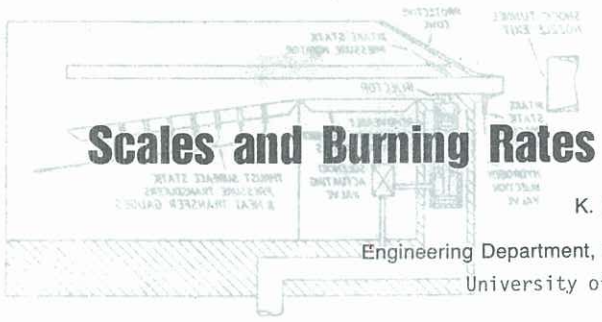
9th AUSTRALASIAN
FLUID MECHANICS CONFERENCE,
AUCKLAND, 8-12 DECEMBER 1986



Scales and Burning Rates in Premixed Turbulent Flames

K. N. C. BRAY

Engineering Department, University of Cambridge, England.

University of Cambridge, England.

ABSTRACT

Two models of turbulent burning in premixed flames are described. Both assume that chemical reaction is confined to thin strained laminar flames embedded in the turbulent flow. The first model leads to a modification of a traditional mixing limited reaction rate expression to allow for quenching in highly strained flamelets. The second model uses a fractal description of a distorted flame surface to describe the range of scales in the wrinkled flame. The two models are shown to predict qualitatively similar behaviour.

INTRODUCTION

There is currently a strong interest in the combustion of premixed fuel-air mixtures with applications to spark ignition engines and industrial furnaces. The combustion chamber flowfield is almost always turbulent. Theoretical and experimental evidence shows that premixed turbulent flames typically consist of thin moving interfaces separating regions of unburned and fully burned mixture. Combustion occurs only within these interfaces. At low turbulence intensities the interface forms a single continuous wrinkled laminar flame but with increasing turbulence it can rupture to create pockets of unburned and/or fully burned mixture. In either case the overall rate of combustion is determined by the surface area and structure of the burning interfaces.

If turbulent mixing is sufficiently intense the laminar flames which form these interfaces are so stretched and curved by the turbulence that the reaction rates within them are reduced and may even be quenched. The turbulent mixing rate may be characterised for example by u'/ℓ_t where u' is the rms turbulence velocity and ℓ_t the integral length scale of the velocity field. If u'/ℓ_t is progressively raised from a low initial value the turbulent mean heat release rate will at first increase, because flame area is enlarge, but flame stretch and quenching will eventually lead to a reduction in heat release, Abdel-Gayed et al (1984).

There is a need to understand and predict the balance between these conflicting processes. Clearly both fluid mechanics and combustion chemistry are important. Both are highly complex and they interact strongly with each other. Laminar flamelet models, in which combustion within a turbulent flame is assumed to be confined to thin moving laminar flamelets embedded in the turbulent flow, provide a means of addressing these problems, Peters (1986). The modelling may then be divided into two quite separate stages, Bray (1985). The first is the calculation of the structure and properties of laminar flames under appropriate conditions of temperature, pressure, composition, strain rate, etc., in order to build up a "library" of laminar flamelet solutions. As much detail as is judged appropriate may be included in the description of the chemical kinetic mechanism and molecular transport processes. The second separate stage is to calculate the turbulent flow using suitable model equations. Chemical reaction effects are represented by an appropriate ensemble of laminar flame solutions from the "library".

This two part approach has been successfully applied to nonpremixed turbulent combustion, with extensive hydrocarbon kinetic mechanisms, Liew et al (1984), Rogg et al (1986). However the premixed combustion case is more difficult to describe because the flamelets move relative to the flow and interact strongly with it.

