THEORY OF GASEOUS COMBUSTION

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I - BASIC CONSIDERATIONS

I.1. Two feed-back mechanisms

The combustion processes are characterised by two non linear feedback mechanisms producing self-acceleration. One is of a thermal nature and the other is purely chemical.

The first one results from the fact that the overall chemical reaction involved in combustion is exothermal with a rate that is a strongly increasing function of the temperature. This produces a self-acceleration of the combustion process that is saturated by the reactants consumption

$$\nu'_F F + \nu'_O O \longrightarrow P + Q \qquad (1.1)$$

Fuel   Oxidant   Products   Heat
     Reactants   release
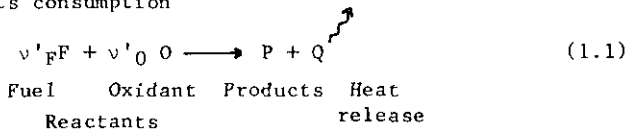
ν' are the stoichiometric coefficients.
For simplicity the reverse reaction is neglected in (1.1).
Let's define W_F, W_O and W_P as the mass consumption (per unit time and per unit volume of reactive mixture) of fuel, oxidant and products respectively. From (1.1) one has :

$$W_F = W_O/\nu = -W_P/(1+\nu), \qquad (1.1')$$

with $\quad \nu = \nu'_O M_O/\nu'_F M_F \quad$ where M_i are the molar mass.

The thermal feedback is described by the nonlinear Arrhenius law :

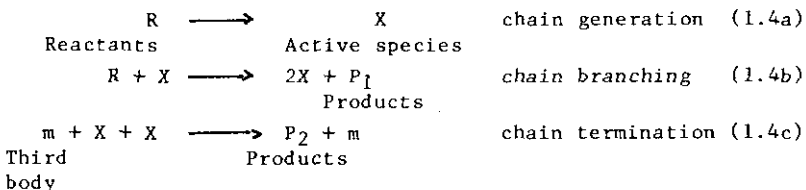$$W_F = \rho B \; Y_F^{n_F} \; Y_O^{n_O} \; e^{-E/RT} \qquad (1.2)$$

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Where Y_i, n_i and E are the mass fractions ($Y_i = \rho_i/\rho$) the order of reaction and the activation energy respectively. B is the frequency factor whose temperature dependance can be neglected in front of $\exp(-E/RT)$. $n_i \neq \nu'_i$ results from the fact that (1.1) is not an elementary reaction governed by collisions. For ordinary hydrocarbons flames the number of elementary reactions required to transform the fresh mixture into burnt products is of the order of 300 with 50 intermediate species ! This precludes a complete quantitative description of the combustion. In this course we will focus the attention on the effects that can be described by (1.1) and (1.2). Only few words will be said concerning the effects produced by the complex chemistry and by the diffusion of the intermediate species. The density dependance of B can be easily calculated only in the case of an elementary reaction where $\nu'_i = n'_i = 1$ by noticing that, according to the elementary kinetic theory of gases the number of reactive collisions per unit time and unit volume is given by :

$$\frac{W_F}{\nu'_F M_F} = N_F \; N_O \; \underbrace{K \; e^{-E/RT}}_{\text{reaction constant}} \qquad (1.3)$$

with the molar concentration N_i defined by $N_i = \rho Y_i/M_i$ and where the prefactor K is predicted to be a constant independent of ρ and weakly dependent on T.

The second feedback mechanism is produced by the <u>chain branching reactions.</u> These reactions are <u>autocatalytic</u> reactions that produce more active intermediate species than they consume leading to a <u>self acceleration</u> of chemical process. Such a mechanism can be represented schematically by :

$$R \longrightarrow X \qquad \text{chain generation} \quad (1.4a)$$
Reactants   Active species

$$R + X \longrightarrow 2X + P_1 \qquad \textit{chain branching} \quad (1.4b)$$
Products

$$m + X + X \longrightarrow P_2 + m \qquad \text{chain termination} \quad (1.4c)$$
Third   Products
body

Because of the strong non-linearity in temperature of the Arrhenius law (1.2), the thermal feedback dominates the kinetic one in the ordinary hot flames. And a good insight into the problem can be obtained by ignoring in a first step the details of the chemical kinetics aspects.

I.2. The conservation equations

When the combustion is assumed to be controlled by the overall chemical reaction (1.1) with the rate (1.2), the equations controlling the reacting flow involve the fuel and oxidant mass balance and the conservation of the energy :

SPECIES $\left\{\rho \dfrac{\partial}{\partial t} Y_i + \rho \underline{V} \bullet \underline{V} Y_i - \underline{V} \bullet (\rho D_i \underline{V} Y_i)\right\} = -W_i$, i=F,O

transient convection diffusion production   (1.5)

ENERGY $\left\{\rho \dfrac{\partial}{\partial t}(C_p T) + \rho \underline{V} \bullet \underline{V}(C_p T) - \underline{V}(\lambda \underline{V} T)\right\} = + q W_F$

Fourier law

where the energy released in the reaction per unit mass fuel q is given by :

$$q = Q/\nu'_F M_F \qquad\qquad (1.6)$$

C_p is the specific heat of the reactive mixture. D_i and λ are the molecular diffusivities of the species i and the heat conductivity of the reactive mixture respectively.

Two basic assumptions have been made in writing (1.5). The first concerns the transport properties of the reactive mixture where it has been assumed that the binary Fick law holds. This is well verified when the mixture is diluted in inert gases (as for the example the Nitrogen of the air). The second assumption concerns the equation for the energy conservation where the com-pressible effects have been neglected. These last effects are of a relative order of magnitude of Mach squared, and it is legitimate to neglect them for subsonic combustion but it is worthwhile to mention that they have determinant effects in detonations (supersonic-waves) that will not be considered here. This approx-imation is called the "isobaric approximation" where it is assumed that, according to the perfect gas law,

$\rho T = C^t$ (for simplicity the change in the molecular mass
in also neglected)   (1.7)

But it is clear that because of the presence of the flow field $\underline{V}$, the system (1.5) is not closed. In fact because of the *expansion of the gas (described by (1.7)), the flow field is influenced by the combustion.* Thus, the mass and momentum equations have to be added (in the general case) to the system (1.5)(1.7) and general combustion problems appear as phenomena where hydrody-namics is coupled with diffusion-reaction process. But in some simple cases (as the 1-d and steady case) this coupling disappears.

I.3. *The adiabatic temperature of combustion*

Consider the case of an homogeneous and adiabatic combustion. In this case, eq.(1.5) reduces to

$$-\frac{\partial Y_F}{\partial t} = +\frac{W_F}{\rho} = \frac{\partial(C_p T/q)}{\partial t} = \frac{\partial(Y_0/\nu)}{\partial t} \qquad\qquad (1.8)$$

$$Y_F - Y_0/\nu = Y_{Fu} - Y_{0u}/\nu$$

$$\text{(1.8')}$$

$$Y_F + C_p T/q = Y_{Fu} - C_p T_u/q$$

where the subscript u is for the initial mixture (unburnt gases)

$$\frac{\partial Y_F}{\partial t} = -Y_O^{nO} \, Y_F^{nF} \, B e^{-E/kT} \qquad \text{(1.9)}$$

When $t \to \infty$ the reaction is completed by consumption of the limiting component. Let assume, for example, that F is the limiting component, in that case one has

$$t \to \infty \ , \ Y_F \approx 0 \ , \ Y_O = Y_{Ou} - \nu Y_{Fu}$$

thus, according to (1.8'), the temperature attains a maximum value given by :

$$t \to \infty \qquad T = T_b$$

$$T_b = T_u + \frac{q Y_{Fu}}{C_p} \qquad \text{(1.10)}$$

eq.(1.10) expresses the conservation of the energy between the initial and the final time.

I.4. The two different kinds of combustion process

One can rewrite the species conservation equations (1.5) in the following symbolic manner

$$\mathbb{L}_F(Y_F) = -\frac{W_F}{\rho} \qquad \text{(1.11)}$$

where the linear differential operator $\mathbb{L}_F$ is given by :

$$\mathbb{L}_F = \frac{\partial}{\partial t} + \underline{V} \cdot \underline{\nabla} - D_F \nabla^2 \qquad \text{(1.11')}$$

where ρD_F has been assumed to be constant. A similar operator $\mathbb{L}_O$ and $\mathbb{L}_T$ can be defined for Y_O and T. Let's define the characteristic mechanical time τ_m by the relation :

$$\mathbb{L}_F(Y_F) \sim \frac{Y_{Fu}}{\tau_m} \qquad \text{(1.12)}$$

In steady cases, τ_m can be considered as the shortest mechanical time (convection, diffusion).
The characteristic reaction time $\tau_r(T)$ is defined by :

$$\tau_r^{-1}(T) = B \, e^{-E/RT} \ , \ \frac{W_F}{\rho} = \frac{Y_F^{nF} \, Y_O^{nO}}{\tau_r(T)} \qquad \text{(1.13)}$$

The equation (1.11) leads to :

$$\mathbb{L}_F(Y_F) = - \frac{Y_F^{nF} \, Y_O^{nO}}{\tau_r(T)} \qquad \text{(1.14)}$$

Two extreme cases can be considered from (1.12) and (1.14) :

(1) $\qquad \tau_r \gg \tau_m \qquad \qquad$ **Frozen-flow**

the chemical reaction can be ignored in (1.14) that reduces to

$$\mathbb{L}_F(Y_F) = 0 \qquad \text{(1.15a)}$$

(2) $\tau_r \ll \tau_m$ **Equilibrium flow**

in that case the chemical equilibrium must be realized

$$W_F = 0 \qquad\qquad (1.15b)$$

and according to the <u>irreversible</u> reaction (1.1) and (1.2) this
is possible only in two cases

$$Y_O = 0 \qquad \mathbf{or} \qquad Y_F = 0 \qquad\qquad (1.15b')$$

One introduces the Damköhler number Da by

$$Da = \frac{\tau_m}{\tau_r}$$

in such a way that the frozen flow corresponds to the small
Damköhler nb limit (Da→0) and the equilibrium flow to large
Damköhler nb limit (Da→∞), in regions of small T and high T, resp.

Let us consider the instructive example of the combustion
developed at the leading edge of a mixing layer of fuel and oxi-
dant :

In the early stage of the mixing layer the mixing time is
shorter than the reaction time (Da≁0) and a frozen reactive pre-
mixed mixture is obtained with a rich composition on the side of the
fuel flow and with a lean composition on the side of the oxidant
flow. Then a combustion proceeds in this premixed mixture to trans-
form the frozen flow in an equilibrium flow (Da≁∞). This called a
<u>premixed combustion</u>. But because of the two different types of
composition (lean and rich) in the frozen flow, the burnt gases
in the equilibrium flow present two different regions of equili-
brium composition. One is defined by $Y_O = 0$ but with $Y_F \neq 0$
(burnt gases of a premixed combustion in a rich mixture where
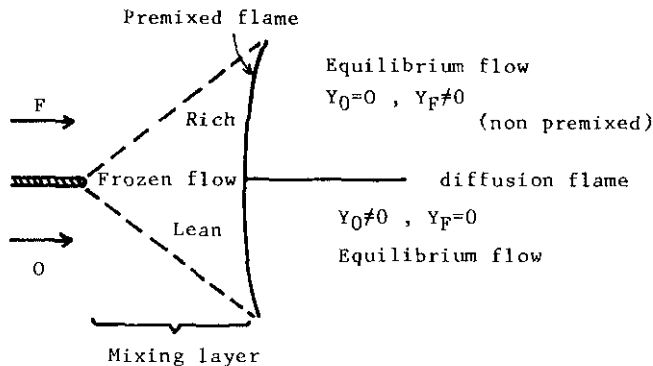there is an excess of fuel) and the other characterized by $Y_F = 0$

Premixed flame

F

Rich

Frozen flow

Lean

O

Equilibrium flow
$Y_O=0$, $Y_F\neq0$
        (non premixed)

———————— diffusion flame

$Y_O\neq0$, $Y_F=0$

Equilibrium flow

Mixing layer

Fig.1.1

(burnt gases of a lean mixture) but with $Y_0 \neq 0$. Then, the combustion takes place at the boundary of these two regions of equilibrium flow in the form of what it is called a diffusion flame to burn the fuel of one equilibrium flow with the oxidant of the other equilibrium flow.

1.5. The large activation energy

The very existence of frozen premixed mixtures as well as the thin transition layers shown in Figure 1.1 are due in fact, mainly to the high sensitivity of the reaction rate (1.2) to the temperature, associated with the large values of the activation energy encountered in combustion, $E \gg RT$, and to the exothermicity of the reaction.

Introducing the reduced activation energy β defined by :

$$\beta = \frac{E}{RT_b} \frac{(T_b - T_u)}{T_b} \quad \text{(Zeldovich number)} \tag{1.16}$$

ordinary values of β are close to 10;

$$\varpi^{-1} = \frac{\tau_r(T)}{\tau_r(T_b)} = \frac{e^{+E/RT}}{e^{+E/RT_b}} = \exp\left\{ + \frac{\beta(1-\theta)}{1+\alpha(\theta-1)} \right\} \tag{1.17}$$

where θ is the reduced temperature $\theta = \frac{T-T_u}{T_b - T_u}$, $(0 < \theta < 1)$, and α is the gas expansion parameter $\alpha = (T_b - T_u)/T_b$ (in ordinary flames $0.8 < \alpha < 1$). Thus, for $\beta \simeq 10$ and $\alpha \simeq 0.8$, eq.(1.17) leads to $\tau_r(T_u) \simeq 2.10^{22} \tau_r(T_b)$. As $\tau_r(T_b)$ is known to be of the order of 10^{-4}s, the reaction time at the ordinary temperature $T_u \backsim 300°K$ is of the order of

$$\tau_r(T_u) \simeq 2.10^{18}s \tag{1.17'}$$

that can be considered as an infinite time at the human scale!

