

LEWIS NUMBER EFFECTS ON THE STRUCTURE AND EXTINCTION
OF DIFFUSION FLAMES DUE TO STRAIN

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In turbulent diffusion flames chemical reaction and mixing occur simultaneously in thin strained and distorted laminar mixing layers separating fuel from the oxidizer.

If the reaction can be modelled in terms of an irreversible reaction



the relative importance of chemical production and transportation terms in the conservation equations is measured by the Damkohler number, or ratio of the characteristic mixing time t_m and the characteristic chemical time t_c . A typical mixing time is the inverse of the straining rate γ , while t_c^{-1} is proportional to the frequency factor of the reaction times the Arrhenius exponential $\exp(-E/RT)$ involving the ratio of the activation energy of the reaction E to the thermal energy TR . Combustion reactions are exothermic and with large values of the ratio E/RT , and, as a result we find in the flow-field regions of low temperature, where the Damkohler number is very small and, therefore, the chemical reaction is frozen. These regions coexist with regions of high temperature where because the reaction is so fast, one of the reactants is depleted, so that either the local concentration of the fuel or of the oxidizer must be zero.

Thus in flows with combustion reactions we find regions in the flow field without fuel separated from regions without oxidizer by thin diffusion flames, where the reactions take place by a process controlled by the rate of diffusion of the reactants towards this surface. These equilibrium regions can be separated from regions of frozen flows, where the reactants coexist, by thin premixed flames that move relative to the unburned mixture leaving behind the reactant that was in excess. See Liñan and Crespo (1976).

For very reactive mixtures the regions of frozen flow cover a small fraction of the flowfields. The diffusion flames are anchored at the injector rim and the chemical

reaction is almost everywhere diffusion controlled. However in many cases the flame is blown completely off the flowfield or lifted from the injector rim, so that a region of mixing without significant effects of the chemical reaction appears, bounded from the downstream region of diffusion controlled combustion by premixed flames.

A criterium for the validity of the diffusion controlled assumption, and the conditions leading to local extinction due to flame strain can only be obtained from an analysis of the structure of the thin reaction zones. See Liñan (1974) and Peters (1980) and Peters and Williams (1980). These analyses show that due to finite rate effects the temperature in the reaction zone is lower than the asymptotic flame temperature value associated with the diffusion controlled limit, and that it decreases with decreasing values of the Damkohler number; then due to the large sensitivity of the reaction rate with temperature no diffusion controlled combustion is possible below an extinction value of the Damkohler number.

With the assumption of infinite reaction rates and if the Lewis number of the reacting species is unity, the passive scalar approach, see for example Bilger (1976), can be used to reduce the problem of describing the reactions in turbulent flows in unpremixed systems to a turbulent mixing problem; this being specially the case if the effects of density changes due to chemical heat release are neglected, although they may be very important in increasing the coherence of the large eddy structures in turbulent combustion.

The purpose of the following is to illustrate the effect of the Lewis number of the fuel in the structures of a strained laminar mixing layer between adjacent eddies of fuel and oxidizer. If a constant positive strain is maintained for some time, the mixing layer will reach a steady state described by the following conservation equations:

$$\gamma Z Y_{OZ} + D Y_{OZZ} + \nu B Y_O Y_F e^{-T_a/T} = 0 \quad (1)$$

$$\gamma Z Y_{FZ} + L^{-1} D Y_{FZZ} + B Y_O Y_F e^{-T_a/T} = 0 \quad (2)$$

$$\gamma Z T_Z + D T_{ZZ} - (Q/c_p) B Y_O Y_F e^{-T_a/T} = 0 \quad (3)$$

to be solved with the boundary conditions

$$Y_O = Y_F - 1 = T - T_O = 0 \quad \text{for } Z \rightarrow -\infty \quad (4)$$

$$Y_O = Y_{O\infty} = Y_F = T - T_O = 0 \quad \text{for } z \rightarrow \infty \quad (5)$$

giving the mass fractions Y_O , Y_F of the oxidizer and fuel, and the temperature T , in terms of the distance to the reference stagnation plane. We consider, for simplicity, that the flow field is not modified due to changes in density, so that the velocity in the Z direction is $(-\gamma Z)$, where γ is the straining rate. We also consider the diffusivity of the oxidizer D to be constant and equal to the thermal diffusivity, so that the Lewis number for the oxygen is taken equal to unity, which is not an unreasonable assumption; the Lewis number of the fuel is L different from unity.

The reaction between fuel and oxidizer is modelled by an Arrhenius reaction of frequency factor B , activation temperature $T_a = E/R$, mass stoichiometric coefficient oxidizer/fuel ν , and heat release Q per unit mass of fuel. The temperature of both approaching streams is T .

