

Ignition and Extinction of Catalytic Reactions on a Flat Plate

AMABLE LIÑÁN

CÉSAR TREVIÑO

Abstract—In this paper ignition and extinction processes of catalytic reactions in a flat plate boundary layer flow are analyzed. The catalytic plate has finite thickness and thermal conductivity. It is assumed a global one-step and irreversible chemical reaction with Arrhenius kinetics and large activation energy. It is further assumed adiabatic boundary conditions for the lower surface and in both edges of the plate. For this case, the critical Damköhler number for ignition is not strongly affected by the axial heat conduction through the plate. On the other hand, the finite thermal conductivity has a big influence on the extinction process. An analytical expression for the critical Damköhler number for extinction is obtained.

INTRODUCTION

Several works have appeared in the literature with the objectives to study the ignition and extinction of catalytic reactions in boundary layer flows. Artyuk *et al.* (1961) solved numerically the governing equations for the flow of a gaseous mixture over an adiabatic flat plate. They used the local similarity concept, reaching the erroneous conclusion of the existence of multiple solutions for this problem. Lindbergh and Schmitz (1969, 1970) studied numerically the ignition and extinction processes for a flat plate and wedge type boundary layer flows. This analysis was made for the limiting cases of adiabatic and perfect conducting plates. They showed that the solution to this problem is unique if the boundary layer assumption holds at the leading edge of the plate. If the boundary layer has a stagnation point, multiple solutions of the steady state equations can exist. Also they showed that for an adiabatic wall it is impossible to have multiple solutions, which result if an inadequate numerical solution is used.

Mihail and Teodorescu (1975) used a refined numerical analysis to solve the integral governing equations using the Lighthill approximation for high Prandtl and Schmidt numbers (Lighthill, 1950). This study supports the results obtained by Lindbergh and Schmitz (1969). Ahluwalia and Chung (1980) analyzed the same problem, but they solved the integral governing equations through the erroneous utilization of the Laplace method. The studies made by Lindberg and Schmitz (1969), Mihail and Teodorescu (1975) and Ahluwalia and Chung (1980) show, for an adiabatic plate, the transition from a kinetically controlled process close to the leading edge to a diffusion controlled process downstream. In a very recent paper, Liñán (1983) showed that this transition occurs abruptly at a well defined distance if the ratio of the activation energy to the thermal energy is large enough. This transition has a universal character. None of the works referred above has taken into account a finite value of the plate thermal conductivity. Only the two limiting cases of zero and infinite thermal conductivity were studied.

The objectives of the present work is to study, using asymptotic methods, the ignition and extinction processes in the flow of a reacting mixture over a flat plate with the inclusion of the longitudinal heat transfer due to finite values of the thermal conductivity. It is assumed further a high ratio of the activation energy for the catalytic heterogeneous reaction to the thermal energy.

ANALYSIS

A gaseous combustible mixture flows over a catalytic flat plate with finite thickness and thermal conductivity. The governing integro-differential equations are the following:

$$-k_0 C^n \exp\left(-\frac{T_a}{T}\right) = 0.332 D \sqrt{\left(\frac{u_\infty}{\nu x}\right)} Sc^{1/3} \int_{C_\infty}^C K(\bar{x}, x) d\bar{C} \quad (1)$$

$$\lambda_p d \frac{d^2 T}{dx^2} + (-\Delta H) k_0 C^n \exp\left(-\frac{T_a}{T}\right) = 0.332 \lambda \sqrt{\left(\frac{u_\infty}{\nu x}\right)} Pr^{1/3} \left[\int_{T_i}^T K(\bar{x}, x) d\bar{T} + (T_i - T_\infty) \right] \quad (2)$$

with the kernel $K(\bar{x}, x)$ given by

$$K(\bar{x}, x) = \left\{ 1 - \left(\frac{\bar{x}}{x}\right)^{3/4} \right\}^{-1/3}.$$

Here the Lighthill approximation (Lighthill, 1950) for high Prandtl and Schmidt numbers has been introduced. However this gives good results for Prandtl and Schmidt numbers of order unity. k_0 represents the pre-exponential term of the catalytic irreversible reaction of the Arrhenius type; n is the reaction order; T_a is the activation temperature of the reaction; T and C correspond to the temperature and the reactant concentration on the surface of the plate, respectively; $(-\Delta H)$ is the heat release per unit mole of fuel consumed; λ and λ_p correspond to the thermal conductivities of the gas and the plate, respectively; D is the mass diffusion coefficient; ν is the kinematic coefficient of viscosity; d corresponds to the thickness of the plate; u_∞ , T_∞ , and C_∞ are the velocity, temperature and reactant concentration for the free stream, respectively; T_i is the temperature on the leading edge of the plate. In Eq. (2) it was assumed that the plate temperature is uniform in the transversal direction, that is

$$3\lambda_p \sqrt{\left(\frac{\nu L}{u_\infty}\right)} \gg \lambda d Pr^{1/3}, \quad (3)$$

where L corresponds to the length of the plate.