In fact eq.(1.17) shows clearly that the relative reaction rate (compared to the one at the adiabatic flame temperature) is transcendentally $O(e^{-\beta})$ small everywhere except when the temperature is close enough to the adiabatic flame temperature that is precisely when $1-\theta = O(1/\beta)$. See fig.1.2.
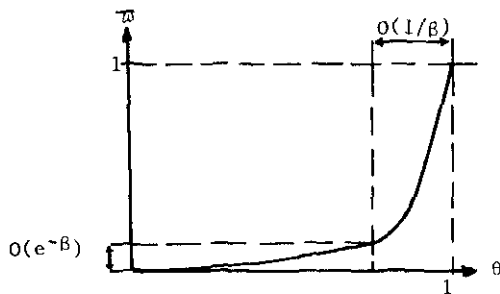

Fig.1.2

Thus it is interesting to notice that, in the limit of $\beta \to \infty$, $\omega = \tau_r^{-1}(T)/\tau_r^{-1}(T_b)$ goes to the singular limit $\omega = 0$ for $0 < \theta < 1$ and $\omega = 1$ for $\theta = 1$. This behavior illustrates the high non-linearity *of the sensitivity of the reaction rate to the temperature.*

II - PREMIXED FLAMES

II.1. Position of the problem

A premixed flame is a subsonic chemical wave propagating in a premixed frozen mixture under the diffusive transport mechanism of mass and energy. In fact it appears as a thin transition layer between the frozen mixture ($Da \to 0$) and the equilibrium mixture ($Da \to \infty$). It turns out experimentally that the mass flux of frozen mixture crossing this transition surface is a characteristic not only of the thermodynamics conditions (temperature and pressure) and of the chemical composition of the frozen mixture but also of the geometrical configuration of the flame front and of the flow. The simplest case is the planar front moving with a constant velocity. In this case, the equations (1.5) written in the moving frame of the front reduces to much simpler one dimensional and steady equations. $\underline{V} = (u,0,0)$ and the total mass conservation implies that the mass flux $m = \rho u$ is constant across the front. A further simplification occurs when the mixture is far from the stoichiometric composition. In this case, one can neglect the change in the mass fraction of the abundant species and the combustion is controlled only by the limiting species. Then the system of equation (1.5) reduce to two coupled equations. In fact, in these 1-d and steady solutions, there is no direct coupling with the hydrodynamics and the deflagration waves are described by ordinary equations of diffusion-reaction :

$$m\frac{d}{dx} Y - \rho D \frac{d^2}{dx^2}Y = -W$$

$$m \frac{d}{dx} (C_p T) - \lambda \frac{d^2 T}{dx^2} = +qW \qquad (2.1)$$

with, according to (1.2), $\quad W = \rho K\ Y^n\ e^{-E/RT}$

where $K = BY^n j$ (the subscript j referring to the abundant species) and with the boundaries conditions :

			(2.1')
Unburnt gases	$x = -\infty$	: $Y = Y_u$, $T = T_u$	(Frozen flow)
Burnt gases	$x = +\infty$	: $Y = Y_b = 0$	(Equilibrium flow)

See the shape of the corresponding profiles in fig. 2.0 The unknowns of the problem are the concentration and temperature profiles (that determines the flame structure) as well as the mass flux m appearing as an eigenvalue of the problem and defining the laminar flame velocity u_L (defined in the fresh mixture)

$$m = \rho_u\ u_L = \rho_b\ u_b \qquad (2.2)$$

In the moving frame of the flame front, u_L and u_b represent the flow velocity in the upstream fresh mixture and in the downstream burnt gases respectively, u_L and u_b can also be considered as the flame velocity relative to the fresh and burnt mixture respectively. Notice that because of the gas expansion $(\rho_b/\rho_u=T_u/T_b)$, the flame velocity defined relative to the burnt gas, u_b, differs from the flame velocity relative to the fresh mixture, u_L. A direct integration of (2.1) from $x=-\infty$ to $x=+\infty$ shows that $T=T_b$ at $x=+\infty$ where T_b is given by (1.10). Thus, introducing the reduced quantity

$$\psi = Y/Y_u \quad \text{and} \quad \theta =(T-T_u)/(T_b-T_u) \qquad (2.3)$$

the boundaries conditions (2.1') for θ and $1-\psi$ appear to be identical

$$x=-\infty \quad : \quad \theta=1-\psi =0 \quad \text{and} \quad x=+\infty \quad : \quad \theta= 1-\psi =1 \qquad (2.3')$$

Furthermore the equations of θ and $1-\psi$ _differ only_ by the value of the diffusion coefficient :

$$m \frac{d}{dx} \psi - \rho D \frac{d^2}{dx^2} \psi = -\frac{1}{Y_u} W \qquad (2.4)$$

$$m \frac{d}{dx} \theta - \rho D_{th} \frac{d^2}{dx^2}\theta= \frac{1}{Y_u} W$$

where the thermal diffusivity is defined by $D_{th}= \lambda/\rho C_p$. Thus, when the Lewis number $Le = D_{th}/D$ is unity, the two equations of (2.4) are identical with the same boundary conditions, and it turns out that

$$\theta = 1-\psi \qquad x\epsilon(-\infty, +\infty) \qquad (2.5)$$

and the problem is reduced to solve only one non linear _thermal_ equation _of reaction-diffusion type_ :

$$m \frac{d}{dx} \theta - \rho D_{th} \frac{d^2}{dx^2} \theta = \frac{\rho}{\tau_r(T_b)} \omega(\theta) \qquad (2.6)$$

with
$$\qquad (2.6')$$

$$\tau_r^{-1}(T_b) = \frac{K}{Y_u} \exp(-E/RT_b) \quad \text{and} \quad \omega(\theta)=(1-\theta)^n\exp\left\{-\frac{\beta(1-\theta)}{1+\alpha(\theta-1)}\right\}$$

$$\omega(\theta)=(1-\theta)^n \varpi(\theta) \quad \text{where} \; \varpi \; \text{has been}$$

defined in § I.5 .
With the boundary conditions

$$x=-\infty \quad : \quad \theta=0 \quad ; \quad x=+\infty \quad : \quad \theta=1 \qquad (2.6'')$$

From an historical point of view, _Mallard and Le Chatelier_ (1883) were the first not only to consider a premixed flame as a progressive chemical wave but also to give the basic mechanism of propagation and to provide the first experimental data on flame speed. They introduce the notion of inflammation temperature T_i under which the reaction is quenched and they consider the thermal propagation of a flame as successive inflammations of slices of frozen flow. A part of the heat released in a reacting slice is used to warm up the frozen slice just ahead where the combustion will start when the temperature will reach T_i. Thus, the combustion process was explained _to possibly propagate in a frozen flow._
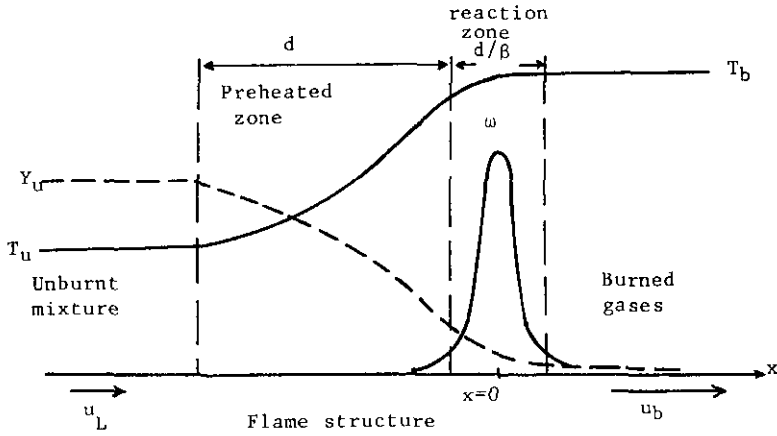
Flame structure

Fig.2.0

Taffanel (1913) and Jouguet (1913) wrote the corresponding differential equation similar to (2.6) and Taffanel obtained the correct expression of the laminar flame speed in terms of D_{th} and of the characteristic chemical time τ_r :

$$u_L \; \alpha \; \sqrt{D_{th}/\tau_r(T_b)} \qquad (2.7)$$

Such an expression can be directly obtained by a dimensional analysis. With $D_{th} \sim 0.3$ cm^2/s and $\tau_r(T_b) \sim 10^{-4}$s one obtains $u_L \sim 55$cm/s.

II.2. Existence and unity

II.2.1. The cold boundary difficulty

From a mathematical point of view, the problem (2.6,6',6") is hill posed. A necessary condition for the existence of the solution is that the production term be zero in the upstream condition (frozen flow) ;

$$\omega(\theta=0) = 0 \qquad (2.8)$$

This condition is not exactly satisfied by the Arrhenius law (2.6'). But from a physical point of view, as shown by (1.17') and the discussion under fig.1.2, this problem is rather academic for the usual combustion problem. From a mathematical point of view, the problem has to be treated as an unsteady problem($\rho \frac{\partial}{\partial t} \theta$ must be added on the left hand side of 2.6) and according to Aldushin, Khudyaev and Zeldovich (1981) one has to look for travelling waves in a non steady, but homogeneous medium that evolves "in bulk" with the characteristic chemical time of the frozen flow :

$$\frac{\partial}{\partial t}\,\theta = \frac{1}{\tau_r(\theta)} \quad , \ \theta \ \text{close to } 0 \Rightarrow \tau_r \ \text{close to } \tau_r(T_u) \qquad (2.9)$$

This problem can be accurately solved by a two time scales method when the two time scales $\tau_r(T_u)$ and $\tau_r(T_b)$ are largely different ($\varpi_u \ll 1$). But, according to (1.17'), ϖ_u is so small in combustion problems ($\varpi_u \sim 10^{-22}$) that $\omega(\theta=0)$ can be physically considered as zero. In the past many different tentatives have been developed to modify the Arrhenius law in the "unburnt" side but, clearly, this modification has not to appear in the final result. It will be seen in the following that the introduction of such modifications is not necessary and that the problem is completely cured by considering the asymptotic limit $\beta \to \infty$.

II.2.2. The unicity

But, even when (2.8) is satisfied (cold boundary difficulty cured), it turns out that the uniqueness of solutions depends critically on the behavior of $\omega(\theta)$ near $\theta=0$. Since the work of Fisher (1937) and of Kolmogorov, Petrovsky and Piskonov (1937), it is known that (2.6,6") may admit a continuous set of solutions corresponding to a continuous spectrum of travelling speeds, m, as soon as $\omega_0' = \frac{d}{d\theta}\,\omega(\theta)\big|_{\theta=0} > 0$. The problem is to determine what are the solutions selected by the physical situations. In the above mentioned work of (K.P.P.)(concerned with a biological problem where $\omega(\theta)\alpha\ \theta(1-\theta)$), it has been shown that the asymptotically stable solution (that is the only one relevant from a physical point of view) corresponds to the lower bounds m_{KPP} of the spectrum. Moreover m_{KPP} is found to be directly proportional to $\sqrt{\omega'_0}$. But on the other hand in the case of an inflammation temperature where :
$$\omega(\theta)= 0 \ \text{ for } 0<\theta<\theta_i<1 \ \text{ and } \ \omega(\theta)>0 \ \text{ for } \theta_i<\theta<1 \qquad (2.10)$$
and where the inflamation temperature θ_i is a given positive constant ($0<\theta_i<1$), it has been proven that the system (2.6.6") admits only a unique solution (see Zeldovich (1948), Johnson-Nachbar (1963) and Gel'fand (1959)). As this unique solution corresponds to $m\neq 0$, it is clear that this solution is not related to the K.P.P. solution .The problem has also been proved to have a unique solution when $\omega_0 < 0$ and when $\omega(\theta)$ has only one zero for $0<\theta<1$. An intensive literature has been devoted to the general problem of the propagation of plane wave fronts controlled by equations of reaction and diffusion (see f.e. P. Fife (1978))and also Murray (1977)), but few comments are usually found concerning the transition from the K.P.P. solution to the unique solution of the θ_i-model.. The most pertinent ones have been developed by authors concerned by combustion phenomena namely Adulshin, Kudyaef & Zeldovich (1981). It is also worthwhile to consult the books of Frank-Kamenetskii (1969) and the one of Zeldovich & co-authors (1980). Interesting comments

can also be found in the monography of P. Fife (1979).

After having cured the cold boundary difficulty as in the paper of Aldushin & Co (1981), the production term (2.6') reduces to

$$\omega(\theta) = (1-\theta)^n \left\{ \exp(\beta(\theta-1)) - \exp(-\beta) \right\} \qquad (2.11)$$

For simplicity one has neglect the term $\alpha(\theta-1)$ in (2.6') that will be proved to not be important. The shape of the production term (2.11) appears as an intermediate case that goes from a "mild" to a "sharp" non linear form as β increases from 0 to infinity (see fig. 2.1). For very small values of β $\omega(\theta) \sim \beta$ $\theta(1-\theta)$ and for large values, when the transcendentally small terms $O(e^{-\beta})$ can be neglected, $\omega(\theta)$ can be considered as a θ_i model but, in addition, with $1-\theta_i = O(1/\beta)$. This last property allows to neglect the term $\alpha(\theta-1)$ in eq.(2.6') as well as the density change in the r.h.s. of eq(2.6) where ρ can thus be replaced by ρ_b. These approximations are used here for simplicity but they can be removed without difficulties A simple change of space variable put the eq(2.6) in the following simpler form

$$\xi = x/d \ , \quad d = \sqrt{\rho D_{th} \tau_r(T_b)/\rho_b} \quad \text{and} \quad \rho D_{th} = C^t \qquad (2.12)$$

$$M \frac{d\theta}{d\xi} - \frac{d^2}{d\xi^2} \theta = \omega(\theta) > 0 \qquad (2.13)$$

With the boundaries conditions $\xi = -\infty$: $\theta=0$ Fresh mixture
$\xi = +\infty$: $\theta=1$ Burnt gases

and with $0<\theta<1$ for $\omega<\xi<+\infty$

the reduced front velocity M is related to m by :

$$M = m \tau_r(T_b)/\rho_b d = m \sqrt{\tau_r(T_b)/\rho_b \rho D_{th}}.$$

In the following, the attention is restricted to the cases $\omega(\theta)>0$ and $(0<\theta<1)$.