Heat Release Rate and Scalar Dissipation

A progress variable c, defined, Bray and Moss (1977), as a normalised product species mass fraction, obeys an equation of the form

$$\frac{\partial \rho c}{\partial t} + \frac{\partial \rho u_k c}{\partial x_k} = \frac{\partial}{\partial x_k}\left(\rho D \frac{\partial c}{\partial x_k}\right) + w \qquad (1)$$

where D is a diffusion coefficient and w a chemical source term. If Eq. (1) is averaged and the turbulence Reynolds number is assumed large the result assuming stationarity is

$$\frac{\partial}{\partial x_k}\left(\overline{\rho u_k c}\right) = \overline{w}. \qquad (2)$$

Our objective is to predict $\overline{w}$ which is the mean of the source term w.

In the laminar flamelet combustion regime thin moving laminar flames separate regions of unburned and fully burned mixture. The probability density function (p d f) of c at a location $\underline{x}$ may then be written

$$p(c;\underline{x}) = \alpha(\underline{x})\,\delta(c) + \beta(\underline{x})\,\delta(c-1) + \gamma(\underline{x})\,f(c;\underline{x}) \qquad (3)$$

where α, β and γ are the probabilities of unburned fully burned mixture, and intermediate burning* states, respectively, occurring at $\underline{x}$; $\delta(c)$ and $\delta(c-1)$ are Dirac delta functions representing unburned gas ($c=0$) and fully burned gas ($c=1$), respectively, and $f(c;\underline{x})$ is the burning mode p d f. Because the burning interfaces are thin the burning mode probability is small, i.e. $\gamma(\underline{x}) \ll 1$ everywhere.

If turbulent mixing is much slower than reaction the source term $\overline{w}$ may be seen, Bray (1979), to be proportional to the rate at which turbulent motion brings unburned gas into contact with flamelets. By combining balance equations for the mean and variance of c assuming $\gamma \ll 1$ it is found that $\overline{w}$ is proportional to the Favre mean scalar dissipation function $\tilde{\varepsilon}_c$. This is the mean rate at which fluctuations in c are decreased by molecular diffusion, i.e.

$$\tilde{\varepsilon}_c = 2\rho D\left(\frac{\partial c}{\partial x_k}\right)^2 / \overline{\rho} \qquad (4)$$

The required relationship is

$$\overline{w} = \overline{\rho}\,\tilde{\varepsilon}_c/(2c_m - 1) \qquad (5)$$

* Strictly γ is the probability that $\varphi < c < 1-\varphi$ where $\varphi \ll 1$ is specified. In some circumstances the "burning" mode γ may represent quenched flamelets whose combustion has been extinguished by intense turbulence.

BRAY

where $c_m = \overline{cw}/\overline{w}$. An analagous expression for nonpremixed combustion was obtained by Bilger (1976).

The main difficulty in exploiting (5) is the representation of $\tilde{\varepsilon}_c$. Classical turbulence modelling suggests

$$\tilde{\varepsilon}_c \simeq \widetilde{c''^2}\,\tilde{\varepsilon}/\tilde{k} \qquad (6)$$

where $\tilde{k}$ and $\tilde{\varepsilon}$ are the Favre averaged turbulence kinetic energy and its dissipation function and $\widetilde{c''^2} = \overline{\rho c''^2}/\bar{\rho}$. Borghi and Dutoya (1979) have proposed a separate balance equation for $\tilde{\varepsilon}_c$. The validity of these approaches is difficult to assess. They ignore the fact that in laminar flamelet combustion the composition gradient $\partial c/\partial x_k$ in Eq. (4) occurs only in coherent structures (laminar flames) rather than quasi-randomly as in conventional turbulence. With (6), Eq. (5) suggests that $\bar{w}$ will increase without limit if the turbulence time scale $\tilde{k}/\tilde{\varepsilon}$ is reduced. No allowance is made for flamelet quenching due to finite reaction rates.

Strained Laminar Flame "Library"

A stretched laminar flame solution may be characterised by a value of the dimensionless Karlovitz number

$$\kappa = \frac{\delta_L^o}{S_L^o}\,\frac{1}{A}\,\frac{DA}{Dt} \qquad (7)$$

where δ_L^o and S_L^o are the thickness and burning velocity of an unstrained laminar flame, A represents flame surface area and D/Dt the material derivative. In turbulent flow, Peters (1986)

$$\frac{1}{A}\,\frac{DA}{Dt} \simeq \left(\frac{\varepsilon}{\nu}\right)^{\frac{1}{2}} \qquad (8)$$

where ν is the kinematic viscosity and ε the instantaneous value of the viscous dissipation function.