This problem was analyzed for large values of the nondimensional activation energy T_a/T_O , in the particular case $L=1$ by this author (1974), and the results were later used by Williams (1975) to describe the structure of diffusion flamelets in turbulent combustion. The analysis showed the existence of a premixed flame regime, in addition to the diffusion controlled regime that appears for large values of the Damkohler number B/γ . Because in most applications the ratio $Y_{O\infty}/\nu$ is small, typically 0.06, it turns out that extinction condition occur in the premixed flame regime that we shall describe, in the following, for $L \neq 1$.

For large values of the nondimensional activation energy T_a/T_O the reaction in the premixed flame regime takes place only at a thin flame region $Z = Z_f$ to be determined as a function of B . The region $Z < Z_f$, toward the fuel side, is a region of near-equilibrium, $Y_O = 0$, while the chemical reaction is frozen in the region $Z > Z_f$, where the fuel and oxidizer coexist. Thus fuel leaks through the reaction zone toward the oxidizer side. The mass fraction of oxidizer on the near-equilibrium side of the flame is small of order T_O/T_a for $Y_{O\infty}/\nu$ of order 1 but becomes negligible if $Y_{O\infty}/\nu \ll 1$.

The mass fractions Y_O and Y_F are then given in terms of $X = Z \sqrt{\gamma/2D}$ by the relations

$$Y_O = 0, \quad Y_F = 1 - A_1 (2 - \operatorname{erfc} X \sqrt{L}) \quad (6)$$

for $X < X_f = Z_f \sqrt{\gamma/2D}$, and

$$Y_O = Y_{O\infty} \left[1 - \frac{\operatorname{erfc} X}{\operatorname{erfc} X_f} \right], \quad Y_F = A_2 \operatorname{erfc} X \sqrt{L} \quad (7)$$

for $X > X_f$

The continuity of the fuel concentration at the flame implies that

$$A_2 \operatorname{erfc} X \sqrt{L} = 1 - A_1 (2 - \operatorname{erfc} X \sqrt{L}) = Y_{Ff} \quad (8)$$

The mass consumption rate of oxidizer per unit flame surface is given by:

$$(\rho D Y_z)_{z_f} = \rho D Y_{O\infty} \frac{\sqrt{\gamma/2D}}{\sqrt{\pi}} \frac{2}{\operatorname{erfc} X_f} \frac{\exp(-X_f^2)}{\operatorname{erfc} X_f} \quad (9)$$

Fuel and oxidizer are consumed at stoichiometric proportions at the flame, so that

$$A_1 - A_2 = \sqrt{L} (Y_{O\infty}/\nu) \frac{\exp\{X_f^2 (1-L)\}}{\operatorname{erfc} X_f} \quad (10)$$

and taking into account Eq (8) we obtain

$$2A_1 = 1 + \sqrt{L}(Y_{O\infty}/\nu) \frac{\operatorname{erfc}(X_f \sqrt{L})}{\operatorname{erfc} X_f} \exp\{X_f^2 (L-1)\} \quad (11)$$

thus determining the concentration distributions in terms of the flame position X_f that will be found below in terms of the Damkohler number from an analysis of the reaction zone structure.

To calculate the temperature distribution we notice that $Y_o/\nu + c_p T/Q$ behaves as an inert species, so that

$$c_p (T-T_o)/Q + Y_o/\nu = (Y_{O\infty}/2\nu) (2-\operatorname{erfc} X) \quad (12)$$

In particular, the flame temperature T_f is given by

$$T_f - T_o = (Q Y_{O\infty}/\nu c_p) \left(1 - \frac{1}{2} \operatorname{erfc} X_f\right) \quad (13)$$

Before giving the results of the analysis of the reaction zone structure, let us indicate that the outer structure of the diffusion flame, in the diffusion-controlled Burke-Schumann limiting case, $B/\gamma \rightarrow \infty$, is given by the above equations if we write $A_2 = 0$, to insure that no fuel leaks toward the oxidizer side of the reaction zone. Then, the flame position is $X_f = X_e$, given by the relation

$$\frac{Y_{O\infty}}{\nu} = \frac{\operatorname{erfc} X_e \exp\{X_e^2 (1-L)\}}{\sqrt{L}(2-\operatorname{erfc} X_e \sqrt{L})}, \quad (14)$$

and the flame temperature $T_f = T_e$ given by

$$c_p (T_e - T_o)/Q + Y_{O\infty}/\nu = 1 - \frac{1}{2} \operatorname{erfc} X_e \quad (15)$$

Only in the case $L=1$ does the flame temperature in the diffusion controlled regime coincide with the adiabatic flame temperature T_{ea} , given by:

$$c_p (T_{ea} - T_o) \nu / Q Y_{O\infty} = (1 + Y_{O\infty} / \nu)^{-1}, \quad (16)$$

If $Y_{O\infty} / \nu$ is small the temperature gradient at the flame toward the fuel side is small compared with the gradient toward the oxidizer side. This simplifies the analysis of the reaction zone structure in the premixed flame regime given by Liñán (1974) which can be used without changes in this case to give the following relation

$$\frac{B}{\gamma} \pi \nu \left[\frac{\nu c_p T_f^2}{Q Y_{O\infty} T_a} \right]^2 Y_{Ff} [\operatorname{erfc} X_f]^2 \exp(2X_f^2 - T_a/T_f) = 1 \quad (17)$$

between the Damkohler number and flame position.