II.2.3. Orbits in the phase space

In order to get a better insight into the problem, it is worthwhile to consider the phase space (θ,P) with P defined by :

$$P = M \ d\theta/d\xi \qquad (2.14)$$

and eq(2.13) takes the form :

$$\frac{1}{M^2} \frac{dP}{d\theta} = \frac{P-\omega}{P} \qquad (2.15)$$

The singular points $(\omega=0)$ are $(1,0)$ and $(0,0)$. The first one, corresponding to the burnt gases, is a saddle (see fig.II.2a) with two principal directions $Q_{\pm}^b$ $(Q_-^b<0, Q_+^b>0)$. Only the negative one Q_-^b is relevant because when $\omega>0$ one must have P>0 as well as $\theta<1$.

$$Q_{\pm}^b = \frac{M^2}{2} (1 \pm \sqrt{1-4\omega_1^{\,\prime}/M^2}) \qquad (2.16)$$

fig.2.1a 1   fig.2.1b 1   fig.2.1c 1   fig.2.1d θ_i 1
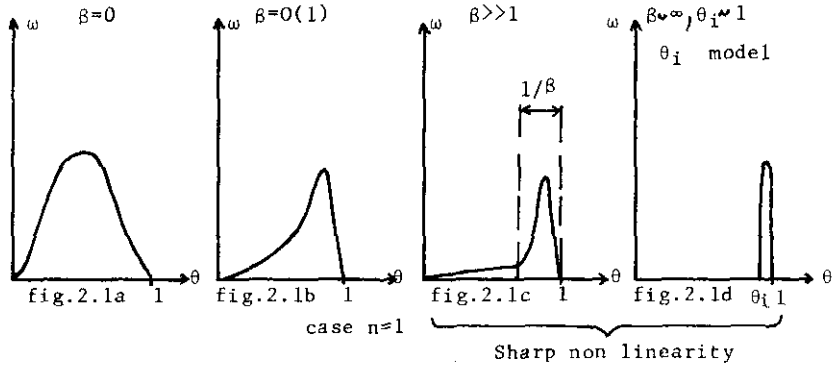
case n=1

Sharp non linearity

Fig.2.1

where $\omega_1' = \frac{d\omega}{d\theta}\big|_{\theta=1} < 0$ for n=1. $(\omega_1' = 0, n=2)$

The second singular point (0,0) is related to the unburnt mixture (fresh gases), it is a spiral point when $M < 2\sqrt{\omega_1'}$ and a node in the opposite case (see fig.II.2b)

$$M > 2\sqrt{\omega_o'} \qquad (2.17)$$

When $\omega > 0$, the solutions are associated with non negative values of θ and thus one has to consider only the case (2.17). No travelling waves can be obtained from (2.13) when the condition (2.17) is not satisfied. The two principal directions at the mode have a positive slope :

$$Q_{\pm}^u = \frac{M^2}{2} (1 \pm \sqrt{1-4\omega_o'/M^2}) > 0 \qquad (2.18)$$

where

$$\omega_o' = \frac{d\omega}{d\theta}\big|_{\theta=0} > 0$$

The solutions (2.13) are represented in the phase space by orbits leaving the saddle point (1,0) with the slope Q_-^b to reach the mode (0,0) with one of the two possible slopes Q_-^u Q_+^u . The differential equation (2.13) being of first order, for each value of M one cannot have more than one trajectory linking the two singular points. The question is to determine the set of values of M (spectrum)associated with a solution. It is worthwhile to notice the following points :
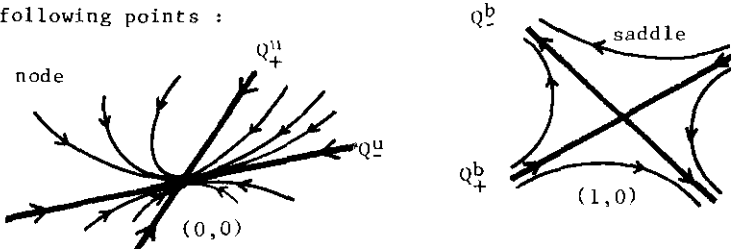

Fig.2.2

- a) For a given value of M, only one orbit can leave the saddle point tangent to Q_-^b and also only one can reach the node with a tangent equal to Q_+^u. But this is not the case for the other principal direction Q_-^u where a family of orbits $P_\kappa(\theta)$ tangent to Q_-^u can reach the node with the following behavior

$$P_\kappa(\theta) \quad Q_-^u \ \theta + \kappa\theta^{(M^2-Q_-^u)/Q_-^u} + \ldots \qquad (2.19)$$

where κ is an arbitrary constant (Notice that according to (2.18) $\dfrac{M^2}{Q_-^u} - 1) > 1$)

- b) In the limit $M \to \infty$, $P = \omega(\theta)$ is, according to (2.15), the trajectory as soon as $dP/d\theta$ remains bounded everywhere.

- c) $0 < |Q_-^b| < |\omega_1'|$ and $M^2 > Q_+^u > 2\omega_o' > Q_-^u > \omega_o'$. Thus the trajectory $P(\theta)$ has to cross $\omega(\theta)$ where according to (2.15) $\dfrac{dP}{d\theta} = 0$.

- d) For the minimum value $M = 2\sqrt{\omega_o'}$, $Q_+^u = Q_-^u = 2\omega_o$. For $M \to \infty$: $Q_+^u \to M^2$ and $Q_-^u \to \omega_o$

Before presenting the detailed analysis of a simplified model, let us present some general results.

II.2.4. General results

- i) When the curve $\omega(\theta)$ is concave as in fig. 2.1a, it has been shown by Kolmogorov & Co (1937) that a solution satisfying $0 < \theta < 1$ exists for all values of M larger than a lower bound called M_{KPP}. The KPP solution is governed by the behavior at the unburnt boundary condition $\theta = 0$:

$$M_{KPP} = 2\sqrt{\omega_o'} \quad \text{with} \quad \omega_o' = \frac{d\omega}{d\theta}\Big|_{\theta=0} \qquad (2.19)$$

It has also been proved that the KPP solution is the physically relevant one in the sense that this solution is reached asymptotically in time ($t \to \infty$) from ordinary initial conditions ($t=0$)
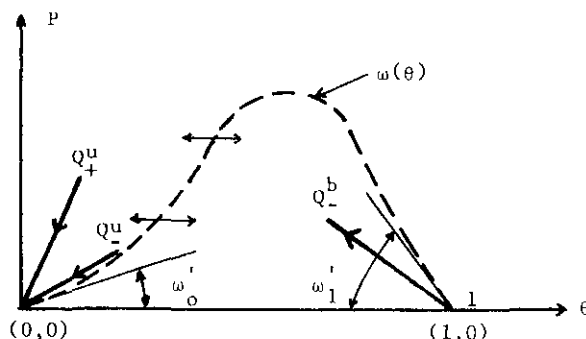

Fig.2.3

including a heavyside step function (see Fife 1979 and also Aronson & Weinberger 1978 for recent reviews). All these solutions $M > M_{KPP}$, including the KPP one, are tangent to the "ordinary" principal direction Q^u_- at the node of the cold boundary condition.

ii) When the production curve is <u>no more concave</u> everywhere in the interval $\theta \in [0,1]$, the lower bound can be higher than M_{KPP} defined by (2.19)(see Fife 1979). Let us call M_L the lower bound in this case, $M_L > M_{KPP}$. The corresponding L-solution is still the relevant one from a physical point of view but presents a different structure from all the other in the spectrum $M > M_L$. The L solution is the only one reaching the node (0,0) at the cold boundary tangent to the "extraordinary" principal direction Q^u_+. To the best of our knowledge, this property that has not been stressed enough before Aldushin & Co (1981) is of primary importance in premixed flames. In fact the relevant travelling wave solution that is always associated with the lower bound of the spectrum, changes of nature when the non linear term $\omega(\theta)$ becomes sharper and sharper. Such a sharpening can be obtained with the production term (2.11) by increasing the reduced activation energy β of the Arrhenius law. Notice that large values of β correspond to a large difference between the characteristic time scales τ_b and τ_u of the chemical production rate at its maximum value $\tau_b = \beta^n \tau_r(T_b)$ and close to the boundary controlled by $\omega_o = O(\beta e^{-\beta})$, $\tau_u = \dfrac{e^\beta}{\beta} \tau_r(T_b)$:

$$\beta \to \infty \; , \; \tau_b/\tau_u \to 0 \; , \quad \tau_b/\tau_u = O(\beta^{n+1} e^{-\beta}) \tag{2.20}$$

As we will see in the next section, for large values of $\beta(\beta \to \infty)$, the L-solution goes to a limiting value that was obtained in 1983 by Zeldovich and Frank Kamenestkii

$$\lim_{\beta \to \infty} M_L = M_{ZFK}$$

The important point is that this ZFK solution is proved to not depend on τ_u but only on τ_b. But on the contrary, for $\beta \to 0$ the KPP solution holds and, as shown by eq(2.19), the solution is completely controlled by τ_u. Thus, the L-solution must insure a transition between these two extreme cases. In fact the L-solution, if it exists, is the only one that is not tangent to Q^u_- at the cold boundary and thus it is the only one in the spectrum that is not controlled by τ_u when $\omega'_o \to 0$. All the other solutions corresponding to $M > M_L$ contain in the upstream part of their temperature profile a long tail associated with τ_u which is determined by ω'_o. But according to the order of magnitude (1.17') the corresponding length scale is prohibitively long to be meaningful in ordinary experimental conditions. The L-solution is the only one that has a thin flame thickness controlled (as u_L, see eq.2.7) by D_{th} and τ_b. Contrarly to the other solutions ($M > M_L$), the chemical reaction is not necessary for matching the cold boundary condition $T = T_u$ in the upstream part of the L-solution where the heat conduction is the dominant phenomenon. This peculiarity of the L-solution is related to the principal direction Q^u_+ .

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Furthermore the unique solution of the θ_i -model goes to the Z.F.K. solution in the limit $\theta_i \to 1$:

$$\lim_{\theta_i \to 1} M_{\theta_i} = M_{ZFK} \qquad (2.22)$$

II.2.5. The exact solution for a particular model

As shown by Aldushin et al. (1981), the KPP solution (2.19) holds for (2.11) in a finite domain of β around zero. There exists a critical value $\beta*$ at which the L-solution $(M_L \geqslant M_{KPP})$ appears. In order to better understand this transition let us study the following model that can be exactly solved (another model is presented by Aldushin et al. (1981)) ;

$$\omega(\theta) = \begin{cases} \omega_o' \cdot \theta & ; & 0 < \theta < 1-\varepsilon \\ \dfrac{1}{\varepsilon^2} h(1-\theta) & ; & 1-\varepsilon < \theta < 1 \quad (\text{see fig.2.4}) \end{cases} \qquad (2.22')$$

with $0 < \varepsilon < 1$ and where one of the two parameters h and ω_o' can be removed through adequate scaling. For convenience, let's keep ω_o' fixed (M_{KPP} fixed) and let vary h and ε.

In this model, the orbit leaving the saddle point (1,0) tangent to Q_-^b as well as the one reaching the node (0,0) tangent to Q_+^{Ψ} are straight lines for $(1-\varepsilon) < \theta < 1$ and $0 < \theta < 1-\varepsilon$ respectively. For h and ε given, let us consider the modification of the orbits (solution of the problem 2.13) when M decreases. For $M = \infty$, the orbit is $P = \omega(\theta)$ (see -b) and when M decreases two scenario are possible depending on the values of h and ε :
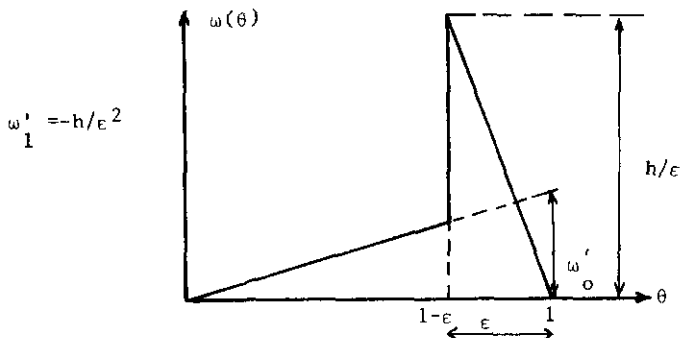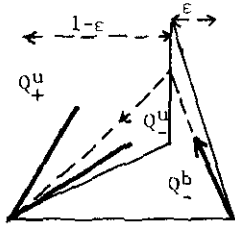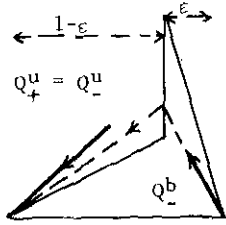

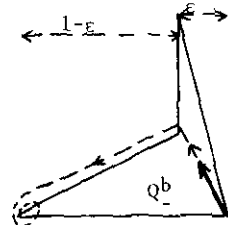$$\omega_1' = -h/\varepsilon^2$$

Fig.2.4

fig.2.5a   fig.2.5b   fig.2.5c

Fig.2.5

$$Q_+^u \cdot (1-\varepsilon) > |Q_-^b| \varepsilon \quad \text{for all} \quad M > M_{KPP} = 2\sqrt{\omega_0} \quad \text{(see fig.2.5)} \qquad (2.23)$$

The intersection of the extraordinary principal direction Q_+^u with $\theta=1-\varepsilon$ above the intersection of the orbit with $\theta=1-\varepsilon$ for all $M > M_{KPP}$. The extraordinary principal direction cannot be used and all the possible trajectories reach the node $(0,0)$ with the slope Q_-^u. Notice that in the fig.2.5b corresponding to the limiting case $M = M_{KPP}$, the orbit does not correspond to the straight line $P = Q_+^u \theta$ for $0 < \theta < 1-\varepsilon$.
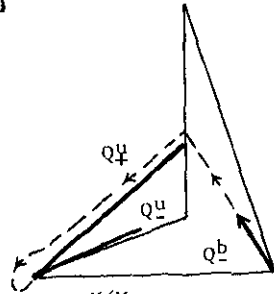
fig.2.6a   fig.2.6b   fig.2.6c

Fig.2.6

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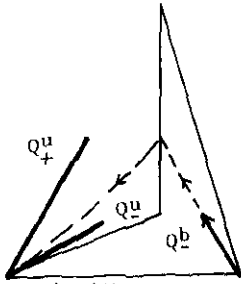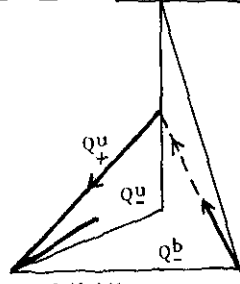
L-scenario : $\boxed{h>(1-\epsilon^2)\omega_o}$

There exists a value M_L of M (with $M_L>M_{KPP}$) such that

$$Q_+^u \cdot (1-\epsilon) = |Q_-|\epsilon \tag{2.24}$$

corresponding to $\quad M_L = \left\{ \dfrac{h}{1-\epsilon} + (1-\epsilon)\omega_o \right\} / \sqrt{\dfrac{h}{1-\epsilon} - \omega_o} \tag{2.24'}$

For $M>M_L$ the situation is similar to the fig.(2.5a), $Q_+^u(1-\epsilon)>(Q_-^b)\epsilon$

For $M=M_L$ the orbit consists of the two straight lines Q_+^u and Q_-^b

For $M<M_L$ the orbit has to cross $\theta=0$ before reaching the node $(0,0)$
and the corresponding solution cannot be retained.

Transition : $\boxed{h =(1-\epsilon^2)\omega_o}$

$$M_L \approx M_{KPP} = 2\sqrt{\omega_o} \tag{2.25}$$

The cases $M>M_{KPP}$ and $M<M_{KPP}$ are represented by figures similar to fig.(2.5a) and fig.(2.5c) respectively. When $M=M_{KPP}$ the orbit consists of the two straight lines Q_+^u and Q_-^b but contrarly to the fig.(2.6b), $Q_+^u=Q_-^u$ in the fig.2.7. When $h=(1-\epsilon^2)\omega_o$, the KPP solution is the L solution because $Q_+^u = Q_-^u$.