In a turbulent flame burning will be represented by a finite number of strained laminar flames with Karlovitz numbers κ_0, κ_1 .... κ_n which are assumed to occur with probabilities $p_0(\underline{x})$, $p_1(\underline{x})$ .... $p_n(\underline{x})$ where $\sum_{s=0}^{n} p_s(\underline{x}) = 1$.

It is assumed that all effects of flame curvature and stretch are described in this way. These discretised probabilities represent the conditional probabilities that the Karlovitz number κ at $\underline{x}$ lies within a specified range of a value κ_s at times when a flamelet exists at $\underline{x}$. In the present state of knowledge it is necessary to follow the precedent from nonpremixed combustion models and assume that κ is uncorrelated with the occurrence of flamelets, i.e. of values of c in the range $\phi < c < 1 - \phi$ where $\phi << 1$. This assumption is unlikely to be strictly valid particularly in the premixed case where the possibility exists for the flamelet to move away from regions of excessive strain rate. Assuming statistical independence the instantaneous viscous dissipation may be modelled as a log-normal distribution.

Unstrained laminar flame solutions with the relevant initial conditions of temperature, pressure and composition, and the chosen Karlovitz numbers κ_s, then provide temperature, density, composition and w profiles through the flamelets, either in the form $T_s(c)$, $\rho_s(c)$, $Y_{is}(c)$ (i = 1,2 ...), $w_s(c)$, or as functions of physical distance z through the flamelet. These properties plus the burning velocities S_L^s and flamelet thicknesses δ_L^s form the flame library.

First Burning Rate Model

This model starts with the observation that the mean of w is

$$\bar{w}(\underline{x}) = \int_0^1 w(c)\, P(c;\underline{x})\, dc$$

but the p d f P(c; $\underline{x}$) is given by Eq. (3) so

$$\bar{w}(\underline{x}) = \gamma(\underline{x}) \int_0^1 w(c)\, f(c;\underline{x})\, dc \qquad (9)$$

Now in flamelet combustion burning occurs only in laminar flamelets so the shape of the burning mode p d f is determined by the flamelet profiles. For flamelets with Karlovitz number κ_s we have

$$f_s(c) = \left[\frac{dc}{d(z/\delta_L^s)}\right]_s^{-1} \qquad (10)$$

Equation (9) becomes

$$\bar{w}(\underline{x}) = \gamma(\underline{x}) \sum_{s=0}^{n} P_s(\underline{x}) \int_0^1 w_s(c)\, f_s(c)\, dc \qquad (11)$$

The mean mass fraction of a species i is

$$\bar{Y}_i(\underline{x}) = \gamma(\underline{x})\, Y_i(o) + \beta(\underline{x})\, Y_i(1) + \gamma(\underline{x}) \sum_{s=o}^{n} P_s(\underline{x}) \int_0^1 Y_{is}(c)\, f_s(c)\, dc \qquad (12)$$

in which $Y_i(o)$ and $Y_i(1)$ are the mass fractions of i in burned and unburned mixtures respectively.

The burning mode probability $\gamma(\underline{x})$ in the above equations is as yet undetermined. An additional physical input to the model is required for this purpose and, in the present state of knowledge, further empiricism appears necessary. For this purpose we shall assume that γ, which is the probability that $\phi < c < 1 - \phi$, is independent of flamelet quenching. Equations (5) and (6) provide a dissipation rate expression for $\bar{w}$ in the absence of quenching. The corresponding flamelet expression for $\bar{w}$ without quenching is obtained by setting $p_o(\underline{x}) = 1$ and $P_s(\underline{x}) = 0$ $(s \geq 1)$ in Eq. (11). Equating the two $\bar{w}$ results it is found that