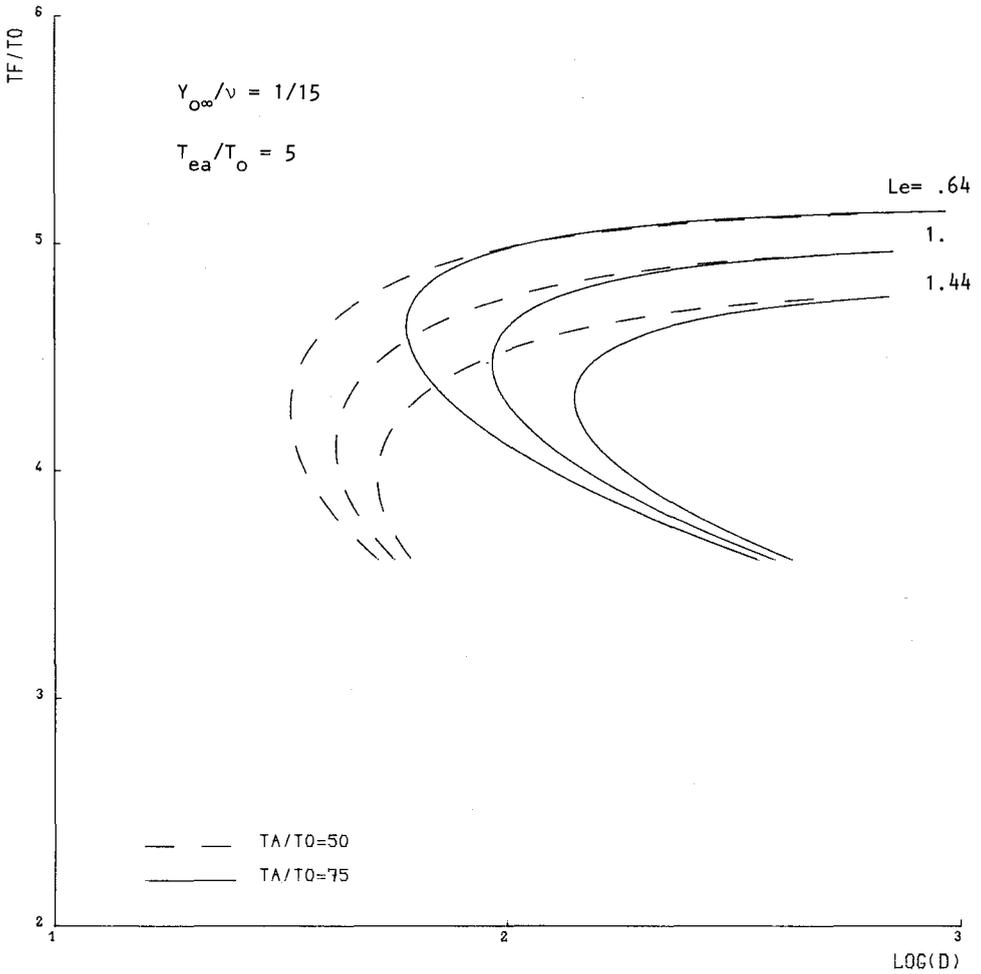
In summary the system of algebraic equations (8), (11), (13) and (17) determines in parametric form, with the flame position X_f as parameter, the relation between the flame temperature and the Damkohler number B/γ involving the straining rate; this relation if, as it has been assumed, T_a/T_o is large is multi-valued for values of $B/\gamma > \gamma(B/\gamma)_E$ an extinction value below which neither the premixed flame regime nor the diffusion controlled regime is possible.

The effect of the Lewis number on the relation between the flame temperature and Damkohler number is shown in the figure for the premixed flame regime. The lower branch of each curve corresponds to unstable solutions of the equations.

The multiplicity of solutions would not exist if time derivative terms representing transient effects were retained in Eqs. (1)-(3). The time derivatives must necessarily be retained if the straining rate γ changes with time; however a coordinate transformation as the one used by Corcos (1980) can be used to transform the problem to that of the unsteady unstrained mixing layer between two half-spaces of fuel and oxidizer, with a slight modification of the reaction rate term. Then the analysis by Liñán and Crespo (1976) can be used to describe the mixing layer structure.

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Flame temperature T_F as a function of $\log(D)$, for different values of Le . The variable D is given by

$$\frac{B}{Y} \pi \nu \exp\left(-\frac{T_a}{T_{ea}}\right) \left(\frac{\nu c_p T_{ea}^2}{Q Y_{O\infty} T_a}\right)^2$$

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