The boundary conditions are given by the assumption that both edges of the plate are adiabatic,

$$\frac{dT}{dx} = 0 \quad \text{at } x = 0 \quad \text{and } x = L \quad (4)$$

We introduce the following non-dimensional variables of the form,

$$x = \frac{x}{L}; \quad \theta = \frac{T - T_\infty}{T_A - T_\infty}; \quad Y = \frac{C}{C_\infty}. \quad (5)$$

Here, T_A corresponds to the adiabatic equilibrium temperature given by

$$T_A = T_\infty \left\{ 1 + \frac{(-\Delta H)DC_\infty Sc^{1/3}}{T_\infty \lambda Pr^{1/3}} \right\}. \quad (6)$$

The non-dimensional governing equations are then reduced to

$$-\frac{\delta}{\Gamma} Y^n \exp\left(\frac{\Gamma\theta}{1 + \beta_1\theta}\right) = \frac{1}{\sqrt{\chi}} \int_1^Y K(\bar{\chi}, \chi) d\bar{Y} \quad (7)$$

and
$$\alpha \frac{d^2\theta}{d\chi^2} + \frac{\delta}{\Gamma} Y^n \exp\left(\frac{\Gamma\theta}{1 + \beta_1\theta}\right) = \frac{1}{\sqrt{\chi}} \left[\int_{\theta_1}^\theta K(\bar{\chi}, \chi) d\bar{\theta} + \theta_1 \right], \quad (8)$$

where the non-dimensional parameters are defined as follows:

$$\beta_1 = \frac{(-\Delta H)DC_\infty Sc^{1/3}}{T_\infty \lambda Pr^{1/3}}; \quad \Gamma = \frac{T_a \beta_1}{T_\infty} \quad (9)$$

$$\delta = \frac{k_0 C_\infty^{n-1} \Gamma \sqrt{(\nu L)} \exp(-T_a/T_\infty)}{0.332 D \sqrt{(u_\infty)} Sc^{1/3}}; \quad \alpha = \frac{\lambda_p d \sqrt{(\nu)}}{0.332 \sqrt{(u_\infty L)} Pr^{1/3} \lambda L}$$

Here, the parameter β_1 gives the ratio between the energy released by the catalytic reaction to the thermal energy of the free stream mixture. This parameter is of order unity in problems related to combustion. Γ is the non-dimensional activation energy which in general is a large number. δ is the Damköhler number and represents the ratio between the characteristic diffusion time to the characteristic reaction time and α represents the ratio of the ability of the plate to carry heat in the streamwise direction to the ability of the gas to carry heat from the plate. The non-dimensional boundary conditions reduce to

$$\frac{d\theta}{d\chi} = 0 \quad \text{at } \chi = 0 \quad \text{and } \chi = 1 \quad (10)$$

For small values of δ , such as $\delta \rightarrow 0$, the solution to Eqs. (7), (8) and (9) gives $\theta = \theta_l = 0$ and $Y = 1$, which correspond to the frozen conditions. On the other hand, for $\delta \rightarrow \infty$ corresponding to chemical equilibrium, we obtain $\theta = \theta_l = 1$ and $Y = 0$. For exothermic reactions with β_1 of order unity and high values of the non-dimensional activation energy ($\Gamma \gg 1$), the problem shows multiple solutions if $\alpha \neq 0$ in the range of δ given by $\delta_E < \delta < \delta_I$. These limits are to be obtained in the following sections. That is, in a diagram of θ_l or $\theta_M = \theta(1)$, as a function of δ , we obtain the classical S-shaped curve which shows the existence of bifurcation points associated to the values of δ_E and δ_I of extinction and ignition, respectively.

In the following sections asymptotic techniques are used for high activation energies to obtain the solution of the governing equations close to ignition and extinction conditions.

IGNITION REGIME

This regime corresponds to values of δ of order unity with values of $1 - Y$ and θ of order $1/\Gamma$. It is appropriate to redefine the non-dimensional variables as

$$Y = 1 - \frac{y}{\Gamma}; \quad \theta = \frac{\phi}{\Gamma} \quad (11)$$

with y and ϕ of order unity. The non-dimensional governing equations are transformed to

$$\delta \left(1 - \frac{\varepsilon y}{\beta_1}\right)^n \exp\left(\frac{\phi}{1 + \varepsilon \phi}\right) = \frac{1}{\sqrt{\chi}} \int_0^y K(\bar{\chi}, \chi) d\bar{y} \quad (12)$$

$$\alpha \frac{d^2 \phi}{d\chi^2} + \delta \left(1 - \frac{\varepsilon y}{\beta_1}\right)^n \exp\left(\frac{\phi}{1 + \varepsilon \phi}\right) = \frac{1}{\sqrt{\chi}} \left[\int_{\phi_l}^{\phi} K(\bar{\chi}, \chi) d\bar{\phi} + \phi_l \right] \quad (13)$$

where ε is a small number given by $\varepsilon = \beta_1/\Gamma \rightarrow 0$. The reduced boundary conditions are

$$\frac{d\theta}{d\chi} = 0 \quad \text{at} \quad \chi = 0 \quad \text{and} \quad \chi = 1 \quad (14)$$

We seek the solution to Eqs. (12) to (14) through a perturbation series of the form

$$\begin{aligned} \phi &= \phi_0 + \varepsilon \phi_1 + \varepsilon^2 \phi_2 + \dots \\ y &= y_0 + \varepsilon y_1 + \varepsilon^2 y_2 + \dots \\ \delta &= \delta_0 + \varepsilon \delta_1 + \varepsilon^2 \delta_2 + \dots \end{aligned} \quad (15)$$

We obtain the following set of equations:

$$\alpha \frac{d^2\phi_0}{d\chi^2} + \delta_0 \exp(\phi_0) = \frac{1}{\sqrt{\chi}} \left[\int_{\phi_{0i}}^{\phi_0} K(\bar{\chi}, \chi) d\bar{\phi}_0 + \phi_{0i} \right] \quad (16)$$

$$\delta_0 \exp(\phi_0) \sqrt{\chi} = \int_0^{y_0} K(\bar{\chi}, \chi) d\bar{y}_0 \quad (17)$$

for terms of order ε^0 ,

$$\alpha \frac{d^2\phi_1}{d\chi^2} + \delta_0 \exp(\phi_0) \phi_1 - \frac{1}{\sqrt{\chi}} \left[\int_{\phi_{1i}}^{\phi_1} K(\bar{\chi}, \chi) d\bar{\phi}_1 + \phi_{1i} \right] \quad (18)$$

$$= \delta_0 \exp(\phi_0) \left(\frac{ny_0}{\beta_1} - \frac{\delta_1}{\delta_0} + \phi_0^2 \right)$$

$$\delta_0 \exp(\phi_0) \left(\phi_1 + \frac{\delta_1}{\delta_0} - \frac{ny_0}{\beta_1} - \phi_0^2 \right) \sqrt{\chi} = \int_0^{y_1} K(\bar{\chi}, \chi) d\bar{y}_1 \quad (19)$$

for terms of order ε^1 , etc. Equation (18) determines δ_1 independent of Eq. (19).