$$\gamma(\underline{x}) = \frac{\bar{\rho}(\underline{x})\, \tilde{\varepsilon}_c(\underline{x})}{[2\, c_m(\underline{x}) - 1] \int_0^1 w_o(c)\, f_o(c)\, dc} \qquad (13)$$

where $\tilde{\varepsilon}_c$ is to be evaluated from (6). Substituting (13) into (11) the chemical source term is obtained as

$$\bar{w}(\underline{x}) = \frac{\bar{\rho}(\underline{x})\, \tilde{\varepsilon}_c(\underline{x}) \sum_{s=o} p_s(\underline{x}) \int_0^1 w_s(c)\, f_s(c)\, dc}{[2\, c_m(\underline{x}) - 1] \int_0^1 w_o(c)\, f_o(c)\, dc} \qquad (14)$$

The dissipation controlled rate expression of Eqs. (5) and (6) describes an assumed fast chemistry limit in which burning is controlled by the rate at which turbulent motion brings unburned gas into contact with the flamelets. In Eq. (14) this eddy break up rate is modified by a term describing the reduction in reaction rate due to effects of flamelet stretch. A criticism of this burning rate expression is that it involves using Eq. (6) to evaluate the scalar dissipation function $\tilde{\varepsilon}_c$. This expression is largely empirical with little physical input. It is also difficult to test it experimentally. The second model aims to overcome this weakness.

Second Burning Rate Model

This model makes use of two separate formulations for $\bar{w}$. Each formulation is at present incompletely developed so a composite model has been formed from them both. An important advantage of these new approaches is that they deal in quantities which are experimentally accessible so it should be possible to improve them systematically.

The first formulation is based upon Gouldin's (1986) description of the surface area of a laminar flame in turbulent flow in terms of the theory of fractals.

According to Gouldin (1986)

$$\frac{A}{A_o} = (f \ell_t/\eta)^{D-2} \qquad (15)$$

where A is the true flamelet area, A_o is the smaller area which would occur if the flame wrinkles could be smoothed out. As before ℓ_t is the integral length scale of the velocity field, while η is the Kolmogorov microscale and

$$f = 1 - (1 - a_T^{-\frac{1}{4}} R_\ell^{-\frac{3}{4}}) \exp\left[- a_t^{\frac{1}{4}} R_\ell^{-\frac{1}{4}} \frac{u'}{S_L^o} \right] \qquad (16)$$

allows for the effect of a finite laminar burning velocity in smoothing out small scale flame wrinkles. The quantity D is known as the fractal dimension.

Gouldin (1986) recommends $D = 2.37$. He relates η to ℓ_t by

$$\frac{\ell_t}{\eta} = a_T^{-\frac{1}{4}} R_\ell^{\frac{3}{4}} \qquad (17)$$

where $a_T = 0.37$ and $R_\ell = u'\ell_t/\nu$. Using these expressions he predicts turbulent burning velocities which are in satisfactory agreement with experiment.

Now if the flamelet area per unit volume is the reciprocal of a length scale ℓ_c the mean burning rate is

$$\overline{w}(\underline{x}) = \frac{\rho_r}{\ell_c(\underline{x})} \sum_{s=o}^{n} P_s(\underline{x}) \, S_L^s \qquad (18)$$

where ρ_r is the density of unburned mixture and S_L^s is the burning velocity of a strained laminar flame of type s. Gouldin's fractals description of flame area leads to

$$\frac{1}{\ell_c} = \frac{1}{\ell_t} (f \ell_t/\eta)^{D-2} \qquad (19)$$

Unfortunately this approach does not properly describe the spatial variation of $\ell_c(\underline{x})$ since a fractal simulation of a rough surface is statistically homogeneous in space. We shall apply Eqs. (18) and (19) at the centre of the flame, where homogeneity does exist, and determine the spatial variation separately.