From the eq(2.23) and (2.24), the propagating wave speed can be plotted in terms of h for different given values of ϵ. The characteristic shape is plotted in fig. 2.8.
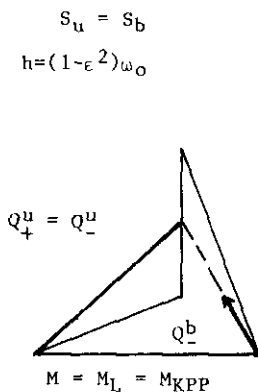

$S_u = S_b$
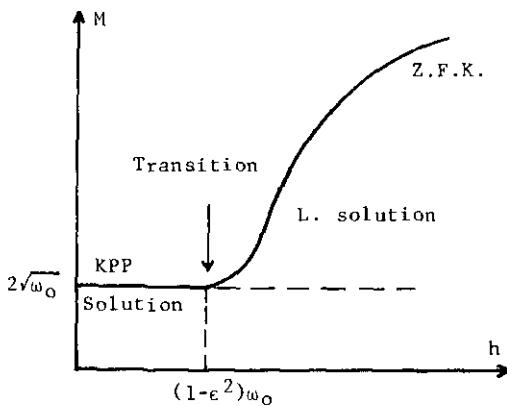
$h=(1-\epsilon^2)\omega_o$

$Q_+^u = Q_-^u$

Q_-^b

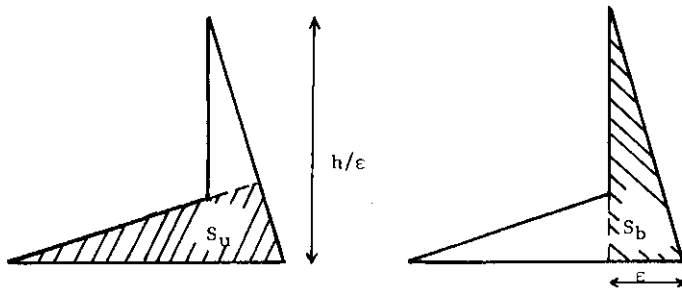$M = M_L = M_{KPP}$

Fig.2.7

Fig.2.8

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Fig.2.9

By noticing that $\frac{h}{\bar{\omega}_0} + \epsilon^2$ is the ratio of two surfaces S_b and S_u plotted in fig. 2.9, the critical condition for the transition between the K.P.P.-solution and the L-solution takes a very simple form :

$$S_u > S_b \quad : \quad \text{KPP solution}$$
$$S_u < S_b \quad : \quad \text{L solution} \qquad (2.26)$$

Such a criterium cannot be straight forward extended to general production terms as (2.11) to give precisely the corresponding critical value β^* of the Zeldovich number β.

$$\beta < \beta^* \quad : \quad \text{KPP solution}$$
$$\beta > \beta^* \quad : \quad \text{L solution} \qquad (2.26')$$

An estimate of β^* can be obtained by an approximate version of (2.26) involving the total aera $S_t = \int_o^1 d\theta\omega(\theta)$

$$S_t = 2S_u \qquad (2.27)$$

where S_u is the area under the slope at the origin[+]. For the production term (2.11), the criterium (2.27) gives $\beta^* \sim 6$ and $\beta^* \sim 8$ for n=1 and n=2 respectively. The numerical determination carried out by Higuera (1983) yields $\beta^* = 3.04$ and $\beta^* = 5.11$ for n=1 and n=2. These numerical results are in good agreements with the time dependent numerical analysis of Aldushin et al. (1981). Furthermore the critical condition has been obtained by Higuera (1983) for other models as the following one :

[+] The criterium (2.27) was suggested by Zeldovich - private communication, July 1983.

$$\omega(\theta) = \theta(1-\theta)e^{\beta\theta} \quad , \quad \beta^* = 1.64 \qquad (2.28)$$

used by Zeldovich (1948) for an exothermic chain branching reaction (1.4b) with unity Lewis number for both the limiting component R and the intermediate X. The corresponding threshold for the onset of the L-solution, β^*=1.64, is found to be much more lower than for the model (2.11). These numerical values of β^* can be compared with the values of the Zeldovich number associated with the overall activation energy and the flame temperature occurring in ordinary flames (see fig. 2.10).

E kcal/mole $T^\circ K$	20	30	40	50
300	0	0	0	0
350	4.10	6.16	8.22	10.27
1500	5.37	8.05	10.74	13.42
2000	4.28	6.42	8.56	10.7
2500	3.54	5.32	7.08	8.86

Values of the Zeldovich number (1.16) for T_0=300°K

Fig.2.10

It turns out that, even for cool flames observed in the low temperature range of the hydrocarbon oxidation ($T_b \sim 600°K$), the Zeldovich number β seems to be too large for the K.P.P. solution. But in such cool flames the multiple step-chemistry is expected to be a fundamental process and definitive conclusions cannot be obtained by the simplified model (2.6). For ordinary flames, $E \gtrsim 30$Kcal and $1500°K < T_b < 2500°K$, the KPP solution is found to not be relevant and the solution appears to be more likely controlled by the L-solution. In addition, the corresponding values of β are large enough ($\beta \sim 10$) to make the exact solution accurately approximated by the dominant orders of an asymptotic expansion in large values of β ($\beta \to \infty$). This approach based on the early works of Zeldovich and Frank Kamenetskii (1938) is presented in the next section.

Let us finally recall that the study of the model (2.22') shows that the transition "K.P.P. solution→L solution" can be produced only by changing the "hot part" (θ=1) of $\omega(\theta)$. Thus, the selection criterium that has been proved to be relevant for selecting the K.P.P. solution (see Zeldovich 1948) cannot be

uniformly valid because it is based only on the linearized form
of $\omega(\theta)$ around the cold boundary ($\theta=0$). This comment emphasizes
the limits of validity of selection criteria such as the one
proposed recently by Die and Langer (1983) in the context of pro-
pagating patterns.

II.3. The asymptotic expansion

In the limit of an infinitely large Zeldovich number β, the
ratio of the characteristic times of reaction at T and T_b becomes
singular (see fig.I.2) :

$$\lim_{\beta \to \infty} \quad , \quad \frac{\tau_r^{-1}(T)}{\tau_r^{-1}(T_b)} = \begin{cases} 0 \ , \ T_o < T < T_b \\ 1 \ , \ T = T_b \end{cases}$$

For large values of β, the reaction can be considered as thermally
quenched everywhere inside the flame except for temperature suffi-
ciently close to the maximum value T_b , $(T_b-T)/(T_b-T_u)=1-\theta= O(1/\beta)$.
And according to eq(2.6'), the reduced reaction rate $\omega(\theta)$ is negli-
gible except in a thin reaction zone of thickness d/β separating
the preheated zone where the flow is frozen(ω is trascendentally
small) from the burned gases at equilibrium, $\psi=0$ $\omega=0$ (see
fig. 2 .0). Because of the quasi-similarity of the profiles of tem-
perature and limiting component, the consumption of the reactant
stops the reaction soon after its initialisation.

In 1938 Zeldovich and Frank Kamenestkii developed an approx-
imate solution of the flame propogation described by the
L-solution of eq(2.6). This approximation valid for $\beta \gg 1$ has now
been proved to be the dominant order of the asymptotic expansion
first developed independently by Bush and Fendell (1970) for the
model (2.6) and by Liñan (1971) for exothermic chain branching
reaction. From eq(2.6) it appears clearly that the heat released
by the chemical reaction is partly consumed by heating the react-
ing gas through the convective term $m\frac{d}{dx}\theta$ and partly carried away
by heat conduction. When the reaction zone is thin, its tempera-
ture change is negligible and, at the dominant order, the chemi-
cal production is balanced by the heat conduction ;

reaction zone : $- \rho D_{th} \frac{d^2}{dx^2}\theta = \frac{\rho}{\tau_r(T_b)} \quad \omega(\theta)$ (2.29)

After multiplication by $\frac{d}{dx}\theta$ the eq(2.29) can be easily integrated
to compute the energy flux that leaves the reaction zone by heat
conduction for preheating the frozen flow :

$$\rho D_{th} \frac{d\theta}{dx} = \sqrt{2 \frac{\rho D_{th}}{\tau_r(T_b)}} \rho b \ I_\theta$$ (2.30)

where according to (2.6) and (2.6')

$$I_\theta = \int_\theta^1 d\theta' \omega(\theta') = \frac{1}{\beta^{n+1}} \int_{\beta(\theta-1)}^0 d\theta\ \theta^n \exp\left\{\frac{\theta}{1+\alpha\beta^{-1}\theta}\right\} \quad (2.30')$$

The main difficulty is to prescribe the lower bound appearing in I_θ and corresponding to the boundary between the reaction zone and the preheated zone. Because of its marked exponential temperature, the reaction rate falls so sharply with a decrease in temperature that, when β is large, the lower bound can be taken to be $-\infty$ ($\beta(\theta-1) \to -\infty$) without modifying notably the value of I_θ :

$$I_\theta = \frac{1}{\beta^{n+1}}\ \Gamma(n+1) + O\left(\frac{1}{\beta^{n+2}}\right) \quad (2.31)$$

with $\Gamma(n+1) = n!$ when $n \in N$

The heat conduction flux (2.30) entering the preheated zone balances the convection flux of energy leaving this zone only for a well defined value of the mass flux m corresponding to the unknown flame velocity. The solution of eq(2.6) in the preheated zone (where ω can be neglected) shows that the value of the convection flux is simply m :

preheated zone : $\quad \theta = e^{x/d}$ $\quad\quad\quad\quad\quad\quad\quad\quad$ (2.32)

with $d = \frac{\rho D_{th}}{m}$ and where the origin of the x-axis has been chosen such that $\theta(x=0)=1$. Eq(2.32) yields :

$$\rho D_{th}\ \frac{d\theta}{dx}\bigg|_{x=0_-} = m = \rho_u\ u_L \quad (2.33)$$

And eq(2.30) and (2.33) provide the expression of the laminar flame speed u_L. This approach can be systemized by an asymptotic expansion whose the first and second order are presented below. The main purpose of such a systematic expansion is not only to obtain a more accurate analytical solution of the planar flame but also to provide a framework that can be used to solve more complex cases as wrinkled fronts in non homogeneous flow. The corresponding works are briefly outlined in the following section and a more detailed presentation can be found in a recent review article (Clavin 1984). Let us consider the model (2.6) but where ρD_{th} is not necessarily assumed to be constant. When the independent variable $\xi = \int_0^x \frac{m}{\rho D_{th}} dx$ is introduced, eq(2.6) takes the form :

$$\frac{d\theta}{d\xi} - \frac{d^2\theta}{d\xi^2} = \Lambda\ A(\theta)\omega(\theta) \quad (2.34)$$

where

$$\Lambda = \frac{(\rho D_{th})_b \rho_b K_b}{m^2 \tau_r(T_b)} \quad (2.35')$$

and where $A(\theta)$ corresponds to the weak temperature dependence of the prefactor in the r.h.s. of (2.34)

$$A(\theta) = \frac{(\rho D_{th})(\rho K)}{(\rho D_{th})_b (\rho K)_b} \qquad (2.35'')$$

According to the result of Zeldovich and Frank Kamenestkii present-
ed above, the unknown quantity Λ/β^{n+1} is expected to remain fi-
nite in the limit $\beta\to\infty$ and one must look for a solution expanded
as follows :

$$\Lambda/\beta^{n+1} = \Lambda_o + \frac{1}{\beta}\ \Lambda_1 + O(\frac{1}{\beta^2}). \qquad (2.36)$$

In the preheated zone $\omega(\theta)$ is transcendentally small and the solu-
tion of eq(2.34) yields :

<u>Outer solution</u> : $\qquad \xi<0 \quad , \quad \theta(\xi) = e^\xi + t.s.t. \qquad (2.37)$

where t.s.t. means transcendentally small terms.
To solve the problem in the reaction zone of thickness d/β loca-
ted around $\xi=0$, the stretched variable η is introduced and consi-
dered as the independent variable in this thin zone :

$$\eta = \beta\xi \quad , \quad \frac{d}{d\xi} = \beta\ \frac{d}{d\eta}$$

Then, the solution is expanded in the following manner

$$(1-\theta) = \frac{\Xi_o(\eta)}{\beta}\ +\ \frac{\Xi_1(\eta)}{\beta^2}\ +\ O(\frac{1}{\beta^3}) \qquad (2.38)$$

and using the corresponding expansion of $\Lambda A(\theta)\omega(\theta)$, eq(2.34)
provides the equations for $\Xi_1, \Xi_2 \dots$

<u>Inner equations</u> $\qquad \dfrac{d^2\Xi_o}{d\eta^2}\ = \Lambda_o\Xi_o^n\ e^{-\Xi_o}$,

$$-\frac{d\Xi_o}{d\eta} + \frac{d^2\Xi_1}{d\eta^2}\ = \begin{cases} \Lambda_1\Xi_o^n\ e^{-\Xi_o} -\Lambda_o\gamma b_1\ \Xi_o^{n+1}\ e^{-\Xi_o} -\Lambda_o\gamma\Xi_o^{n+2}e^{-\Xi_o} \\ \Xi_1\Lambda_o(n\Xi_o^{n-1}\ e^{-\Xi_o} -\Xi_o^n\ e^{-\Xi_o}), \end{cases} \qquad (2.39)$$

where
$$\gamma = \alpha \ ; \ b_1 = \frac{\partial Log(\rho D_{th}\rho K)}{\partial Log\ T}\bigg|_{T=T_b} \quad ; \quad A=1-\gamma b_1\ \frac{\Xi_o}{\beta} + O(\frac{1}{\beta^2}) \quad (2.40)$$

The boundary condition in the burnt gases yields :

$$\eta\to +\infty \quad : \quad \Xi_o\to 0 \quad , \quad \Xi_1\to 0 \qquad (2.41)$$

According to the equations (2.39), the solutions Ξ_o and Ξ_1 pre-
sent the following limiting behavior in the direction toward the
preheated zone :

$$\eta\to\ \infty \ : \ \frac{d\Xi_o}{d\eta} \to Ct\neq 0 \qquad \frac{d^2\Xi_1}{d\eta^2} \to Ct \neq 0 \quad . \qquad (2.42)$$

The matching conditions (Van Dyke 1964, Cole 1968) of the inner
solution (2.38) with the outer solution $\theta(\xi)= \theta_o(\xi)+ \frac{1}{\beta}\theta_1(\xi)+O(\frac{1}{\beta^2})$
of the preheated zone yields :