The boundary conditions are then

$$\frac{d\phi_0}{d\chi} = \frac{d\phi_1}{d\chi} = 0 \quad \text{at } \chi = 0 \quad \text{and} \quad \chi = 1. \quad (20)$$

In defining δ_1 we can use the fact that at the singular point the arbitrary choice of $\phi_{1i} = \phi_1(0)$ brings only errors of order ε in δ_1 . Thus we can set $\phi_{1i} = 0$. The Eqs. (16) to (20) can be solved numerically to find the critical values of δ_{0I} and δ_{1I} as a function of α . These are given in the Table I. Figure 1 shows the variation of ϕ_{0I} and ϕ_{0M} with δ for different values of α indicating clearly the ignition points. From this analysis it can be inferred that the thermal conductivity of the plate has little influence on the ignition process. In the following subsections we analyze the two limiting cases of adiabatic and well conducting plates.

Adiabatic Plate ($\alpha=0$)

This limiting case was studied by Liñán (1983). In this limit it can be readily shown that $y = \phi$. Thus Eq. (13) reduces to

$$\left(1 - \frac{\varepsilon\phi}{\beta_1} \right)^n \exp \left(\frac{\phi}{1 + \varepsilon\phi} \right) = \frac{1}{\sqrt{(\xi)}} \int_0^{\phi} K(\bar{\xi}, \xi) d\bar{\phi} \quad (21)$$

where $\xi = \chi \delta^2$. The inversion of Eq. (21) gives

$$\phi = \frac{\sqrt{3}}{2\pi} \int_0^z \frac{\bar{z}^{1/3} \exp\left(\frac{\bar{\phi}}{1 + \varepsilon \bar{\phi}}\right) \left(1 - \frac{\varepsilon \bar{\phi}}{\beta_1}\right)^n d\bar{z}}{(z - \bar{z})^{2/3}} \quad (22)$$

where $z = \xi^{3/4}$. Equation (22) can be integrated numerically to obtain the evolution of ϕ with z for different values of ε , β_1 and n . The solution of Eq. (22) shows that ϕ grows to very high values compared with unity as z approaches the value of z_I , thus indicating the ignition point. The Damköhler number for ignition is then given by $\delta_I = z_I^{2/3}$. Values of δ_I for different values of ε , β_1 and n are given in Table II. The

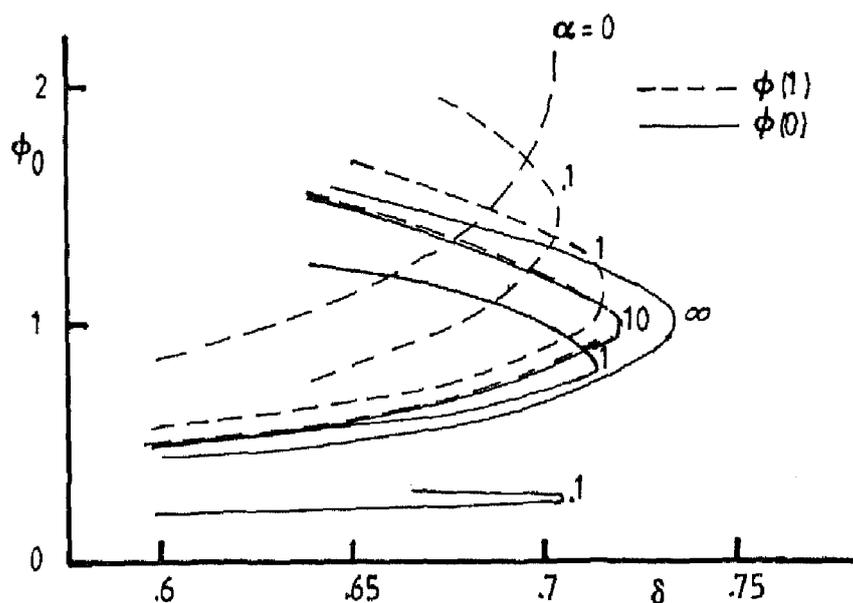


FIGURE 1 Variation of ϕ_I and ϕ_M as a function of δ , for different values of α .

TABLE I
Critical Damköhler number for ignition δ_0 , δ_1 for
different values of α

α	n	β_1	δ_0	δ_1
0.1	1	3	0.713	0.867
0.1	1	4	0.713	0.809
1.0	1	3	0.734	1.022
1.0	1	4	0.734	0.960

first order solution of Eq. (22) shows a universal character, obtaining the value of $\delta_I = 0.711$, independent of β_1 and the reaction order n .