The second independent formulation, which will be used here to obtain this spatial variation, is the time series modelling of Bray et al (1984). The mean reaction rate is written

$$\overline{w}(\underline{x}) = w_F(\underline{x}) \, \nu(\underline{x}) \qquad (20)$$

where $\nu(\underline{x})$ is the number of times per second that station $\underline{x}$ is crossed by a flamelet and

$$w_F = \int_F w \, dt \qquad (21)$$

is the average chemical change per crossing. If the flamelets are thin the progress variable $c(\underline{x},t)$ observed at a fixed point $\underline{x}$ is a square wave time series, which may be represented as a random telegraph signal. A simple analysis then leads to the result

$$\nu(\underline{x}) = \frac{g \, \overline{c}(\underline{x}) \, [1 - \overline{c}(\underline{x})]}{\hat{T}(\underline{x})} \qquad (22)$$

where $\hat{T}$ is the integral time scale of the square wave time series and g lies between 1 and 2. Results of this analysis are well verified experimentally. A modelled balance equation describes the variation of $\hat{T}$ through the flame, Bray et al (1984, 1986).

Assuming strained laminar flamelets the chemical term in (20) is modelled as

$$w_F(\underline{x}) = \frac{K}{\overline{V}(\underline{x})} \sum_{s=o}^{n} p_s(\underline{x}) \int_F w_s(z) \, dz \qquad (23)$$

where $\overline{V}$ is the magnitude of the mean flow velocity, K is an unknown factor, and subscript F indicates integration through a flamelet.

Thus this model also is incomplete since K is not known. The composite model evaluates Kg by equating $\overline{w}$ at mid flame from the fractal model, Eq. (18), to $\overline{w}$ from the time series model from Eq. (20). The result is

$$Kg = \frac{4 \rho_r \overline{V}_{\frac{1}{2}} \hat{T}_{\frac{1}{2}} \overline{S}_{L(\frac{1}{2})} \left[\frac{1}{\ell_t} (f \ell_t/\eta)^{D-2} \right]_{r\frac{1}{2}}}{\left[\sum_{s=o}^{n} P_s \int w_s \, dz \right]_{\frac{1}{2}}} \qquad (24)$$

where subscript $\frac{1}{2}$ indicates conditions where $\overline{c} = \frac{1}{2}$, subscript r refers to reactants and

$$\overline{S}_{L(\frac{1}{2})} = \left[\sum_{s=o}^{n} P_s \, S_L^s \right]_{\frac{1}{2}}$$

Application

For purposes of illustration we shall reduce the flamelet "library" to only two entries: unquenched flamelets for which $0 \leq \kappa < \kappa_2$, approximated as unstrained flamelets; and highly strained flamelets with $\kappa \geq \kappa_2$ for which negligible reaction occurs. The limiting Karlovitz number at quenching may be determined from laminar flame calculations. With κ_2 chosen the corresponding viscous dissipation is

$$\varepsilon_q = \nu_v [\kappa_q \, S_L^o / \delta_L^o]^2$$

For a log-normal distribution the probability of unquenched flamelets is, Liew et al (1984)

$$p_o(\underline{x}) = \tfrac{1}{2} \, erfc[(\ell n \, \tilde{\varepsilon}/\varepsilon_q - \tfrac{1}{2}\sigma^2)/\sqrt{2}\,\sigma]$$

where $erfc$ is the complementary error function while $\sigma(\underline{x})$ is related to the standard deviation of the log-normal distribution.

These expressions may be used to simplify our two burning rate models. The result from the first model is

$$\overline{w} = \frac{\overline{\rho} \, p_o \, \tilde{\varepsilon} \, \overline{c} \, (1 - c)}{(2 c_m - 1) \, \tilde{k}} \qquad (26)$$

from (14).