$\eta\to-\infty$:

$$: \ \Xi_o(\eta) = (\frac{\partial\theta_o}{\partial\xi}\big|_{\xi=0_-})\eta + \theta_1(\xi=0_-)+ t.s.t.$$
$$\qquad (2.43)$$

$$\Xi_1(\eta) = (\frac{\partial^2\theta_0}{\partial\xi}\big|_{\xi=0_-})\frac{\eta^2}{2} + (\frac{\partial\theta_1}{\partial\xi}\big|_{\xi=0_-})\eta + \theta_2(\xi=0) + t.s.t.$$

According to the result (2.37), this yields
$\eta \to -\infty$:

$$\Xi_0(\eta) = \eta + t.s.t.$$

$$\Xi_1(\eta) = \frac{\eta^2}{2} + t.s.t. \tag{2.44}$$

The eigenvalues Λ_0 and Λ_1 are determined by prescribing the boundary conditions (2.41) and (2.42) (see Joulin & Clavin 1976) :

$$\Lambda_0 = \frac{1}{2\Gamma_{n+1}}$$

$$\Lambda_1 = \Lambda_0 \left\{ b_1 \gamma \frac{\Gamma_{n+2}}{\Gamma_{n+1}} + \gamma \frac{\Gamma_{n+3}}{\Gamma_{n+1}} - \frac{1}{\Lambda \Gamma_{n+1}} \right\}_n \right\} \tag{2.45}$$

where $\qquad \mathcal{J}_n = \int_0^\infty d\Xi (1 - \sqrt{\frac{1}{\Gamma_{n+1}} \int_0^\Xi dx \; x^n \; e^{-x}})$

As already mentioned, the dominant order Λ_0 is identical to the solution of Zeldovich and Frank Kamenestkii u_{ZFK}. The numerical evaluation of $\mathcal{J}_{n=1}$ yields : $\mathcal{J}_{n=1} = 1.344$, (see Fendell 1972). For $n=1$ and $\gamma=0.85$, the flame velocity u_L is, according to (2.35) and (2.45), given by :

$$u_L = u_{ZFK} (1 - \frac{0.57}{\beta} + 0(\frac{1}{\beta^2})) \qquad \text{for} \quad b_1 = -\frac{3}{2} \quad ,$$
and
$$u_L = u_{ZFK}(1 - \frac{1.2}{\beta} + 0(\frac{1}{\beta^2})) \qquad \text{for} \quad b_1 = 0. \tag{2.46}$$

According to the values of β given in fig. 2.10, the results (2.46) shows that the first correction is not always negligible. By comparison with numerical solutions the results (2.46) are found to be accurate with less than 10% error for $\beta > 3$ (Bush & Fendell 1971). For $\beta > 5$, the error is less than 2%. In fact the very limitation of the asymptotic method toward the small value of the Zeldovich number β is the critical value β^* corresponding to the onset of the KPP solution. The coefficient γ appearing in the first term in the bracket of eq(2.45) is not present in the result of Fendell (1972) concerning n=1 but $L_e \neq 1$. In order to get rid of the cold boundary difficulty, $A(\theta)$ was approximated by θ^{b_1} in the model used by Fendell. Such a modification of the Arrhenius law is not necessary in the framework of the asymptotic expansion $\beta \to \infty$ and *can lead to irrelevant corrective terms when the hot boundary is modified.*

This asymptotic method has been successfully applied to other one dimensional and steady cases such as : non unity Lewis number (Bush and Fendell 1970), volumetric heat losses for describing the thermal extinction (Buckmaster 1976, Joulin Clavin 1976), monopropellant droplet burning (Fendell 1972, Liñan 1976), *stretch effect of a planar front stabilised in a stagnation point*

flow (Buckmaster 1982, Libby and Williams 1982), influence of flame holders and of the spherical geometry (Deshaies and Co 1981, Clarke and McIntosh 1980), in this last case the temperature in the burnt gas can decrease toward a room temperature small compared to the flame temperature and the corresponding inner zone structure is more complex (than the one presented above) and has been first studied by Linan (1974) in the context of diffusion flames. The study of the effects of two limiting components for reactive mixtures close to the stoichiometric composition has been studied by Joulin & Mitani 1981). More recently, the asymptotic method was successfully applied by Liñan and Clavin (1984) to a multiple step, kinetic scheme introduced by Adams and Stock (1953) to model the reactions with Hydrogen and Halogens. These approaches are very promising but, presently, they are limited to the cases where the complete chemical scheme can be reduced to few steps. For example, such a drastic reduction has not yet been performed successfully for the simplest hydrocarbons. Performance numerical methods are now available to solve the structure of flames sustained by the most complex kinetic scheme. But because of the huge amount of physico-chemical parameters necessary to describe the structure of flames sustained by complex kinetic scheme, the analysis of the corresponding numerical results are difficult. A promising avenue is to combine numerics and analytical treatments.

II.4. Dynamics of flame front

Let us consider the motion of flame fronts in flows that can be unsteady and non-uniform. When the length and time scales of the initial flow are larger than those associated with the planar flame (the flame thickness d and the transit time d/u_L where u_L is the laminar flame speed), the flame front can be considered, in first approximation, as a surface of discontinuity whose motion is controlled by two distinct factors : the normal burning velocity u_n associated with the mass flux of fresh mixture crossing the front and the value at the front of the flow velocity field. Each point of the front moves with a velocity equal to the difference between the values (at this point) of the upstream flow velocity and the normal burning velocity oriented toward the fresh mixture in the direction normal to the front.

As soon as one is concerned with wrinkled fronts and/or inhomogeneous flows, the flame **cannot be described by a pure reaction-diffusive model**. Because of the gas expansion produced by the temperature increase in the preheated zone, the streamlines are deflected across the tilted front and a strong coupling with hydrodynamics is developed. When the size D of the wrinkles of the front is large compared to the flame thickness d, the corre-

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ponding fluid mechanical effects can be split in two distinct parts :

-i) The flame structure is locally influenced by the convective transfer produced in the preheated zone by the deflection of the streamlines.

-ii) Outside the flame where the gas density ρ and the temperature T are uniform, the flow field is also modified (from its initial value without combustion) upstream and downstream the flame on a distance D from the front.

The first effects i) produce a change of the normal burning velocity $u_n \neq u_L$. It must be noticed that, in addition to the convection transfer produced by the gas expansion, the diffusion fluxes of heat and mass play also a great part in this modification to flame structure of wrinkled fronts.

The second effects ii) results in a modification to the gas flow at the front.

Both of these effects i) & ii) influences the motion of the front, but the second is the stronger one at long wave lengths.

When the modification to flame structure is neglected, $u_n = u_L$ the flame could be considered as a passive surface in the sense that the motion is completely prescribed by the value of the flow at the front. Even in this case, the second effect ii) produces a strong hydrodynamical feedback in the motion of the front. This effect was first described in the pioneering works of Darrieus (1938) and Landau (1944) who computed the flow field induced by the front wrinkling when $u_n = u_L$ and d=0. The analysis was carried out at the linear approximation in the amplitude of the front corrugations and the induced flow velocity was found to be in phase with the front wrinkles. The resulting motion of the front reveals a strong instability mechanism of planar flames in uniform flows. The least fluctuation around the planar steady state solution (described in the preceding sections) is amplified under the hydrodynamical effect ii). As the wavelength becomes shorter, the front is more unstable and Darrieus and Landau concluded that planar fronts freely propagating in uniform mixture cannot exist. The instability mechanism appeared to be so strong that they conclude also that the combustion must be a self-turbulizing phenomena. In fact, only two parameters being involved in this theory, the gas expansion parameter γ and the laminar flame speed u_o, the growth rate σ of the instability is found to be proportional to the modulus k of the wave vector of the front wrinkles

$$\sigma = \sigma_1(\gamma)u_L k \qquad (2.47)$$

where $\sigma_1(\gamma)$ is a positive adimentional quantity vanishing only in the unrealistic limit $\gamma \to 0$ (zero gas expansion, $\rho_u = \rho_b$).

The first attempt to take into account the effect of the
modification to flame structure was performed in the fifty[th] by
Markstein (see his review paper 1965) who assumed the following
phenomenological relation between u_n and the mean radius of cur-
vature of the front R (R>0 when the front is concave toward the
unburnt gases) :

$$\frac{u_n - u_L}{u_L} = \frac{\mathcal{L}}{R} \qquad (2.48)$$

where $\mathcal{L}$ is a phenomenological length (called Markstein length)
that was assumed to be proportional to the flame thickness d and
whose the expression is a characteristic of the reactive mixture.
It can easily be anticiped from eq(2.48) that the effects asso-
ciated with the modification to flame structure can only change
the dispersion relation (2.47) through a k^2 -term. And thus the
large wavelength can never be stabilized by such a mechanism.
Another stabilizing mechanism must be present in order to explain
the large planar front observed experimentally.

The first analysis of the wrinkled flame structure was
carried out by Barenblatt, Zeldovich and Istratov (1962) but in
the diffusive-thermal model where the gas expansion effects i)
and ii) are neglected. This model was extensively used these ten
last years to culminate in the derivation by G. Sivashinsky (1977)
of a non linear differential equation for the flame motion describ-
ing a self turbulizing behavior of the cellular structures
(Michelson & Sivashinsky 1977). The asymptotic technique applied
to solve this model in the limit of large values of the Zeldovich
number $\beta \to \infty$, is presented in the paper of Joulin & Clavin (1979)
that is devoted to the dynamical properties in the presence of
heat losses that can produce the thermal extinction. Travelling
and spinning waves as well as oscillatory fronts have been predict-
ed by this model (for a review see the book of Buckmaster and
Ludford 1982 and the review article of Sivashinsky 1983). But even
as modified by Sivashinsky to take into account a weak gas expan-
sion, this model underestimates the hydrodynamical effects that has
to play a dominant role (see eq(2.47)).

Recently, the coupling between diffusion and hydrodynamics
has been properly taken into account for describing the wrinkled
flame structure in an analytical work by Clavin & Williams (1982).
The asymptotic expansion $\beta \to \infty$ is used together with a multiscale
method based on the assumption $\varepsilon = d/D$ smaller than unity. The
corresponding result was used by Pelcé & Clavin (1982) to study
the stability limits of planar fronts propagating downward. The
results can be summarized as follow :
a) - In the approximation of a one step overall chemical reaction,
the modification to flame structure by wrinkling is predicted to
be a stabilizing mechanism for most of the ordinary hydrocarbon-

mixtures; whatever the equivalence ratio may be; the only exception could be a mixture of very light reactive components (as hydrogen) diluted in nitrogen. This conclusion contradicts the result obtained by the diffusive-thermal model and appears as a typical effect of the mechanism i).

b) - The gas viscosity has a neutral effect on the stability properties of planar fronts.

c) - The acceleration of gravity g associated with the effects of the modification to flame structure by wrinkling can counterbalance the hydrodynamical instability for all the wave numbers when the flame velocity is low enough. The cellular threshold is predicted to be observable for flame velocity u_L varying between 5cm/s and 17cm/s with rich mixture of ordinary fuel for low flame velocities ($u_L < 12$cm/s) and with lean composition for higher velocity.

d) - The cell size at the threshold can be expressed in terms of only the variable g, u_L and γ ; the detailed properties (chemical kinetics, transport processes...) do not enter into the final expression.

These predictions are in good agreements with the recent experiments of Quinard et al. (1983). Furthermore the induced velocity field has been recently recorded in the unburnt mixture by Searby et al. (1983) in the case of stable fronts stabilized in weakly "turbulent" flows. As predicted by the theory for planar stable flames, the induced velocity field is found to be out of phase with the front corrugations leading to a blocking of the low frequencies in the turbulence approaching the front (see the lecture of L. Boyer at the present summer school).

The analysis of Clavin & Williams (1982) concerning the flame structure of wrinkled fronts in a non homogeneous flows has been extended independently by Matalon & Matkowsky (1982) and by Clavin & Joulin (1983) to the nonlinear case of finite amplitudes of the front corrugations. As anticipated by the early phenomenological analysis of Karlowitz et al. (1953), the modification to the normal burning velocity u_n produced by the front curvature and by the flow inhomogeneities can be expressed in terms of only one geometrical scalar i.e. the total flame stretch experienced by the front.

$$u_n - u_L = - \mathcal{L} \; (\frac{1}{\sigma} \frac{d\sigma}{dt}) \qquad (2.49)$$

where σ is the surface element of the front and $\frac{d}{dt}$ its time derivative when each point of the flame moves as described at the beginning of this section. $\mathcal{L}$ is the Markstein length that depends, as the laminar flame velocity u_L, on the physico-chemical properties of the reactive mixture (transfer properties, chemical kinetics, etc...). The corresponding expression of $\mathcal{L}$ has been obtained for different cases (see the review article by Clavin 1984).

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Except its limitation to the weak stretch, this surprisingly simple result is general and can be used in any flow configuration : stagnation point flow, spherical flames, turbulent flames... etc... The effects of the strong stretch has been recently investigated by Libby, Linan and Williams (1983) in the particular case of a planar front in a stagnation point flow. Once again, the effect of the gas expansion is proved to be important ; for example the flame extinction under strong stretch predicted by the "diffusive-thermal model" (γ=0) for one overall chemical reaction is no more accessible when the effects i) are properly taken into account).

It is worthwhile to express the result (2.49) in terms of the mean radius of curvature of the front R. At the same order, the modification to normal burning velocity can be expressed as (see Clavin & Joulin 1983) :

$$u_n - u_o = \mathcal{l} \; u_L \; \left\{ \frac{1}{R} + \frac{1}{u_L} \; \underline{n} \bullet \underline{\underline{\nabla u}} \bullet \underline{n} \right\} \tag{2.50}$$

where $\underline{n}$ is the unit vector normal to the front and $\underline{\underline{\nabla u}}$ is the "rate of strain tensor" of the upstream flow evaluated at the flame position. Each of the two terms in r.h.s. represents a contribution to the total flame stretch. The term $-u_L/R$ represents the stretch of the front moving in a uniform flow with a constant normal velocity u_L. This term is the effect of the non planar geometry of the front. The term $\underline{\nabla} \bullet \underline{u} - \underline{n} \bullet \underline{\nabla u} \bullet \underline{n}$ is known to represent the stretch of a surface convected by the flow field $\underline{u}$. (Here $\underline{\nabla} \bullet \underline{u} = 0$ outside the flame). This second term is the effect of the non homogeneity of the flow.