TABLE II
Critical Damköhler number for ignition δ_1 for
different sets of parameters and $\alpha=0$

ε	n	β_1	δ_1
0.00	—	—	0.711
0.01	1	3	0.723
0.05	1	3	0.777
0.10	1	3	0.870
0.01	1	4	0.722
0.05	1	4	0.773
0.10	1	4	0.857
0.01	2	4	0.724
0.05	2	4	0.785
0.10	2	4	0.893

Well Conducting Plate ($\alpha \rightarrow \infty$)

For high thermal conductivity of the plate, the temperature shows little variation along the longitudinal coordinate. To find the critical condition for ignition we assume a solution to Eqs. (12) to (14) of the form

$$\psi = \sum_{n=0}^{\infty} \frac{\psi_n(\varepsilon, \chi)}{\alpha^n} = \sum_{n=0}^{\infty} \frac{1}{\alpha^n} \sum_{m=0}^{\infty} \varepsilon^m \psi_{nm}(\chi)$$

where ψ stands for ϕ , δ or y . We obtain the following set of equations grouping the terms with the same power of $1/\alpha$:

$$\frac{d^2\phi_0}{d\chi^2} = 0 \tag{23}$$

$$\frac{d^2\phi_1}{d\chi^2} + \delta_0 \left(1 - \frac{\varepsilon y_0}{\beta_1}\right)^n \exp\left(\frac{\phi_0}{1 + \varepsilon\phi_0}\right) = \frac{\phi_0}{\sqrt{\chi}} \tag{24}$$

$$\frac{d^2\phi_2}{d\chi^2} + \delta_0 \left(1 - \frac{\varepsilon y_0}{\beta_1}\right)^n \exp\left(\frac{\phi_0}{1 + \varepsilon\phi_0}\right) \left(\frac{\phi_1}{1 + \varepsilon\phi_0} + \frac{\delta_1}{\delta_0}\right) \tag{25}$$

$$= \frac{1}{\sqrt{\chi}} \left[\int_{\phi_1}^{\phi_1} K(\bar{\chi}, \chi) d\bar{\phi}_1 + \phi_{11} \right]$$

$$\delta_0 \exp(\phi_0) = \frac{1}{\sqrt{\chi}} \int_0^{y_0} K(\bar{\chi}, \chi) d\bar{y}_0, \text{ etc.} \tag{26}$$

The boundary conditions for these equations are

$$\frac{d\phi_0}{d\chi} = \frac{d\phi_1}{d\chi} = \frac{d\phi_2}{d\chi} = 0 \quad \text{at } \chi = 0 \quad \text{and } \chi = 1 \quad (27)$$

The solution of Eq. (23) indicates that ϕ_0 is independent of χ . After integration of Eq. (24) we obtain

$$\delta_0 \left(1 - \frac{\varepsilon \sigma n}{\beta_1} \right) \exp\left(\frac{\phi_0}{1 + \varepsilon \phi_0} \right) = 2\phi_0 \quad (28)$$

where

$$\sigma = \int_0^1 y_0 d\chi.$$

The solution to Eq. (26) gives

$$y_0 = \frac{\sqrt{3}}{2\pi} \frac{\Gamma(4/3)\Gamma(1/3)}{\Gamma(5/3)} \delta_0 \exp(\phi_0) \sqrt{\chi} \quad (29)$$

and

$$\sigma = \frac{\Gamma(4/3)\Gamma(1/3)}{\sqrt{3} \pi \Gamma(5/3)} \delta_0 \exp(\phi_0) \doteq 0.4873 \delta_0 \exp(\phi_0) \quad (30)$$

To find the solution to Eq. (28) we assume the expansion for the variables given by

$$\phi_0(\varepsilon) = \phi_{00} + \varepsilon \phi_{01} + \dots$$

$$\delta_0(\varepsilon) = \delta_{00} + \varepsilon \delta_{01} + \dots$$

obtaining thus the following set of equations:

$$\delta_{00} \exp(\phi_{00}) = 2\phi_{00} \quad (31)$$

$$[\delta_{00} \exp(\phi_{00}) - 2]\phi_{01} = \delta_{00} \exp(\phi_{00}) \left(-\frac{\delta_{01}}{\delta_{00}} + \phi_{00}^2 + \frac{\sigma n}{\beta_1} \right) \quad (32)$$

From Eqs. (31) and (32) we deduce that the critical Damköhler number for ignition is

$$\delta_{0I} = \frac{2}{e} \left| 1 + \varepsilon \left(1 + \frac{0.9746n}{\beta_1} \right) \right| + O(\varepsilon^2) \quad (33)$$

From Eq. (24) we have

$$\frac{d^2\phi_{10}}{d\chi^2} = \frac{\phi_{00}}{\sqrt{\chi}} - \delta_{00} \exp(\phi_{00}) = \frac{1}{\sqrt{\chi}} - 2 \quad (34)$$

the solution to which is

$$\phi_{10} = \frac{4}{3}\chi^{3/2} - \frac{2}{3}\chi^3 + \phi_{10l} \quad (35)$$

Also from Eq. (25) we obtain

$$\frac{d^2\phi_{20}}{d\chi^2} = \frac{8}{3}F_1\chi - \frac{8}{3}(F_2 + 1)\chi^{3/2} - \delta_{10}e + \phi_{10l}\left(\frac{1}{\sqrt{\chi}} - 2\right) \quad (36)$$

where

$$F_1 = \int_0^1 \frac{u \, du}{(1-u)^{1/3}} = \frac{\Gamma(2)\Gamma(2/3)}{\Gamma(8/3)} = 0.890$$

and

$$F_2 = \int_0^1 \frac{u^{5/3} \, du}{(1-u)^{1/3}} = \frac{\Gamma(8/3)\Gamma(2/3)}{\Gamma(10/3)} = 0.725$$

After integration of Eq. (36) and applying the boundary condition (27) we obtain

$$\delta_{10} = \frac{1}{e} \left(\frac{4}{3}F_1 - \frac{16}{15}(F_2 + 1) + \frac{1}{3} \right) = -\frac{0.32}{e} \quad (37)$$

