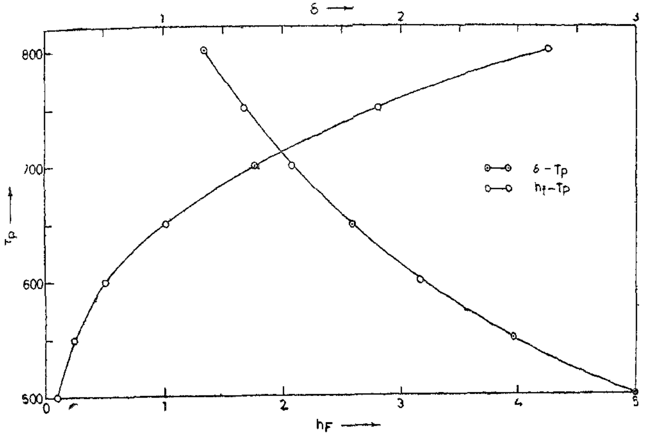

FIG. 2. Variation of δ (energy transport parameter) and h_f (Thiele modulus) with particle temperature.

For all the three cases it is evident that the steady state profiles are not unique. In fact dependent on the starting conditions and the transient operation, it is likely that the initial kinetic regime can be completely bypassed and the entire profiles obtained in the high temperature pore diffusion regime.

Luss [8] has shown that the steady state in a catalyst particle is unique if

$$\beta^{+} \leqslant \frac{4}{(\gamma - 4)} \tag{15}$$

where

$$\gamma = E/RT_0; \quad \beta^{+} = \frac{J}{T_0}\frac{D_s}{\lambda_e} = \frac{\bar{J}D_s}{\lambda_e}$$

Since a catalyst particle can exhibit multiple steady states, the heterogeneous packed bed reactor whose analysis is complicated by the macroscopic considerations of heat and mass transport in the interstitial fluid phase, ought to exhibit multiple steady states for the same reason. For equal Peclet numbers for such transport processes, Halvacek [9] has shown that for uniqueness of steady state..

$$\bar{J} \leqslant \frac{4}{(\gamma - 4)} \tag{16}$$

Since for gas-solid systems, $(D_s/\lambda_s) \leqslant 1$, equation (16) implies equation (15). With external transfer resistance and a reaction confined to the catalyst surface, the inequality criterion is obtained by Cardoso and Luss [10] as:

$$\beta + \gamma \leqslant \frac{4\,(N_u)_m}{(S_h)_m} + 4\beta \tag{17}$$

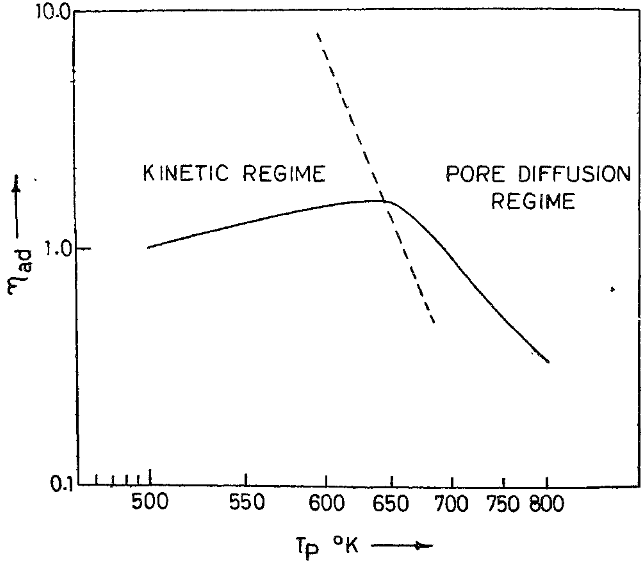

FIG. 3. Temperature adiabatic effectiveness factor excursion in catalytic reactor.