Finally let us mention that the eq(2.49) and (2.50) provide a non linear equation for the front in a non uniform and/or unsteady flow. But, as already mentioned, the value of the flow field appearing in this equation is not a given quantity and, because of the hydrodynamics effects ii), this flow is, in fact, a functional of the flame surface. This aspect of the problem of the flame dynamics has been solved only in the linear approximation (see L. Boyer 1983). Nevertheless, for turbulent wrinkled flames, and when the corresponding random process is assumed to be stationary and homogeneous, the local equation for the front evolution provide an expression for the turbulent flame speed. The time average of the modification to normal burning velocity is found to be zero and the turbulent flame speed is proved to be given by simply the laminar flame speed times the mean area increase of the front.

III. DIFFUSION FLAMES

III.1. Position of the problems

In the broadest sense a diffusion flame is defined, see

Williams 1965, as any flame in which the fuel and the oxidizer
are initially separated ; the term diffusion flame is synonymous
with nonpremixed combustion. In diffusion flames mixing and chemi-
cal reaction take place simultaneously.

In a restricted sense, a diffusion flame is defined as a
non-premixed flame in which most of the reaction occurs in a
thin zone that separates the fuel from the oxidiser, and that,
following Burke and Schumann 1928, it can be approximated by a
surface.
       Two types of problems may be encountered in the analysis of
chemical reactions in unpremixed systems : (a) Problems of the evo-
lution type, like unsteady mixing and combustion in mixing layers
and boundary layers without a stagnation point, and (b) quasy
steady problems like mixing and reaction in the stagnation region
and quasi-steady droplet combustion.

For large activation energies, multiple solutions exist for
the conservation equations in problems of the elliptic, quasi-steady
type within a range of Damköhler numbers, bounded by an extinc-
tion Damköhler numbers, and by an ignition Damköhler number ; these
solutions correspond to different combustion regimes,(Linan 1974).
In problems of the evolution type the conservations equations are
parabolic, because the terms representing the diffusive effects
have second order spatial derivatives, while those terms represent-
ing the local heat accumulation or convective effects are first
order with respect to time or with respect to a spatial derivative,
that does not appear in the diffusive terms. Then the solution is
uniquely determined in terms of the initial and boundary conditions
With increasing values of the time-like variable the flow changes
from nearly-frozen, with incipient effects of the chemical reaction,
to a near-equilibrium, diffusion controlled mode of combustion
(see fig.1.1); the transition occurs through premixed flames, of
the deflagration or of the detonation type (see Liñan and Crespo
1976).
       In the following, we shall present a detailed analysis of
the diffusion flame structure, using as an example of quasi-
steady problems, the diffusion flame at the stagnation region
between to opposed jets of fuel and oxidiser. The results are,
however, applicable to any general configuration. The analysis
will be carried out for reactions that can be modelled by an
Arrhenius overall irreversible reaction, but the analysis can be
generalised for more general reactions.

The qualitative structure of diffusion flames is not strong-
ly dependent on the value of the Lewis number of the species. The
analysis simplifies considerably when we write $\rho D_\alpha = \lambda/C_p = \rho D_{th}$,

corresponding to the equidiffusional approximation. In this case the transport operators on eq(1.5) coincide for all species, and when we take into acount (1.1'), the coupling functions, or Schwalb-Zeldovich variables,

$$Y_b - \nu Y_F \quad \text{and} \quad T + Y_F q/C_p$$

are found to diffuse as passive scalars.
Thus the systems of eqs(1.5,1',2) can be written in the form

$$\mathbb{L}(Y_F) = -BY_F^{n_F} \, Y_0^{n_0} \, e^{-E/RT} \tag{3.1}$$

$$\mathbb{L}(Y_0 - \nu Y_F) = 0 \quad , \quad \mathbb{L}(T + Y_F q/C_p) = 0 \tag{3.2}$$

and also $L(Y_N)=0$ for any inert species. Here $\mathbb{L}$ is defined by :

$$\mathbb{L}(Z) = \frac{\partial Z}{\partial t} + \underline{v} \cdot \underline{\nabla}(Z) - \frac{1}{\rho} \underline{\nabla} \cdot (\rho D_{th} \underline{\nabla} Z) \tag{3.3}$$

If we assume that we have, as in the example of fig. 1.1, two independent feed streams, one with fuel, with mass fraction Y_{F0} and temperature T_{F0}, and the other with oxidiser with mass fraction Y_{00} and temperature T_{00}, and no heat or mass flux on all the other boundary surfaces, then it is possible to write the solution of eq(3.2) in terms of the solution Z (mixture fraction) of the problem of eq(3.3) for an inert species, of unit concentration, $Z=1$, in the fuel feed stream, and zero concentration at the oxidiser stream (see for example Bilger, 1975, and Peters 1983).
Thus we can write the following Schvab-Zeldovich relations

$$Y_0 - \nu Y_F = Y_{00} - (\nu Y_{F0} + Y_{00})Z \tag{3.4}$$

and

$$T + Y_F q/C_p = T_{00} + (T_{F0} - T_{00} + Y_{F0} \, q/C_p)Z \tag{3.5}$$

independent of the kinetics, that appears only in eq(3.1).
In the non-reacting limit $Be^{-E/RT} \to 0$, when the chemical reaction is frozen, eq(3.1) simplifies to

$$\mathbb{L}(Y_F) = 0 \tag{3.6}$$

so that

$$Y_F = Y_{Ff} = Y_{F0} \, Z$$

$$Y_0 = Y_{0f} = Y_{00} \, (1-Z) \tag{3.7}$$

$$T = T_f = T_{00} + (T_{F0} - T_{00})Z$$

In the opposite limiting case (the Burke-Schumann limit), of very fast chemical reactions, $Be^{-E/RT} \to \infty$, we have chemical equilibrium, with

$$Y_0 = 0 \quad , \quad Y_F = -Y_{00}/\nu + (Y_{F0} + Y_{00}/\nu)Z$$

$$T = T_{F0} + (T_{00} - T_{F0} + Y_{00} q/\nu C_p)(1-Z) \tag{3.8a}$$

for $Z > Z_e$, on the fuel side, and

$$Y_F = 0 \quad , \quad Y_0 = Y_{00} - (\nu Y_{F0} + Y_{00})Z$$

$$(3.8b)$$

$$T = T_{00} + (T_{F0} - T_{00} + Y_{F0} \, q/C_p)Z$$

for $Z < Ze$, on the oxidizer side

A thin flame, located at $Z=Ze$ given by

$$Ze = Y_{00}/(Y_{00} + \nu Y_{F0}) \qquad (3.9)$$

There $Y_0 = Y_F = 0$ and $T = T_e$, given by the adiabatic flame temperature value

$$T_e = T_{00} + (T_{F0} - T_{00} + Y_{F0} \, q/C_p)Ze \qquad (3.10)$$

The flame sheet separates the fuel from the oxidiser.

To calculate the flame sheet position, $Z=Ze$, and the temperature *and reactant concentration distributions, given by* (3.8), we must solve the transport problem (3.3) for the mixture fraction. *These distributions in the Burke-Schumann limit of infinitely fast reactions are diffusion controlled.* It is easy to show, taking into account (3.8), *that* m_F'', *the mass burning rate of fuel per unit flame surface,* and the corresponding value m_o'' for the oxidizer, given by

$$m_F'' = \rho D_F \left(\frac{\partial Y_F}{\partial n} \right)_{e^+} \quad , \quad m_o'' = -\rho D_o \left(\frac{\partial Y_o}{\partial n} \right)_{e^-} \qquad (3.11)$$

are related by

$$\nu m_F'' = m_o'' \qquad (3.12)$$

and the heat release per unit flame surface $\quad q'' = \lambda \left[\dfrac{\partial T}{\partial n} \right]_{e^+}^{e^-}$

is related to m_F'' by

$$q'' = \frac{q}{C_p} \, m_F'' \qquad (3.13)$$

That is fuel and oxidiser reach the flame in stoichiometric proportions, and the heat release by the chemical reaction is conducted away from the flame. The jump relations (3.12,13) are also valid for non-unity Lewis numbers, when the relations (3.4) and (3.5), and therefore (3.9) and (3.10) do not hold. For non-unity Lewis numbers, and diffusion controlled combustion, we must solve the equations $\mathbb{L}_T(T)=0$, $\mathbb{L}_0(Y_0)=0$ on the oxidiser side of the flame where $Y_F=0$; and the equations $\mathbb{L}_F(Y_F)=0$, $\mathbb{L}_F(T)=0$, on the fuel side where $Y_0=0$. The concentration of both reactants must be zero at the thin flame, and the temperature continuous ; there are jumps however of the concentration and temperature gradients normal to the flame sheet, that satisfy the jump relations (3.12) and (3.13).

In order to describe with some details the transition from the frozen flow distributions of the form (3.7) to the equilibrium distributions of the form (3.8) we shall analyse the structure of counterflow diffusion flames. We shall make this description in the realistic limit of large values of the non-dimensional activation energy E/RT_e, when multiple solutions of the conservation equasions may exist, with associated bifurcation points, where

jumps from a nearly frozen state to a near-equilibrium state, and
vice versa, occurs.

In counterflow diffusion flames two streams, one of fuel and
the other of oxidiser flow in opposite directions, setting up a
diffusion flame between them where the chemical reaction takes
place. The qualitative structure and the main characteristics of
diffusion flames do not change when the effects, associated with
density changes, of the heat release on the flow field are neglect.
We shall, in addition assume for simplicity in the presentation
of the structure, assume that the two jet velocities are equal.
The flow field shown in fig.III.1 is axis-symmetric.
Close to the stagnation point the flow field is given by :

$$u = -Ax \quad , \quad v = Ar/2$$

as a result of the constant density approximation, and for two
identical jets. The factor A is the inverse of a residence time m
the stagnation of the initial diameter D and velocity V of the jets.

It is well known that in the solutions of the conservation
equations in the stagnation region the temperature and concentra-
tions are functions only x, the distance normal to the mixing layer
and, in unsteady problems, of time. We shall look for steady solu-
tions, so that only x is involved as independent variable. The
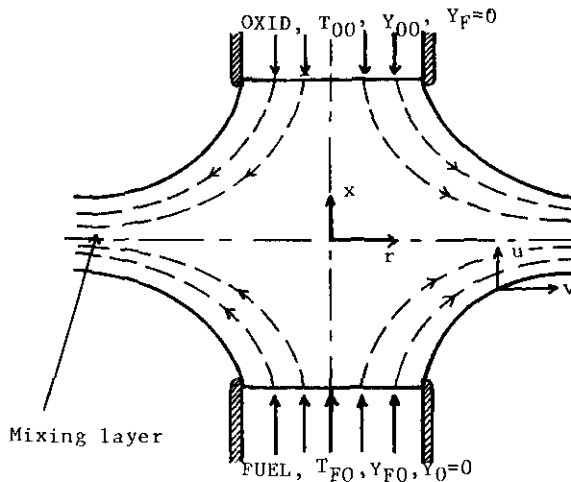mixture fraction Z and the fuel mass fraction Y_F are given by the

Fig.3.1

conservation equations

$$- Ax \frac{dZ}{dx} - D_{th} \frac{d^2Z}{dx^2} = 0 \tag{3.14}$$

$$- Ax \frac{dY_F}{dx} - D_{th} \frac{d^2Y_F}{dx^2} = -Be^{-E/RT} Y_F^{n_F} Y_0^{n_0} \tag{3.15}$$

where we have considered, for simplicity, that both ρ and the ther-
mal diffusivity D_{th} are constant. We shall write these equations in
non-dimensional form in terms of the variable

$$\eta = x/\sqrt{D_{th}/A}$$

where D_{th}/A is the characteristic thickness of the mixing layer.
Thus we obtain

$$\eta Z_\eta + Z_{\eta\eta} = 0 \tag{3.16}$$

$$\eta Y_{F\eta} + Y_{F\eta\eta} = D_\infty e^{-E/RT} Y_F^{n_F} Y_0^{n_0} \tag{3.17}$$

to be solved with the boundary conditions

$$Z=1 \ , \ Y_F = Y_{F0} \qquad \text{for} \quad \eta \to -\infty$$
$$Z=0 \ , \ Y_F = 0 \qquad \text{for} \quad \eta \to \infty$$

if the mixing layer thickness is small compared with the size of
the jets. Y_0 and T are given by eq(3.4,5) in terms of Y_F and Z.
D_∞ is a Damköhler number $D_\infty = B/A$, the product of the frequency
factor B and the characteristic diffusion time, or residence time,
$1/A$ across the mixing layer. The solution of (3.16) can be written
as :

$$Z = (1/2)\text{erfc}(\eta/\sqrt{2}) \tag{3.18}$$

which together with eqs(3.4 and 5) and eq(3.17) determines $Y_F(\eta)$.
In the non-reactive limit $D_\infty e^{-E/RT} \to 0$ the solution was given before
as the frozen solutions eq(3.7). In the limit $D_\infty e^{-E/RT} \to \infty$, of
infinitely large Damköhler numbers, we obtain the Burke-Schumann
(B-S), chemical equilibrium, solution, given by eq(3.8). These
limiting solutions are shown schematically in figs(3.2a, 2b) in
terms of the mixture fraction Z as independent variable.
Notice that in the B-S limit there are jumps in the concentration
and temperature gradients at the flame sheet, $Z=Z_e$, that acts as a
sink for the fuel and oxidiser, and as a source for the products
and thermal energy. The jumps are rounded off, as shown by the
dashed lines in fig.III.2b due to finite rate effects.
The linear form of the profiles, in both limiting cases, when the
mixture fraction Z is used as independent variable can be under-
stood, when we notice that the transport operator appearing in
eq(3.17) can be written in the form

$$\eta Y_{F\eta} + Y_{F\eta\eta} = Z_\eta^2 Y_{FZZ} \tag{3.19}$$

where $Z_\eta^2 = (1/2\pi)\exp(-\eta^2/2)$, the local gradient of the mixture
fraction , is a function of $2Z = \text{erfc}(\eta/\sqrt{2})$, whose variation across
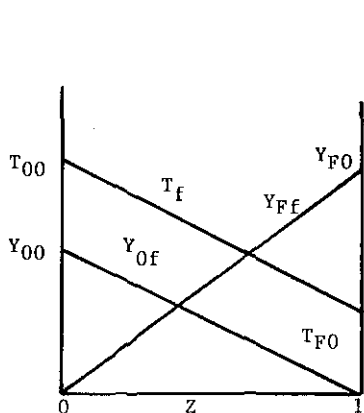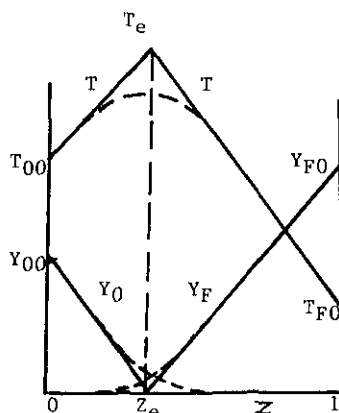the mixing layer accounts for convective effects.