Finally, from Eqs. (33) and (37) we have for the Damköhler number for ignition

$$\delta_I = \frac{2}{e} \left[1 + \varepsilon \left(1 + \frac{0.9746n}{\beta_1} \right) - \frac{0.16}{a} \right] + O(\varepsilon^2, \varepsilon/a, 1/a^2) \quad (38)$$

EXTINCTION REGIME

Near the extinction condition, the temperature of the plate is close to the equilibrium temperature $\theta=1$ and the reactant concentration diverges from zero only in the proximity of the leading edge of the plate in a region of $\chi \sim 1/\Gamma^2 \ll 1$. Far away from this region, that is $\chi \sim 1 \gg 1/\Gamma^2$, the reaction term of Eqs. (7) and (8) reaches the value of $1/\sqrt{\chi}$ (corresponding to the diffusion-controlled process). Thus Eq. (8) reduces to

$$a \frac{d^2\theta}{d\chi^2} + \frac{1}{\sqrt{\chi}} = \frac{1}{\sqrt{\chi}} \left| \int_{\theta_l}^{\theta} K(\bar{\chi}, \chi) d\bar{\theta} + \theta_l \right| \quad \text{for } \chi \gg 1/\Gamma^2 \quad (39)$$

with the boundary condition of $d\theta/d\chi=0$ at $\chi=1$. However, the adiabatic condition at the leading edge has to be changed by the matching condition with the solution of the problem given by Eqs. (7) and (8) for the region $\chi\sim 1/\Gamma^2$, where Y falls from a value of unity to values small compared with unity. If the reaction term had the value $1/\sqrt{\chi}$ from $\chi=0$, the solution of the problem would be $\theta=1$. Because of the finite values of δ , the temperature of the plate changes from unity. If this temperature difference is of order $1/\Gamma_e=(1+\beta_1)^2/\Gamma$, the reaction rate is reduced by a factor of order $1/e$, thus causing extinction. We can anticipate that in the extinction regime $1-\theta\sim 1/\Gamma_e$ throughout the length of the plate. From Eq. (7), the dimension of the reaction zone χ_r , is such that $\delta/\Gamma\cdot\exp[\Gamma/(1+\beta_1)]\sim 1/\sqrt{\chi_r}$. The order of magnitude of $d\theta/d\chi$ is $1/\Gamma_e$ along the entire length of the plate. For values of α of order unity, all the terms in Eq. (8) are of the same order, that is

$$\frac{1}{\Gamma_e\chi_r} \sim \frac{\delta}{\Gamma} \exp\left(\frac{\Gamma}{1+\beta_1}\right) \sim \frac{1}{\sqrt{\chi_r}} \quad (40)$$

We can deduce that the variations of θ in the region close to the leading edge are of order $\chi_r/\Gamma_e\sim 1/\Gamma_e^3$. Due to this fact we can define the quantity Ψ as $\Psi=(1-\theta_i)\Gamma_e$ of order unity and independent of χ . Thus, for values of δ of the order for extinction, such as

$$\Delta = \frac{\delta \exp\left(\frac{\Gamma}{1+\beta_1}\right)}{\Gamma\Gamma_e} \sim 1 \quad (41)$$

there exists a region close to the leading edge $\chi\sim 1/\Gamma_e^2$, where Ψ can be considered constant of order unity. Eq. (7) which determines how Y decreases from unity to values of $Y\ll 1$ in this region, takes the form

$$-\Delta\Gamma_e \exp(-\Psi) Y^n = \frac{1}{\sqrt{\chi}} \int_1^Y K(\bar{\chi}, \chi) d\bar{Y} \quad (42)$$

which can be written as

$$-Y^n = \frac{1}{\sqrt{\xi}} \int_1^Y K(\bar{\xi}, \xi) d\bar{Y} \quad (43)$$

with

$$\xi = \chi \{\Delta\Gamma_e \exp(-\Psi)\}^2 \quad (44)$$

Equation (43) giving $Y(\xi)$ is similar to that deduced by Rosner (1964, 1967) in his study of homogeneous catalytic reactions.

In a first approximation, the second member of Eq. (8) can be set equal to $1/\sqrt{\chi}$. After integration of Eq. (8) we obtain

$$a \left(\frac{d\theta}{dX} \right)_{x_l} = - \int_0^{x_l} \left\{ \Delta \Gamma_e \exp(-\Psi)^n - \frac{1}{\sqrt{X}} \right\} dX \quad (45)$$

where we suppose that $1/\Gamma_e^2 \ll x_l \ll 1$. The second member of Eq. (45) can be written as

$$a \left(\frac{d\theta}{dX} \right)_{x_l} = \{ \Delta \Gamma_e \exp(-\Psi) \}^{-1} b \quad (46)$$

where

$$b = \int_0^\infty \left(-Y^n + \frac{1}{\sqrt{\xi}} \right) d\xi$$

has to be obtained through the solution of the inner problem given by Eq. (43). For $n=1$, the numerical integration gives $b=4.20$.