where $(N_u)_m$ and $(S_h)_m$ are the modified Nusselt and Sherwood numbers respectively. Equation (17) may be simplified to provide the equivalent condition for uniqueness:

$$J \leqslant \frac{4}{(\gamma - 4)}\left(\frac{M}{H}\right) \tag{18}$$

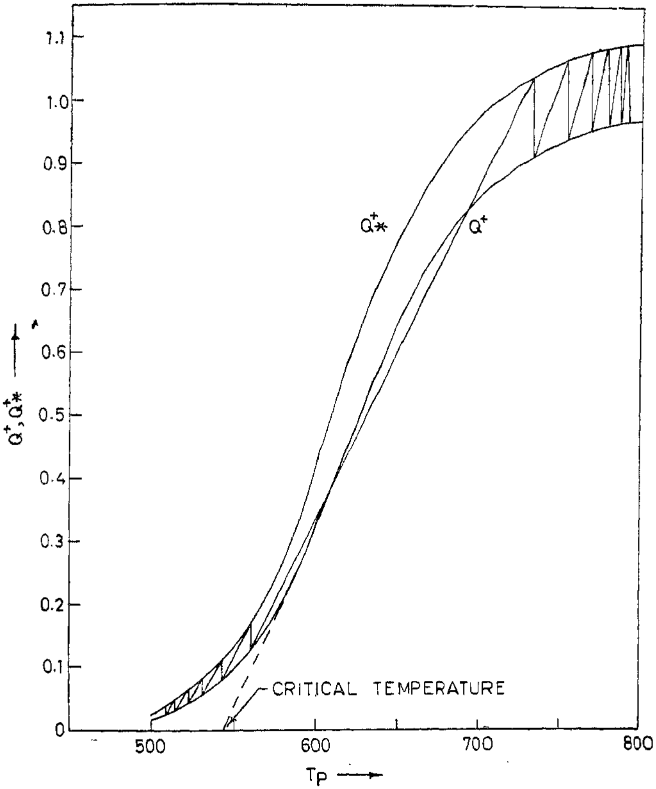

Fig. 4. Graphical marching technique for an adiabatic catalytic reactor (with diffusion limitation).

Since for gas-solid systems, $M > \mathrm{H}$, equation (18) represents a stronger condition than equation (16). When gradients are present both external and internal to the catalyst pellet, the uniqueness condition is obtained by Hlavacek [11] as:

$$\beta^{+} \leqslant \frac{4}{(\gamma - 4)} \left(\frac{\rho_1}{\beta_1}\right)^2 \tag{19}$$

where ρ_1 and β_1 are the first roots of certain transcendental equations.

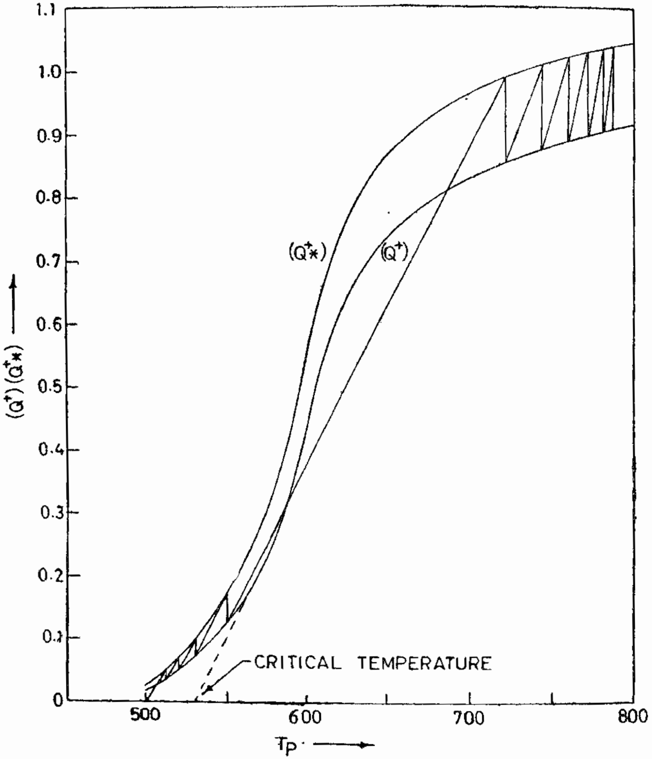

FIG. 5. Graphical marching technique for an adiabatic reactor (with no diffusion limitation)

For the cell model it may be possible to obtain the criterion for uniqueness of steady state if the two following conditions are satisfied:

$$Q^- = (Q^+_*)$$
$$\left(\frac{dQ^-}{dT_p}\right) \leqslant \frac{dQ^+_*}{dT_p} \tag{20}$$