Fig.3.2a   Fig.3.2b

III.2. Ignition regime

For zero Damköhler numbers the temperature and concentration distributions take their frozen values, $Y_{F_f} = Y_{FO} \, Z$, $Y_{O_f} = Y_{OO}(1-Z)$ and $T = T_f = T_{OO} + (T_{FO} - T_{OO})Z$. The deviations from these values, for non zero small values of D_∞, can be calculated in first approximation, by using eq(3.17) with the right hand side evaluated in terms of the frozen solution, i.e. by using the equation

$$Z_n^2 \, Y_{FZZ} = D_\infty e^{-E/RT_f} \, Y_{F_f}^{n_F} \, Y_{O_f}^{n_O} \tag{3.20}$$

with $Y_F(0) = 0$, $Y_F(1) = 1$

The solution gives the first two terms of an expansion of the solution of eq(3.17) in powers of the Damköhler number D_∞. It represents well the temperature and concentration distributions as long as the deviations of the chemical production term from its frozen flow value, appearing in the right hand side of eq(3.20) are small.

For large activation energies, $E/RT \gg 1$, the changes in the Arrhenius factor, $\exp(-E/RT)$, become significant, even with small changes in the temperature from its frozen flow value T_f. That is suffices to have variations of T from T_f small, $(T-T_f)/T_f = O(RT_f/E)$ in order to change the Arrhenius exponential by a factor of order unity, so that it can no longer be approximated by $\exp(-E/RT_f)$, although we can use, because $(T-T_f)/T_f \ll 1$, the Frank-Kamenetskii (1969),linearisation

$$\exp(-E/RT) \simeq \exp(-E/RT_f) \exp E(T-T_f)/RT_f^2 \tag{3.21}$$

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of the Arrhenius exponent, when analysing the diffusion flame in the ignition regime.

Due to the much weaker sensitivity of the reaction rates to concentration changes, the factor $Y_F^{n_F} Y_0^{n_0}$ can often be approximated by its frozen flow value $Y_{F_f}^{n_F} Y_{0_f}^{n_0}$ because in the ignition regime the relative changes in concentration are small of the order of RT_f/E. Although this is not the case when, for example, $T_{00}-T_{F0} \gg RT_{00}^2/E$, when in the ignition regime the chemical reaction occurs on the oxidizer edge of the mixing layer, where the temperature is higher, and where we can write $Y_0 = Y_{00}$ but not $Y_F = Y_{F_f}$ in evaluating the reaction rate. See Liñán 1974.

In the particular case $T_{00} = T_{T0} = T_0$, when $T_f = T_0$, we can except from the solution of (3.20) that $(T-T_0)/T_0$ will be of the order RT_0/E, and therefore we shall be in the ignition regime for values of the Damköhler number such that

$$\frac{q}{C_p T_0} D_\infty e^{-E/RT_0} Y_{F0}^{n_F} Y_{00}^{n_0} = \frac{RT_0}{E} \mathcal{D} \qquad (3.22)$$

with $\mathcal{D}$ a number of order unity.
In this distinguished limiting case, $E/RT_0 \to \infty$ with $D_\infty \to \infty$ so that $\mathcal{D}$ is fixed of order unity, the deviations of Y_0, Y_F and T from their frozen values $Y_{00}(1-Z)$, $Y_{F0}Z$ and T_0 are small of order RT_0/E; and are given in first approximation in terms of the solution, for $\phi = E(T-T_0)/RT_0^2$, of

$$Z_\eta^2 \phi_{ZZ} = -\mathcal{D} e^\phi Z^{n_F} (1-Z)^{n_0} \qquad (3.23)$$

$$\phi(o) = \phi(1) = 0$$

and

$$Y_F/Y_{F0} = Z - \varepsilon_0 \phi \quad , \quad Y_0/Y_{00} = 1-Z-(\nu Y_{F0}/Y_{00})\varepsilon_0 \phi$$

where $\varepsilon_0 = (C_p T_0/q Y_{F0})(RT_0/E)$ is small for large values of the activation energy.

The limiting form eq(3.23) of the conservation equation for T, for large values of E/RT_0, results from linearisation eq(3.21) of the Arrhenius exponent and from the neglect of the reactant consumption in evaluating the reaction rate.

The reduced Damköhler number $\mathcal{D}$, defined by eq(3.22), is the only parameter, aside from the reaction orders n_F and n_0, entering in eq(3.23). When this equation is solved numerically, two solutions are found for all values of the Damköhler number smaller than an ignition value $\mathcal{D}_I$, of order unity, for which the two solutions coincide. No solution of the problem (3.23) exists for values of the Damköhler number $\mathcal{D}$ larger than $\mathcal{D}_I$. Thus, when we plot a certain norm of $\phi(Z)$, such as $\phi_{max} = E(T_{max}-T_0)/RT_0^2$ in terms of $\mathcal{D}$, for fixed values of the reaction orders, the resulting curve is of the form shown in fig. 3.3 that corresponds to $n_F = n_0 = 1$, with a $\mathcal{D}_I = 2.59$.
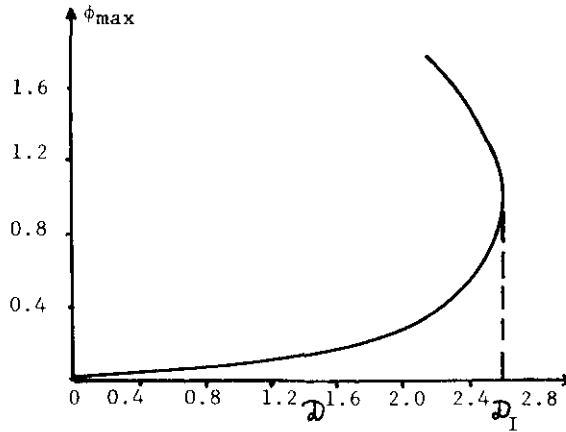
Fig.3.3

The existence of the two solutions is associated with the strong dependence of the reaction rate with temperature. The solution corresponding to the lower branch of Fig. 3.3 shows small temperature increments, associated with small reaction rates ; the solution, for the same Damköhler number, corresponding to the upper branch shows a much larger value of ϕ_{max} associated with larges values of $\exp\phi$. For values of $\mathcal{D} > \mathcal{D}_I$ the increments in temperature, and the corresponding values of $\exp\phi$, are two large to sustain a nearly frozen solution. A stability analysis of the two solutions represented in Fig. 3.3 would show the upper branch to be unstable ; and only the lower branch can be reached for large times in an unsteady process if we begin with initial conditions in an appropriate domain of attraction. When $\mathcal{D}$ is increased slowly by increasing, for example, the reactant or oxidizer concentration in the free streams the solution will follow the lower branch of Fig. 3.3, until a sudden jump from the nearly frozen mode of combustion to a near equilibrium mode occurs if $\mathcal{D}$ is increased slightly above $\mathcal{D}_I$.

III.3. Diffusion controlled regime

We shall now describe the structure of the flame in the limiting case of large Damköhler numbers, $D_\infty \to \infty$, with E/RT_{00} fixed. This is the Burke-Schumann limit. As we indicated before, in this limit an infinitely thin reaction zone, or flame sheet, located at $Z=Z_e$, where the temperature is the adiabatic flame temperature T_e, given by eqs(3.9 and 10), separates a region $Z>Z_e$ where

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$Y_F=0$. The temperature and concentration distributions are given in this limit by eq(3.8), and are shown schematically in fig. 3 .2b. For large, but finite values of D_∞, the distributions are still given by the B-S solution (3.8), outside a thin reaction zone located, as shown in fig. 3 .4, around Z_e. Let $\ell \ll 1$ be the thickness of the reaction zone relative to that of the mixing layer, then the mass fractions of the reactants Y_F/Y_{F0} and Y_0/Y_{00}, that co-exist in the reaction layer are there of order ℓ ; and this is also the order of $C_p(T_e-T)qY_{F0}$, measuring the deviation of T from T_e. We require that all the terms appearing in the form of Schwabb-Zeldovich relations (3.4 and 5) given below

$$C_p(T-T_e)/qY_{F0} = -Y_F/Y_{F0} + \{1-C_p(T_{00}-T_{F0})/qY_{F0}\}(Z-Z_e)$$ (3.24)

$$Y_0/\nu Y_{F0} = Y_F/Y_{F0} - (1+Y_{00}/\nu Y_{F0})(Z-Z_e)$$

are of the same order $\ell \ll 1$.
If we want to relate ℓ to D_∞, we use eq(3.17), noticing that, because Z_η^2 is of order unity (as long as Z_e is not close to 0 or 1), its terms are of order

$$\ell/\ell \quad , \quad \ell/\ell^2 \quad , \quad D_\infty e^{-E/RT_e} \quad \ell^{n_F+n_O}$$

respectively, if, for simplicity, we assume Y_{00} and Y_{F0} to be of order unity. We thus see that the convective term is, of order unity, negligible when compared with the diffusion term, of order $1/\ell \gg 1$, that must be balanced by the reaction term. So that the value of ℓ given by

$$\ell = \{D_\infty e^{-E/RT_e}\}^{-1/(1+n_F+n_O)}$$ (3.25)

must be small compared with unity, if we want the reaction zone to be thin, and thereby the convective term to be negligible compared with the diffusion term. Notice that this approximation is equivalent to replacing the transport operator $\eta Y_{F\eta} + Y_{F\eta\eta}$ by $(Z_\eta^2)_e Y_{FZZ}$, justified because the changes of Z_η^2 accross the reaction zone are small. An additional simplification, when solving eq. (3.17) in the thin reaction zone, results from replacing the Arrhenius exponential by $\exp(-E/RT_e)$, when we notice that for large Damköhler numbers

$$(T_e-T)/T_e \sim (qY_{F0}/c_pT_e)\ell$$

is small, and then

$$\exp(-E/RT) \simeq \exp(-E/RT_e)\exp\{E(T-T_e)/RT_e^2\}$$ (3.26)

and the last factor can be replaced by 1, if

$$(E/RT_e)(qY_{F0}/C_pT_e)\ell \quad \ll 1$$

Therefore, when this last relation holds, for large values, according to eq(3.25), of the Damköhler numbers, the fuel concentration in the thin flame is given by the equation :

$$(Z_\eta^2)_e Y_{FZZ} = D_\infty e^{-E/RT_e} Y_F^{n_F} Y_0^{n_O}$$ (3.27)

to be solved, together with second relation (3.24) and the boundary conditions :

$$Y_F \to 0 \quad \text{for} \quad (Z_e-Z) \to \infty$$
$$Y_0 \to 0 \quad \text{for} \quad (Z-Z_e) \to \infty \tag{3.28}$$

We should however point out that if, for example $0 < n_F < 1$, Y_F comes down to zero at a finite value of (Z_e-Z), to be determined as part of the solution. The decay to zero is exponential for $n_F=1$, and of the form $(Z_e-Z)^{-(2+n_0)/(n_F-1)}$ for $n_F > 1$.

The problem (3.27-28) can be recast in a universal form, Liñan 1961, of the type

$$y_{XX} = y^{n_F}(\widetilde{y}-X)^{n_0} \tag{3.29}$$
$$y_{-\infty} = 0 \quad , \quad (\widetilde{y}-X)_{\infty} = 0$$

in terms of the variables

$$\widetilde{y} = Y_F/Y_r \quad , \quad X=(Z-Z_e)(Y_{F0}+Y_{00}/\nu)/Y_r \tag{3.30}$$

where Y_r, the characteristic value of Y_F in the thin reaction zone, is given by the relation :

$$Y_r^{n_F+n_0+1} = (Z_n^2)_e(Y_{F0}+Y_{00}/\nu)^2 \nu^{-n_0} D_\infty^{-1}\exp(E/RT_e)$$

and

$$Y_0/\nu Y_r = \widetilde{y} - X, (T-T_e)= qY_r/C_p\{-\widetilde{y}+mX\} \tag{3.31}$$

where

$$m = \{1-C_p(T_{00}-T_{F0})/qY_{F0}\}/(1+Y_{00}/\nu Y_{F0}) \tag{3.32}$$

In the particular case when the reaction order is zero for one of the reactants, the boundary conditions of eq(3.29) must be modified. For example if $n_0=0$, the oxidant concentration will come down to zero at a finite value X_0 of X, and the reaction term will be zero for $X > X_0$, where $\widetilde{y}-X = 0$. Then the boundary condition $(\widetilde{y}-X)_\infty=0$ must be replaced by the conditions $y-X=0$ and $y_X=1$ at $X=X_0$ to be determined, as part of the solution, as a function of n_F. If $n_F=1$ the solution of eq(3.29) is of the form $y=A\exp X$ and $A=1/e$ results from the conditions $A\exp X_0=X_0=1$. If $n_F \neq 1$,
$$\widetilde{y}_X = \{2/(n_F+1)\}^{\frac{1}{2}}\widetilde{y}^{(n_F+1)/2} \quad \text{and}$$
$$\widetilde{y}^{(1-n_F)/2} -1 = (X_0-X)(n_F-1)/\sqrt{2(n_F+1)}$$
with X_0 given by $X_0= \{(n_F+1)/2\}^{1/(n_F+1)}$, to insure that $\widetilde{y}_X=1$ at $X=X_0$. Notice that for $n_F < 1$, y will be identically equal to zero for $X < X_1$ when X_1 is given by $X_0-X_1= \sqrt{2(n_F+1)}/(1-n_F)$.

The solution of (3.29), then describes the concentration and temperature profiles within the reaction zone if the Damköhler number is sufficiently large so that $Y_r/Y_{F0} \ll 1$. However, due to the large values that the nondimensional activation energy

$$(E/RT_e)(qY_{F0}/C_pT_e) = \beta_e \tag{3.33}$$

takes in practical cases, the nondimensional temperature drop $E(T_e-T)/RT_e^2$ in the reaction zone, of the order of $(Y_r/Y_{F0})\beta_e$, can become of order unity, and then the Arrhenius exponent can no longer be evaluated at the temperature T_e, but it should be calcu-

lated using the Frank-Kamenetskii approximation (3.26), when descri-bing *the structure of the thin reaction zone.*

III.4. Extinction regime

The extinction regime corresponds to large activation ener-gies $\beta_e \gg 1$, and precisely those Damdöhler numbers that lead to values of Y_r/Y_{F0}, calculated by (3.31), of the order $1/\beta_e$. This is also the order of the thickness of the reaction zone relative to that of the mixing layer.