To determine Ψ or $\theta_l = 1 - \Psi/\Gamma_e$, Eq. (39) has to be solved with the boundary conditions

$$\theta = \theta_l \quad \text{at} \quad X = 0 \quad \text{and} \quad \frac{d\theta}{dX} = 0 \quad \text{at} \quad X = 1$$

Thus, we can obtain $a(d\theta/dX)_0$ as a function of θ_l and a . This has to be introduced in Eq. (46). To do this it is convenient to define u as follows:

$$u = \frac{(\theta - 1)\Gamma_e}{\Psi} \quad (47)$$

Therefore, Eq. (39) takes the form

$$a \frac{d^2 u}{dX^2} = \frac{1}{\sqrt{X}} \left| \int_{-1}^u K(\bar{\chi}, \chi) d\bar{u} - 1 \right| \quad (48)$$

with the boundary conditions given by

$$u = -1 \quad \text{at} \quad X = 0 \quad \text{and} \quad \frac{du}{dX} = 0 \quad \text{at} \quad X = 1 \quad (49)$$

We can obtain here $(du/dX)_0 = p(a)$. Thus, Eq. (46) reduces to

$$ap(a)\Psi = \frac{b}{\Delta \exp(-\Psi)} \quad (50)$$

This equation determines Ψ as a function of Δ and a in the extinction regime. Extinction occurs for $\Psi=1$. The reduced Damköhler number for extinction is then:

$$\Delta_E = \frac{be}{ap(\alpha)} \quad \text{or} \quad \delta_E = \frac{b\Gamma\Gamma_e}{ap(\alpha)} \exp\left(1 - \frac{\Gamma}{1 + \beta_1}\right) \quad (51)$$

In Figure 2 schematically is plotted the characteristic S-shaped curves which show the ignition and extinction conditions as a function of the parameter α . The extinction regime however has a universal character as shown here.

Equation (51) is valid for all α . The dependence of $ap(\alpha)$ on α is shown in Figure 3. For high values of α such as $\alpha \gg 1$, the solution of Esq. (48) and (49) can be found through the following expansion,

$$u = -1 + \frac{u_1}{\alpha} + \frac{u_2}{\alpha^2} + \dots \quad (52)$$

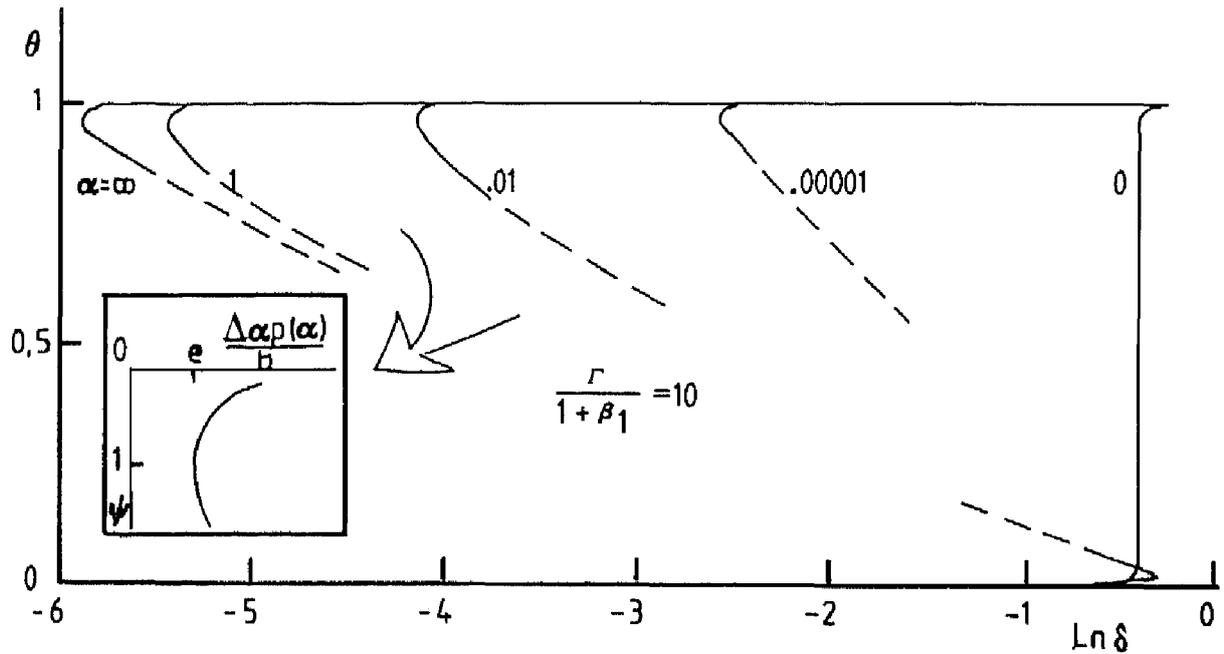


FIGURE 2 Characteristics S-shaped curves showing ignition and extinction as a function of α

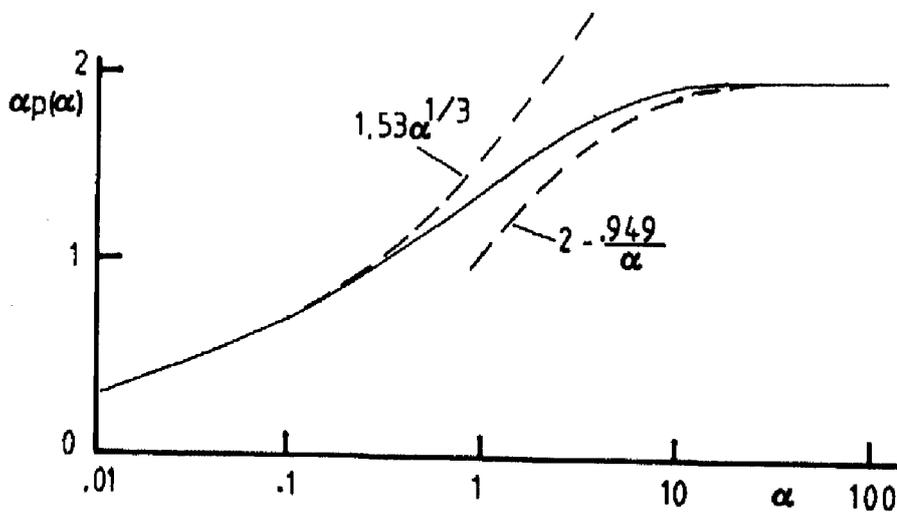


FIGURE 3 Variation of $ap(\alpha)$ as a function of α .