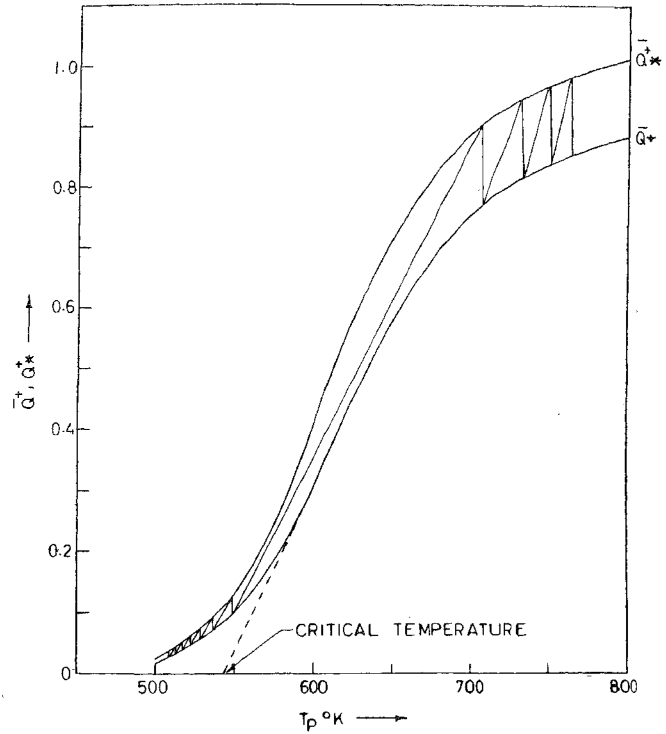

FIG 6. Graphical marching technique for an adiabatic reactor (with isothermal effectiveness factor).

Making use of equation (10) the above conditions are translated into an inequality:

$$J \leqslant \frac{M}{(H+1)} e^{-A} \left(1 - \frac{T_0}{T_p}\right)^2 e^{(\gamma T_0/T_p)} \tag{21}$$

The above inequality may be put in a more conservative form by substituting for $\frac{T_0}{T_p}$:

$$\frac{T_0}{T_p} = \left(1 - \frac{2}{\gamma}\right) \tag{21A}$$

a value which maximises the function ϕ:

$$\phi = \left(1 - \frac{T_0}{T_p}\right)^2 \exp\left(\frac{\gamma T_0}{T_p}\right) \tag{22}$$

The criterion becomes:

$$J \leqslant \frac{4}{\gamma^2} \left(\frac{M}{(H+1)}\right) e^{-A} . e^{(\gamma - 2)} \tag{22 A}$$

For the first time it is believed a part of the dimensionless rate expression K_R, namely, e^{-A} in

$$K_R = e^{(A - E/RT_p)}$$

has intervened in the uniqueness criterion. It may be mentioned that in deriving the criterion given by equation (22 A), the assumption that $\eta = 1$ is implicit in the analysis. For a rigorous treatment it is expected that the temperature dependence of η be adequately considered when it intervenes in the definitition of (Q^+) given by equation (9A). The additional factor that makes its appearance as a consequence is λ^+ which acts as a multiplier to the function ϕ.

$$\lambda^+ = \left[1 - \frac{R}{E} \frac{d \ln \eta}{d(1/T_p)}\right] \tag{23}$$

In a regime of kinetic control, λ^+ is greater than unity and in the pore diffusion regime it is less than unity. Since the criterion of uniqueness is obtained in the region of transition, λ^+ does not affect the validity of equation (22 A).

The foregoing analysis, based on a semi-quantitative description of the interaction of transport and chemical rate processes in catalytic reactor