Similarly from (20), (22), (23) and (24) the second model gives

$$\overline{w} = 4 \rho_r S_L^o \, p_o \left[\frac{1}{\ell_v} \left(\frac{f L_v}{\eta} \right)^{D-2} \right]_{r(\frac{1}{2})} \frac{\overline{V}_{\frac{1}{2}} \hat{T}_{\frac{1}{2}}}{\overline{V} \, \hat{T}} \, \overline{c} \, (1 - \overline{c}) \qquad (27)$$

Trends implied in Eqs. (26) and (27) may be illustrated as follows. Define a turbulence Reynolds number $R_\ell = \tilde{k}^2/\tilde{\varepsilon}\nu_v$, laminar flamelet time $t_L = \delta_L^o / S_L^o$, quenching time $t_q = (\nu/\varepsilon_q)^{\frac{1}{2}}$, so that $\kappa = t_L/t_q$. Let $t_t = \tilde{k}/\tilde{\varepsilon}$. Assume $\nu_v = S_L^o \, \delta_L^o$. Then Eq. (26) may be written

$$W_1 = \frac{y}{2} \, erfc[(\ell n \, (y^2 R_\ell) - \tfrac{1}{2}\sigma^2)/\sqrt{2}\,\sigma] \qquad (28)$$

where $y = t_q/t_t$ and W_1 is a normalised burning rate

$$W_1 = \frac{\overline{w} \, (2 c_m - 1) t_L}{\overline{\rho} \, \overline{c} \, (1 - \overline{c}) \, \kappa} \qquad (29)$$

BRAY

Similarly if a normalised burning rate from Eq. (27) is defined as

$$W_2 = \frac{\overline{w}\,\overline{V}\,\hat{T}\,t_L}{4\,\rho_r\,\overline{V}_{\frac{1}{2}}\,\hat{T}_{\frac{1}{2}}\,\overline{c}(1-\overline{c})\kappa} \qquad (30)$$

then Eq. (27) may be written

$$W_2 = A\,W_1 \qquad (31)$$

where

$$A = (y\,\kappa R_\ell)^{-\frac{1}{2}}\,(f\,a_T^{\frac{1}{4}} R_\ell^{\frac{3}{4}})^{D-2}$$

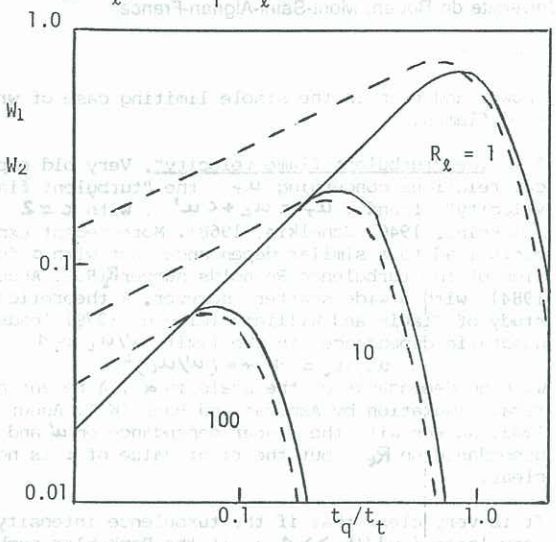


Figure 1: Full curves: W_1 from Eq. (28). Dashed curves: W_2 from Eq. (31).

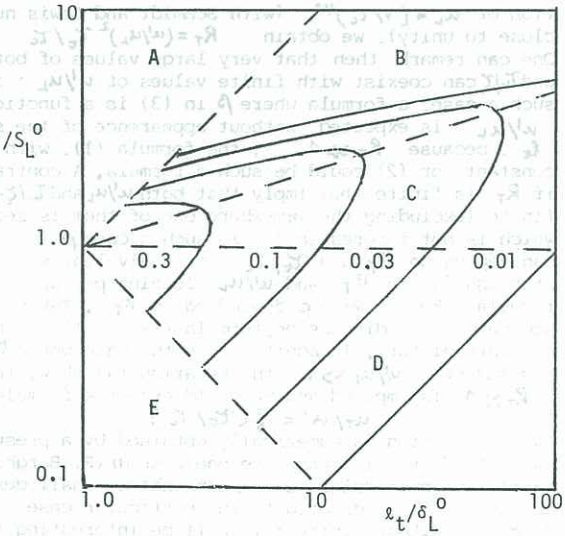


Figure 2: Contours of constant W_1 on a plot showing premixed combustion regimes.