So, we obtain the following set of equations

$$\frac{d^2 u_1}{d\chi^2} = -\frac{1}{\sqrt{\chi}}; \quad \frac{d^2 u_2}{d\chi^2} = \frac{8}{3} \Gamma(4/3) \Gamma(2/3) \sqrt{\chi} - \frac{8\Gamma(2/3)}{3\Gamma(8/3)} \chi \quad (53)$$

the solution of which gives the value of $ap(\alpha)$ as follows

$$ap(\alpha) = \alpha \left(\frac{du}{d\chi} \right)_l = \left(\frac{du_1}{d\chi} \right)_l + \frac{1}{\alpha} \left(\frac{du_2}{d\chi} \right)_l = 2 - \frac{0.949}{\alpha} + O(1/\alpha^2) \quad (54)$$

For small values of α ($\alpha \rightarrow 0$), it is useful to introduce the independent variable ζ , defined by

$$\zeta = \frac{\chi}{\alpha^{2/3}}$$

Equation (45) transforms to

$$\frac{d^2 u}{d\zeta^2} = \frac{1}{\sqrt{\zeta}} \left| \int_{-1}^u K(\bar{\zeta}, \zeta) d\bar{u} - 1 \right|$$

with the boundary conditions given as

$$u = -1 \quad \text{at} \quad \zeta = 0 \quad \text{and} \quad \frac{du}{d\zeta} = 0 \quad \text{at} \quad \zeta = \frac{1}{\alpha^{2/3}} \rightarrow \infty$$

The numerical calculations give

$$\left(\frac{du}{d\zeta} \right)_l = \alpha^{2/3} p(\alpha) = 1.53$$

or,

$$ap(\alpha) \sim 1.53 \alpha^{1/3} \quad \text{as} \quad \alpha \rightarrow 0 \quad (55)$$

In Figure 4 the dependence on α of δ_I and δ_E is plotted. There are four important zones in this figure. In zone I there is only the frozen steady state condition. In zone III the only steady state condition is the vigorous burning beginning at distances close to the leading edge. In zone II there are three steady state solutions one of them is unstable. In zone IV the vigorous burning front is located behind the ignition point, calculated neglecting the axial heat conduction. The plate thermal conductivity is unable to carry the burning front to locations close to the leading edge.

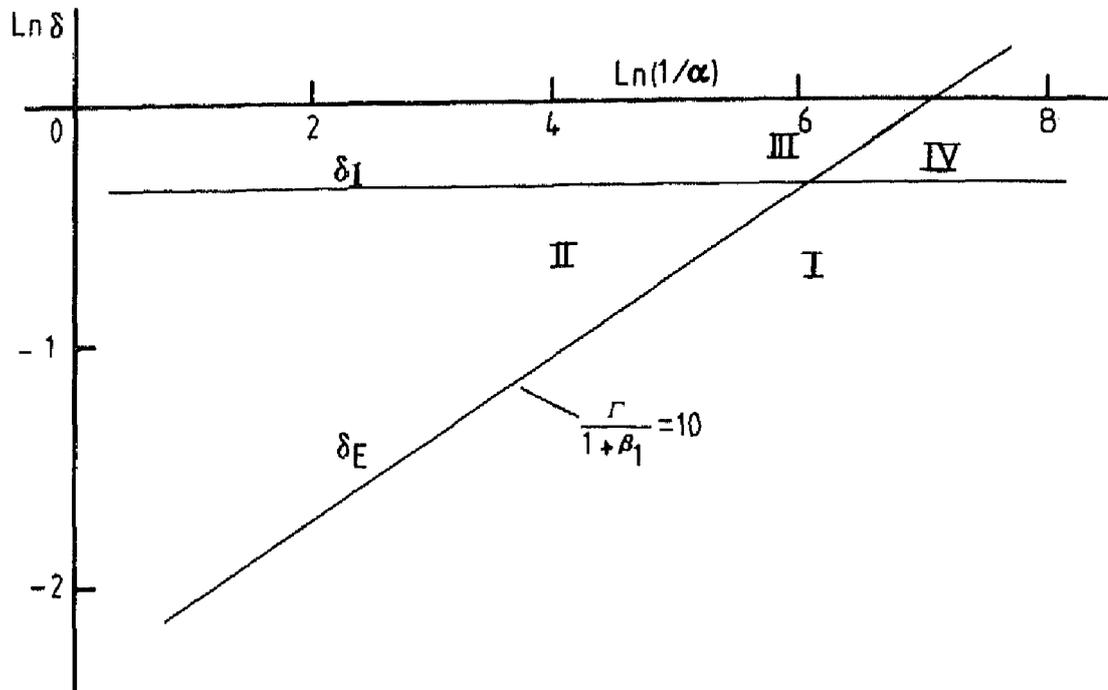


FIGURE 4 Ignition and extinction Damköhler numbers as a function of $1/a$.

An analysis could be made to correct the results retaining higher order terms. However it is desired to present the results from this relatively complex analysis.