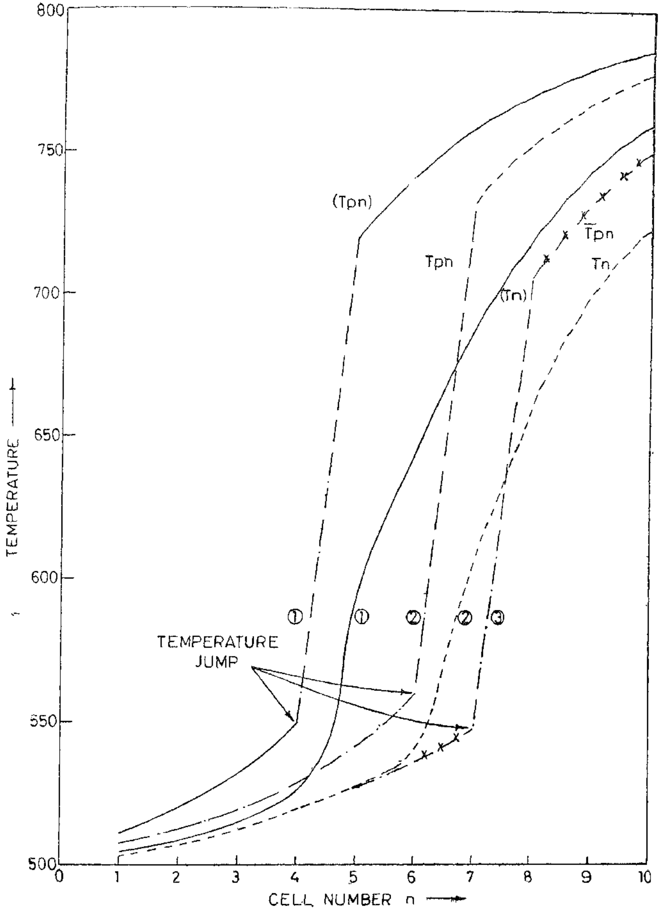

FIG. 7. Particle and fluid temperature profile for an adiabatic reactor.

(1) With diffusion limitation (Tpn)–(Tn)–n

(2) With no diffusion limitation Tpn–Tn–n

(3) With isothermal effectiveness factor Tpn–n

design may introduce an element of rigor in the analysis of situations where simpler assumptions concerning principally the character and variation with temperature of catalyst effectiveness factor may not be justified. If the validity of this argument is granted, the linearized stability analysis of an adiabatic packed bed reactor has to include the appropriate variation of η with particle temperature. This aspect of the problem will be explored presently.

Stability Analysis of n-th cell

Let the following perturbation variables be defined:

$$\begin{aligned} (p - p_s) &= X_1 \\ (T - T_s) &= X_2 \\ (P_p - P_{ps}) &= X_3 \\ (T_p - T_{ps}) &= X_4 \end{aligned} \tag{24}$$

Equations (1 – 4) may be rewritten in perturbation form:

$$-(1 + M)\,X_1 + X_3 = \alpha_1 \frac{dX_1}{d\theta} \tag{25}$$

$$-(1 + H)\,X_2 + X_4 = \alpha_2 \frac{dX_2}{d\theta} \tag{26}$$

$$X_1 - [(1 + K_R\eta)\,p_p - (1 + K_{RS}\eta_s)\,p_{ps}] = \alpha_3 \frac{dX_3}{d\theta} \tag{27}$$

$$X_2 + \beta\,[(K_R \,.\, p_p . \eta - K_{RS} \,.\, P_{ps} \,.\, \eta_s)] - X_4 = \alpha_4 \frac{dX_3}{d\theta} \tag{28}$$

The symbols appearing in equations (25–28) are defined below:

$$\theta = t/\tau_m \;;\; \tau_m = \frac{H_g}{(u/\epsilon)}$$

$$\alpha_1 = 1;\; \alpha_2 = \frac{H}{M};\, \alpha_3 = (1 - \epsilon);\; \alpha_4 = \frac{(1 - \epsilon)}{\epsilon} \frac{\rho_p \,.\, C_s}{\rho_F C_p} \frac{H}{M};$$

$$H_g = \frac{G}{K_g a_v P \,.\, M_m};\; H_1 = \frac{H_h}{\gamma^+ D_p};\; H_h = \frac{GC_p}{h a_v}$$

$$\bar{k}_r = \frac{\rho_p\,(1 - \epsilon)\,S_g \,.\, K_r}{a_v};\; K_R = \frac{\bar{k}_r}{k_g}\; M = \frac{H_g}{\gamma^+ D_\rho};\; H = \frac{H_h}{\gamma^+ D_\rho}$$

$$\beta = \frac{(-\triangle H_r)\,K_g}{h}$$

Linearization

Equations (27) and (28) involve nonlinear difference terms indicated by square brackets. Linearizing these terms through Taylor expansion and neglecting terms of second order and higher, these equations may be rewritten as:

$$X_1 - (1 + K_{RS} \cdot \eta_S)\, X_3 - \left[\frac{K_{RS} \cdot p_{ps} \eta_S \cdot E}{RT^2_{ps}} \cdot (1 + F - G)\right] X_4 = \alpha_3 \frac{dX_3}{d\theta} \quad (29)$$

$$X_2 - \beta \cdot K_{RS} \cdot \eta_S X_3 - \left[1 - \frac{\beta \cdot K_{RS} \cdot P_{ps} \eta_S \cdot E}{RT^2_{ps}} \cdot (1 + F - G)\right] X_4 = \alpha_4 \frac{dX_4}{d\theta} \quad (30)$$

where

$$F = \frac{h_{FS}}{2\eta_S}\left(\frac{\delta\eta}{\delta h_F}\right)_S \quad (31)$$

$$G = \frac{2\delta_0}{\eta_S} \frac{RT_{ps}}{E} \left(\frac{T_{p0}}{T_{ps}}\right)^2$$

Equations (25, 26, 29 and 30) may be cast in vector-matrix notation:

$$\alpha \frac{dX}{d\theta} = \boldsymbol{CX} \quad (32)$$

where

$$\alpha = \begin{bmatrix} \alpha_1 & & & \\ & \alpha_2 & & \\ & & \alpha\alpha_3 & \\ & & & \alpha_4 \end{bmatrix} : \; \boldsymbol{X} = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \end{bmatrix}$$

$$\boldsymbol{C} = \begin{bmatrix} -(1 + \mu_m) & 0 & 1 & 0 \\ 0 & -(1 + \mu_H) & 0 & 1 \\ 1 & 0 & -(1 + K_{RS}\eta_S) & \frac{-E}{RT^2_{ps}} K_{RS} \cdot P_{ps} \cdot \eta_S (1 + F - G) \\ 0 & 1 & \beta K_{RS} \cdot \eta_s & -\left[1 - \frac{\beta E}{RT^2_{ps}} K_{RS} \cdot P_{ps} \cdot \eta_s \; (1 + F - G)\right] \end{bmatrix}$$

The necessary and sufficient conditions of stability of cell n are that all the eigen values of:

$$det\,(\alpha^{-1}C - \lambda I) = 0 \tag{33}$$

be negative definite.

It is possible to introduce a degree of simplicity in the stability analysis if the assumption is made that the catalyst particle has negligible capacity for the accumulation of mass. Then the following steady state equality holds good.

$$P_{ps} = \frac{p_S}{(1 + K_{RS} \cdot \eta_S)} \tag{34}$$

The third column and row of matrix C may be eliminated since α_3 and X_3 are both zero. After some algebraic manipulation, the following characteristic equation is obtained:

$$\begin{aligned} &\lambda^3 + (\phi^+ + M' + H')\,\lambda^2 + [(M' + H')\,\phi^+ + M'H' - 1]\,\lambda \\ &+ M'\,(H'\phi^+ - 1) = 0 \end{aligned} \tag{35}$$

where

$$\phi^+ = 1 - \frac{\beta E K_{RS} \cdot \eta_S p_S}{RT^2_{ps}\,(1 + K_{RS} \cdot \eta_S)}\,(1 + F - G)$$

$$M' = (1 + M)$$

$$H' = (1 + H)$$

Casting the coefficients of equation (35) in a Routh array and expanding the column the following conditions are obtained:

$$(a)\ (\phi^+ + M' + H') > 0 \tag{36}$$

$$(b)\ (\phi^+ + M' + H') \rangle \frac{M'\,(H'\phi^+ - 1)}{[(M' + H')\,\phi^+ + M'H' - 1]}$$

Examining (a), since M' and H' are positive the condition reduces to the inequality:

$$\phi^+ \geqslant 0 \quad \text{or}$$

$$\frac{\beta E K_{RS} \cdot \eta_S \cdot p_S}{RT_{ps}{}^2\,(1 + K_{RS} \cdot \eta_S)}\,(1 + F - G) \leqslant 1 \tag{37}$$