Figure 1 shows W_1 and W_2 plotted against $y = t_q/t_t$ for several turbulence Reynolds numbers assuming for illustration that $\kappa = 1$ and $\sigma = \ell n 10 = 0.679$. Before quenching, the first model, Eq. (29), reduces to $W_1 = y$ independently of R_ℓ. Quenching leads to a rapid reduction in W_1 and this occurs at smaller values of y at higher Reynolds numbers. Qualitatively similar behaviour is shown by the second model although W_2 is not independent of R_ℓ in the unquenched region.

Figure 2 shows contours W_1 = constant on a plot of $\tilde{k}^{\frac{1}{2}}/S_L^o$ against ℓ_t/δ_L^o. According to Borghi (1984) regions on this graph may be interpreted as follows:

A: $(t_L > t_t)$ distributed reaction,

B: $(t_L < t_t,\ t_L > t_\eta)^*$ quenching possible,

C: $(t_L < t_\eta,\ \tilde{k}^{\frac{1}{2}} > S_L^o)^*$ laminar flamelet combustion in pockets,

D: $(\tilde{k}^{\frac{1}{2}} < S_L^o)$ wrinkled laminar flames.

E: $(R_\ell < 1)$ nonturbulent regime.

These regions are identified in Fig. 2. It may be seen that according to the first model W_1 contours are straight in Region D corresponding to negligible quenching in the wrinkled laminar flame regime. The contours are curved due to significant quenching in Region C and quenching is very strong in Region B, as expected. The flamelet model is not applicable in Region A.

REFERENCES

Abdel-Gayed, R. G., Bradley, D., H amid, M. N., Lawes, M. (1984): Lewis Number Effects on Turbulent Burning Velocity. 20th Symp. (Int.) on Combustion, pp. 505-512, Combustion Inst.

Bilger, R. W. (1976): Turbulent Jet Diffusion Flames. Prog. Energy Combust. Sci. 1, 87.

Borghi, R. (1984): Mise au Point sur la Structure des Flammes Turbulentes. J. de Chimie Physique, 81, 321-370.

Borghi, R., Dutoya, D. (1979): On the Scales of the Fluctuations in Turbulent Combustion. 17th Symp. (Int.) on Combustion, pp. 235-244, Combustion Inst.

Bray, K. N. C. (1979): The Interaction Between Turbulence and Combustion, 17th Symp. (Int.) on Combustion, pp.223-233, Combustion Inst.

Bray, K. N. C. (1985): Laminar Flamelet Modelling of Turbulent Combustion. Lecture Notes in Physics 241, pp.3-19, Springer-Verlag, Berlin.

Bray, K. N. C., Moss, J. B. (1977): A Unified Statistical Model of the Premixed Turbulent Flame. Acta Astronautica, 4, 291.

Bray, K. N. C., Libby, P. A., Moss, J. B. (1984): Flamelet Crossing Frequencies and Mean Reaction Rates in Premixed Turbulent Combustion. Comb. Sci. and Tech., 41, 143-172.

Bray, K. N. C., Libby, P. A. (1986): Passage Times and Flamelet Crossing Frequencies in Premixed Turbulent Combustion. Combust. Sci. and Tech: 47, 253-274.

Gouldin, F. C. (1986): An Application of Fractals to Modelling Premixed Turbulent Flames. Sibley School of Mechanical and Aerospace Eng. Rept. Cornell Univ. Ithaca, N.Y.

Liew, S. K., Bray, K. N. C., Moss, J. B. (1984): A Stretched Laminar Flamelet Model of Turbulent Non-premixed Combustion. Comb. and Flame, 56, 199-213.

Peters, N. (1986): Laminar Flamelet Concepts in Turbulent Combustion. Paper to be presented at 21st Symp. (Int.) on Combustion, Munich.

Rogg, B., Behrendt, F., Warnatz, J. (1986): Turbulent Non-Premixed Combustion in Partially Premixed Diffusion Flamelets with Detailed Chemistry. Paper to be presented at 21st Symp. (Int.) on Combustion, Munich.

* The Kolmogorov time scale is evaluated from $t_\eta = (\nu/\varepsilon)^{\frac{1}{2}}$.