CONCLUSIONS

In this paper an analysis was made of the ignition and extinction of catalytic reactions on a flat plate boundary layer with finite thermal conductivity. It was found that the critical Damköhler number for ignition δ_I varies from 0.711 to $2/e$ for $a=0$ and $a \rightarrow \infty$ respectively and is independent of the reaction order in a first approximation. This indicates that the thermal conductivity of the plate does not have strong effects on the ignition process. On the other hand, the finite thermal conductivity of the plate has a strong influence on the critical Damköhler number for extinction δ_E , as given by Eq. (51). One conclusion of practical interest is that the ratio $\delta_I/\delta_E \gg 1$ when $\Gamma \gg 1$ and a is not too small. Thus, for continuous operation it is convenient to work with values of δ far away from that of ignition. Therefore we have to ignite the catalytic combustion with some external aids as for example electrical heating or pre-heated combustible mixture.

Appendix

INTERMEDIATE REGIME

The intermediate branch resulting from the solution to Eqs. (7) and (8), corresponds to an unstable mode and therefore is of little importance. However, we dedicate a

few lines to this regime. Here, the temperature of the plate increases from θ_l at the leading edge of the plate to a critical value θ_c at the position χ_c , where $0 < \chi_c < 1$, maintaining the reaction frozen for $\chi < \chi_c$ and reaching equilibrium for $\chi > \chi_c$. At $\chi = \chi_c$ the reactant concentration changes abruptly from 1 to 0. The energy equation is given then by

$$\alpha \frac{d^2\theta}{d\chi^2} + \frac{H(\theta - \theta_c)}{\sqrt{\chi} \left\{ 1 - \left(\frac{\chi_c}{\chi} \right)^{3/4} \right\}^{1/3}} = \frac{1}{\sqrt{\chi}} \left| \int_{\theta_l}^{\theta} K(\bar{\chi}, \chi) d\bar{\theta} + \theta_l \right| \quad (60)$$

where $H(\theta - \theta_c)$ corresponds to the Heaviside function,

$$H(\theta - \theta_c) = \begin{cases} 1 & \text{for } \theta > \theta_c \\ 0 & \text{for } \theta < \theta_c \end{cases}$$

with the boundary conditions

$$\frac{d\theta}{d\chi} = 0 \text{ at } \chi = 0 \text{ and } \chi = 1; \quad \theta = \theta_c \text{ at } \chi = \chi_c \quad (61)$$

and the continuity of $d\theta/d\chi$ at $\chi = \chi_c$. We can obtain χ_c and θ_l as a function of α and θ_c . From the analysis of the abrupt change in the reactant concentration close to χ_c , we can obtain the value of $\theta_c(\delta)$. We can anticipate that

$$\frac{\delta}{\Gamma^{4/3}} \exp\left(\frac{\Gamma\theta_c}{1 + \beta_1\theta_c}\right) \sim 1. \quad (62)$$

This analysis would fail if the plate thermal conductivity of the plate is very high ($\alpha \rightarrow \infty$). In this case the integration of Eq. (8) gives

$$\frac{\delta}{\Gamma} \exp\left(\frac{\Gamma\theta_c}{1 + \beta_1\theta_c}\right) \int_0^1 Y^n d\chi = 2\theta_c. \quad (63)$$

Equation (7) can be transformed to,

$$- Y^n = \frac{1}{\sqrt{\xi}} \int_1^Y K(\bar{\xi}, \xi) d\bar{Y} \quad (64)$$

with

$$\xi = \chi \left\{ \frac{\delta}{\Gamma} \exp\left(\frac{\Gamma\theta_c}{1 + \beta_1\theta_c}\right) \right\}^2 = \chi \xi_M.$$

Therefore from Eq. (63) we obtain finally

$$\int_0^{\xi_M} Y^n d\xi = 2\theta_c \sqrt{\xi_M} \quad . \quad (65)$$

From Eqs. (64) and (65) we can obtain $\xi_M = \xi_M(\theta_c)$ which in fact provides the value of $\delta = \delta(\theta_c)$.

ACKNOWLEDGEMENT

The participation of the second author was supported by the Fundacion de Estudios e Investigaciones Ricardo J. Zevada A.C. of Mexico. Support was also provided by the Ministerio de Asuntos Exteriores of Spain, the Dirección General de Asuntos del Personal Académico and the Dirección General de Intercambio Académico of the Universidad Nacional Autónoma de México through the Scientific and Cultural Exchange Program between both countries.

- Ahluwalia, R. K., and Chung, P. M. (1980). Extract and approximate solutions of a chemically reacting non-equilibrium flow problem. *Int. J. Heat Mass Transfer* **23**, 627.
- Artyukh, L. Y., Vulis, L. A., and Kashkanov, V. P. (1961). Combustion of gas flowing at the surface of the plate. *Int. Chem. Engng.* **1**, 64.
- Lighthill, M. J. (1950). Contribution to the theory of heat transfer through a laminar boundary layer. *Proc. Roy. Soc.* **A202**, 359.
- Lindberg, R. C., and Schmitz, R. A. (1969). On the multiplicity of steady states in boundary layer problems with surface reactions. *Chem. Engng. Sci.* **24**, 1113.
- Lindberg, R. C., and Schmitz, R. A. (1970). Multiplicity of states with surface reaction on a blunt object in a convective system. *Chem. Engng. Sci.* **25**, 901.
- Liñán, A. (1983). Laminar boundary layer with surface reactions on a flat plate. To be published.
- Mihail, R., and Teodorescu, C. (1975). Laminar boundary layer with non-isothermal surface reactions. *Chem. Engng. Sci.* **30**, 993.
- Rosner, D. E. (1964). Convective diffusion as an intruder in kinetic studies of surface catalyzed reactions. *AIAA Journal* **2**, 593.
- Rosner, D. E. (1967). Convective diffusion limitation of the rates of chemical reactions at solid surfaces—kinetic implications. *Eleventh (International) Symposium on Combustion*, The Combustion Institute, pp. 181–196.