Outside the reaction zone the reaction can be frozen due to the rapidly decreasing values of the Arrhenius exponential when the temperature drops. However, the temperature and concentrations are still given there by the Burke-Schumann solution in first approxi-mation. In the thin reaction zone, in first approximation, Y_F, Y_0 and T are given by the solution of

$$(Z_\eta^2)_e Y_{FZZ} = D_\infty e^{-E/RT_e} e^{E(T-T_e)/RT_e^2} Y_F^{n_F} Y_0^{n_o} \qquad (3.34)$$

together with eq(3.24), and the boundary conditions

$$Y_{FZ} = 0 \quad \text{for} \quad (Z_e-Z) \to \infty \quad ; \quad Y_{0Z} = 0 \quad \text{for} \quad (Z-Z_e) \to \infty \qquad (3.35)$$

obtained from the matching conditions with the Burke-Schumann solu-tion, or first approximation of the outer solution.
The problem (3.34-35) can be recast in a simpler form, similar to (3.29), using variables of the type (3.30) with $Y_r = Y_{F0}/\beta_e$. That is, if

$$y = (Y_F/Y_{F0})\beta_e \quad , \quad \xi = (Z-Z_e)(1+Y_{00}/\nu Y_{F0})\beta_e \qquad (3.36)$$

Then the problem (3.34-35) becomes

$$y_{\xi\xi} = \delta e^{-y+m\xi} y^{n_F} (y-\xi)^{n_o} \qquad (3.37)$$

$$y_\xi = 0 \quad \text{for} \quad \xi \to -\infty \quad , \qquad y_\xi \to 1 \quad \text{for} \quad \xi \to \infty \qquad (3.38)$$

involving the parameters m, defined in (3.32), n_F, n_o and the reduced Damköhler number δ, defined by

$$\delta = (Z_\eta^{-2})_e D_\infty e^{-E/RT_e} \nu^{n_o}(Y_{F0}/\beta_e)^{n_F+n_o-1} (Y_{F0}+Y_{00}/\nu)^{-2} \qquad (3.39)$$

of order unity in the extinction regime.

Notice that due to the presence of the Arrhenius variable factor $exp(-y+m\xi)$ in eq(3.37), *the chemical reaction can be frozen* on one or both sides of the thin reaction zone, and thus we must use for eq(3.37) the boundary conditions (3.38), weaker than those used for eq(3.29). We thus allow for leakage $y_{-\infty}$ of the fuel, or $(y-\xi)_\infty$ of the oxidizer through the reaction zone, due to quenching *of the chemical reaction in the extinction regime. Associated with* this leakage, we shall find concentrations of order $1/\beta_e$ of the fuel on the oxidant side of the flame, and similar concentrations of oxidizer on the fuel side of the flame. The amount of reactants

$y_{-\infty}$ and $(y-\xi)_{\infty}$ leaking through the reaction zone must be calculated from the numerical solution of the problem (3.37-38) ; it is, for given reaction orders n_O and n_F, a function of δ and m.

In order to understand the reasons for finding reactant leakage, notice that $E(T-T_e)/RT_e^2 = -y+m\xi$, so that the temperature decreases with a slope m on the oxidant side of the flame, and with a slope (1-m) on the fuel side. It is then clear that we will not find leakage of fuel if m is zero or negative, when no quenching of the reaction takes place on the oxidant side ; no leakage of oxidant will occur when m>1. The numerical solution of the problem (3.37-38) can be found in Liñan 1974, for the case $n_O=n_F=1$, where $(4\delta)^{1/3}(y-\xi/2)$ was used as dependent variable, $(4\delta)^{1/3}\xi/2$ as independent variable ; the solution was found in terms of $\delta_o = 4\delta$ for several values of $\gamma=2m-1$. When m belongs to the interval (0,1), two solutions of the problem (3.37-38) exist for values of δ larger than an extinction value δ_E, a function of m for fixed values of n_O and n_F, and no solutions exist for $\delta<\delta_E$. This is shown in fig.III.4 where $(y-\xi)_{\infty}$ is plotted in terms of δ for several values of m, with $n_F=n_O=1$. Fig.III.4 can also be used to calculate the leakage of oxidant, for $n_F=n_O=1$ for the symmetrical case when m lies in the interval (0.5<m<1) if m is replaced by 1-m and $y_{-\infty}$ by $(y-\xi)_{\infty}$:
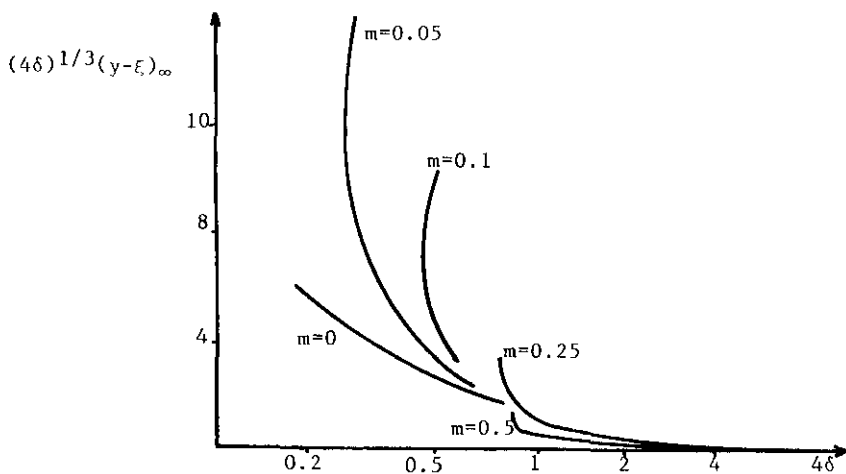

Figure 3.4

A good correlation of the extinction Damköhler number in this case
was obtained by Liñan 1974, yielding

$$\delta_E=(e/2)\{m-2m^2+ 1.04m^3+ 0.44m^4\} \tag{3.40}$$

valid in the range $0<m<0.5$; and also in the range $0.5<m<1$ if m is
replace by l-m.

Of the two solution branches appearing in fig. 3 .4 only
the lower branch, showing smaller deviations from the B-S solu-
tion, can be expected to be stable. The structure of this solution
for large values of δ takes a universal form given by eq(3.29),
where $\tilde{y}=\delta^{1/3}y$,$X =\delta^{1/3}\xi$; the Arrhenius factor $\exp(-y+m\xi) = \exp\{\delta^{-1/3}(-\tilde{y}+mX)\}$ does not deviate significantly from unity in
the reaction zone if $\delta>>1$. The upper branch shows stronger non-
equilibrium effects. For large values of δ the solution merges
if m takes values around 0.5, with the solution corresponding to
an unstable partial burning regime, when both reactants cross the
thin reaction zone and coexist on both sides of the flame sheet.
It merges with a premixed flame regime when m or l-m are negative
or small (see Liñan 1974).

For small values of m, or of (l-m), extinction conditions of
the diffusion flame occur with a premixed flame regime. This can
be shown, using the eq(3.37-38) that describe the reaction zone
structure, as follows. We pose our problem as that of finding
$\delta(b,m)$ that leads to an oxidant leakage $(y-\xi)_\infty =b/m$ with b of
order unity and $m<<1$. Then we anticipate the following structure
of the reaction zone, shown schematically in fig. 3.5

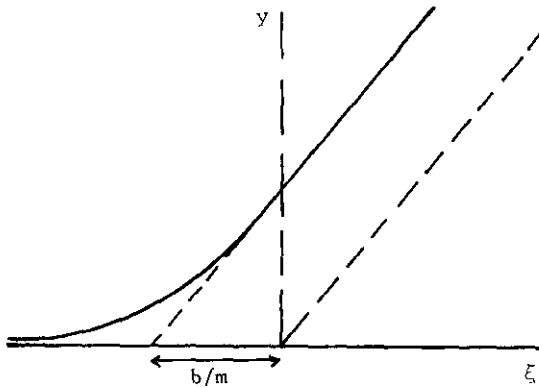Fig.3.5

There is a reaction zone, of thickness of order unity in the ξ variable, located around $\xi = -b/m$, where b of order unity, is negative if m is negative. In this reaction zone y is of order unity, to the right the reaction is frozen, and y tends to zero for large values of $-\xi$. The solution will be written in the form of an expansion in powers of m, using $\zeta = \xi + b/m$ as independent variable. In terms of ζ eq(3.37) takes the form

$$y_{\zeta\zeta} = \delta e^b (b/m)^{n_O} e^{-y+m\zeta} y^{n_F} \{1+m(y-\zeta)/b\}^{n_O} \qquad (3.41)$$

to be solved with the boundary conditions

$$y_\zeta = 0 \quad \text{at } \zeta \to -\infty \quad ; \quad y-\zeta = 0 \quad \text{at } \zeta \to \infty \qquad (3.42)$$

When we introduce in these equations the expansions

$$y = y_O(\zeta) + m \, y_1(\zeta) + \dots$$
$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad (3.43)$$
$$\delta e^b (b/m)^{n_O} = \delta_O \left[1+md+\dots \right]$$

where y_O, y_1, as well as δ_O and d, are assumed to be of order unity for ζ of order unity, we obtain the equation

$$y_{O\zeta\zeta} = \delta_O y_O^{n_F} e^{-y_O} \qquad (3.44)$$

and boundary conditions

$$y_O \to 0 \quad \text{for } \zeta \to -\infty, \quad (y_O - \zeta) \to 0 \quad \text{for } \zeta \to \infty \qquad (3.45)$$

identical to those that describe the reaction zone structure in a premixed flame. Notice that $y_{O\zeta} \to 0$ for $\zeta \to -\infty$ implies that also $y_O \to 0$. A first integral of (3.44) yields, when using (3.45):

$$y_{O\zeta}^2 = 2\delta_O \int_O^{y_O} x^{n_F} e^{-x} \, dx$$

and then $\delta_O^{-1} = 2\Gamma(n_F+1)$, that provides in first approximation, for small values of m, the relation

$$2\Gamma(n_F+1) \, \delta e^b (b/m)^{n_O} = 0 \qquad (3.46)$$

between δ and b. The relation $\delta(b)$ is single-valued, but the inverse relation $b(\delta)$, determining the oxidant leakage, $b=m(y-\xi)_\infty$, in terms of δ, although single-valued for $m<0$, is doubled valued for $m>0$ if δ is larger than an extinction value δ_E, as shown in fig. 3.4 for small values of m. At the extinction value, the Damköhler number is given by

$$\delta_E = (e \, m/n_O)^{n_O} / 2\Gamma_{n_F+1} \qquad (3.47)$$

where Γ_{n_F+1} is the gamma function of order n_F+1.
The equation giving the second term of the expansion (3.43) is

$$y_{1\zeta\zeta} = \delta_O y_O^{n_F} e^{-y_O} \{y_1(n_F/y_O - 1) + d + \zeta + n_O(y_O - \zeta)/b\} \qquad (3.48)$$

to be solved with the conditions $y_{1\zeta} = 0$ for $\zeta \to -\infty$ and $y_1 = 0$ for $\zeta \to \infty$. We notice that $y_{O\zeta}$ satisfies the homogeneous part of this equation. If we multiply both members of (3.48) by $y_{O\zeta}$ we obtain :

$$(d/d\zeta)(y_{O\zeta} y_{1\zeta} - y_{O\zeta\zeta} y_1) = y_{O\zeta} \delta_O y_O^{n_F} e^{-y_O} \{d+\zeta+n_O(y_O-\zeta)/b\}$$

that we can integrate from $-\infty$ to ∞ to obtain

$$d\Gamma_{n_F+1} + (n_o/b)\Gamma_{n_F+2} + \alpha(1-n_o/b) = 0 \qquad (3.49)$$

a relation determining the perturbation d in the Damköhler number in terms of b. Here α is given by the integral

$$2\alpha = \int_{-\infty}^{+\infty} x \frac{d}{dx}(y_{ox}^2)dx = \int_0^\infty (1-y_{ox})dy_o = \mathbf{J_{n_o}}$$

is a function of n_o that can be evaluated numerically without difficulties. If we are simply interested in calculating the new extinction value of δ, we do not need to evaluate this integral, because d can be calculated using the first approximation for the extinction value of b, namely $b=n_o$, in (3.49). Then $d = -(n_F+1)$ and *a two term expansion for the extinction value of the Damköhler number is*

$$\delta_E = \{2\Gamma_{n_F+1}\}^{-1}(em/n_o)^{n_o}\{1-(n_F+1)m+...\} \qquad (3.50)$$

Generalisation to other configurations and kinetic schemes

The analysis presented here was generalized to account for variable gas density and realistic variations of transport *coefficients by Krishnamurthy et al.(1976), who consider a jet of* oxidizer flowing normal to a condensed fuel surface ; the vaporisation rate of the fuel is controlled in this case by the balance between the heat feedback from the flame and the heat required for *gasification. Extinction experiments carried out with this config-*guration have been used to obtain kinetic data for a variety of fuels. See Williams 1981. The quasisteady spherically symmetrical burning of a droplet was analysed by Law, 1975.

For a review of the use of the conserved scalar approach in turbulent combustion see Bilger 1976. When the assumption of infinitely fast chemistry is used together with the equi-diffusional approximation, the concentration of the main reactants and radi-*cals as well as the temperature can be calculated in terms of the* local instantaneous mixture fraction, that can be described in terms of its probability density function. When non-equilibrium effects become important, in addition to the mixture fraction, at *least another "progress" variable must be included in the formu-*lation. A presumed joint pdf for the conserved scalar and for the temperature as a progress variable was used by Peters et al.(1981) to derive a closed form expression for the mean turbulent reaction rate in the limit of large activation energies, showing low quenching would reduce the turbulent reaction rate.

Williams (1975) introduced the concept of laminar diffusion flamelet in turbulent combustion showing how mixing and chemical *reaction occurs in thin regions that are wrinkled and strained by* the turbulent fluctuations, but show a structure similar to that of the counter flow diffusion flames. For recent reviews on these laminar flamelets in diffusion flames, see Peters and Williams 1981 and 1983 and Peters 1983.

For a review of the numerical analysis of diffusion flame structure with multiple kinetics see Peters 1983, who also reviews the work that has been carried out to analyse these flames using asymptotic techniques. The use of these techniques is justified by the fact that the characteristic reaction times associated with the different reactions that enter into a reaction mechanism, differ very often by many orders of magnitude. Thus it is possible to justify by means of asymptotic techniques the use of the "partial equilibrium" assumption for some reactions, and the use of the quasi-steady approximations for some of the radical species.

The first attempts to describe by means of asymptotic techniques the diffusion flame structure with multiple kinetics were those of Clarke 1968 and 1969, see also Clarke 1975 and Allison and Clarke 1980, in connection with the Hydrogen-Air reaction. Melvin and Moss 1970 analysed the structure of Methane-Air flames for large Damköhler numbers. An analysis of diffusion flames involving a one-step forward and the backward reaction has been carried out by Peters 1979. For a review of additional asymptotic analysis of the structure and ignition processes of diffusion flames see Buckmaster and Ludford 1982.

Acknowledgements

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