Equation (37) may be recast into the following form:

$$\frac{(dQ^+/dT_p)_s}{(dE^-/dT_p)_s}(1 + F - G) \leqslant 1 \tag{37 A}$$

If the slope condition is satisfied at the steady state then for the inequality of equation (37 A) to hold good

$$G \geqslant \mathrm{F} \quad \text{or}$$

$$\delta_0 \frac{RT_{ps}}{E}\left(\frac{T_{p0}}{T_{ps}}\right)^2 \geqslant \frac{h_{FS}}{4}\left(\frac{\delta\eta}{\delta_{h_F}}\right)_s \tag{38}$$

The LHS of equation (38) is always positive and as long as the steady state resides in a region of pore diffusion control $(\delta\eta/\delta_{h_F})_s$ is negative and the above inequality is always satisfied. On the contrary in a zone of temperature progression in the kinetic regime, the partial derivative will be positive (unless δ_0 is small) and the inequality may not be satisfied.

Condition (*b*) implies that:

$$(1 + H)\,\phi^+ > 1 \tag{39}$$

$$\text{or} \quad \left(\frac{dQ^-}{dT_p}\right)_s > \frac{(1 + H)}{H}\left(\frac{dQ^+}{dT_p}\right)_s \tag{39 A}$$

The above condition is stronger than the slope condition used to derive equation (38) which therefore represents a conservative criterion.

CONCLUSIONS

A few exothermic catalytic reactions carried out on the industrial scale are characterized by large δ and low h_F values and this feature has necessitated the inclusion of temperature dependent effectiveness factor in the conservation equations of the packed bed reactor modelled as a sequence of well strired gas-solid cells. As a consequence, in the analysis of adiabatic reactor stability, one of the two necessary and sufficient conditions of stability involve the partial derivative $\left(\frac{\delta\eta}{\delta_{h_F}}\right)_s$ that has not intervened in the investigations reported so far. In addition the equations used for computing the steady state profiles by a modified graphical marching technique has formed the basis for predicting the uniqueness criterion for a reacting system influenced by both inter and intra particle diffusion effects. For the first time we believe that the dimensionless frequency factor e^A in the Arrhenius form of expression for the dimensionless reaction rate term K_R, has appeared in the uniqueness criterion.

NOMENCLATURE

A, B: stability parameters, eq. 29
a: half slab thickness
a_v: external transfer area per unit volume of packed bed
C_p, C_s: heat capacity of gas, solid
d_p: catalyst particle diameter
D_s: effective pore diffusivity
E: activation energy
F: function defined by eq. 25 A
G: fluid mass velocity in reactor
H: $(H_h/\gamma^+ \cdot d_p)$
H_h: HTU for external heat transfer
H_g: HTU for external mass transfer
h_p, h_f: Thiele parameter, particle, slab
h; external heat transfer coefficient
I: Idem matrix
j: maximum temperature rise, eq. 7
k_g: external mass transfer coefficient
k_r: heterogeneous reaction rate constant
K_R: dimensionless rate constant, k_r/k_g
M_m: mean mol. wt.
M: $(\mathrm{H}_g/\gamma^+ d_p)$
Nu: Nusselt number, $(k_g RT . a/D_s)$
P: total pressure
p: reactant partial pressure
(Q^+): heat generation function eq. 9A
Q^-: heat abstraction function eq. 9 A
(Q^+): modified heat generation function, eq. 10
R: gas constant
S_g: specific catalyst surface
T: temperature °K
t: time

u: mean fluid velocity in reactor
X: vector of perturbation variables (state)
x_1, x_2, x_3, x_4: perturbation variables

Greek:

α: diagonal matrix eq. 24
α_1, α_4: *see* symbols under eq. 21
β: parameter ($- \triangle Hk_g/h$)
γ^+: small whole number, 1–3
δ: energy-transport number *see* eqn. (13)
ϵ: bed porosity
ρ: density
η: effectiveness factor (adiabatic)
λ: eigenvalue
λ_e: effective catalyst thermal diffusivity
ϕ: function defined under eq. 25 A
$\triangle H_r$: heat of reaction
θ: dimensionless time, t/τ_m
τ_m: $H_g . \epsilon/u$
ϕ: function defined by equation (21 A)
ϕ^+: function defined by equation (35)

Subscripts:

p: particle
o: initial value
s: steady state value
n: cell number
e: effective

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