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TURBULENT PREMIXED FLAMES

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1. INTRODUCTION

Turbulent premixed flames exhibit phenomena not found in other turbulent flows. In some circumstances a thin flame sheet (thinner than the Kolmogorov scale) forms a connected but highly wrinkled surface that separates the reactants from the products. This flame surface is convected, bent, and strained by the turbulence and propagates (relative to the fluid) at a speed that can depend on the local conditions (surface curvature, strain rate, etc.). Typically, the specific volume of the products is seven times that of the reactants, the flame surface being a volume source. Because of this volume source there is a pressure field associated with the flame surface that affects the velocity field and hence indirectly affects the evolution of the surface itself. For the simplest case of a plane laminar flame, this feedback mechanism tends to make the flame unstable.

As well as looking at the detailed structure of a turbulent premixed flame, we can examine mean quantities. Here too, in comparison to other turbulent flows, there are some unusual observations, the most striking being countergradient diffusion. Within the flame there is a mean flux of reactants due to the fluctuating component of the velocity field. Contrary to normal expectations and observations in other flows, it is found that this flux transports reactants up the mean-reactants gradient, away from the products (hence countergradient diffusion). A second notable phenomenon is the large production of turbulent energy within the flame: Behind the flame the velocity variance can be 20 times its upstream value (Moss 1980). Both these phenomena result from the large density difference

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between reactants and products and from the pressure field due to volume expansion.

There is a wide variety of theories and models for premixed turbulent flames. Some take as their prime objective the determination (or correlation) of the turbulent-flame speed u_T as a function of the relevant parameters (Abdel-Gayed & Bradley 1981, Tabaczynski et al. 1980, Andrews et al. 1975). More ambitious are the probabilistic field theories that attempt to calculate statistical properties of the flame as functions of position and time. As an example, in the pdf approach the statistic calculated is the one-point joint probability density function (pdf) of the velocities and compositions.

Here we review, first, our knowledge of the structure of turbulent premixed flames and the fundamental processes involved. Second, we review the application of probabilistic field theories (primarily the pdf approach) to turbulent premixed flames to reveal their achievements, shortcomings, and issues yet to be resolved.

By definition, in a premixed flame the gaseous fuel and oxidant are homogeneously mixed prior to combustion. In applications, because of the explosion hazard, premixing is generally avoided. Nevertheless, there are several important applications of turbulent premixed combustion; the principal one is the (homogeneously charged) spark-ignition engine. Other examples are reheat systems in jet engines, industrial tunnel burners, and gaseous explosions in a turbulent atmosphere (Bray 1980).

There have been several experiments in which the flame within a spark-ignition engine has been studied [see Tabaczynski (1976), Keck (1982), and Abraham et al. (1985) for references]. But most quantitative information about premixed flames comes from experiments in a variety of simpler configurations. Most closely related to engine flames are statistically spherical flames, ignited by a spark and propagating outward into turbulent reactants (Mickelsen & Ernstein 1956, Bolz & Burlage 1960, Palm-Leis & Strehlow 1969, Hainsworth 1985). A variant is the double-kernel technique, in which two spark-ignited flame balls propagate into turbulent reactants and eventually collide (see, e.g., Abdel-Gayed et al. 1984, Groff 1986). Like flames in spark-ignition engines, both the single- and double-kernel flames are not statistically stationary and do not depend upon stabilization.

Jet flames have been extensively studied since the early work of Damköhler (1940). The reactants flow up a cylindrical burner tube, sometimes through a turbulence-generating grid. The approximately conical flame is then stabilized on the rim of the burner. (An annular hydrogen flame may also be used for stabilization.) The early work on these flames has been reviewed by Stambuleanu (1976). Recent investigations have

been performed by Moss (1980), Yoshida & Tsuji (1982), Shepherd & Moss (1982), Gunther (1983), Suzuki & Hirano (1984), and Cheng & Shepherd (1986), among others.

Other configurations to which we give less consideration in what follows are ducted flames stabilized on a cylinder, say, held perpendicular to a high-speed stream (see, e.g., Wright & Zukoski 1962), unconfined flames stabilized in low-speed streams (see, e.g., Dandekar & Gouldin 1982, Cheng 1984, Gulati & Driscoll 1986a,b), and flames stabilized in stagnation flow (Cho et al. 1986).

Recent reviews on turbulent combustion in general have been provided by Williams (1985a), by Libby & Williams (1976, 1980, 1981), and by Jones & Whitelaw (1982, 1984). For turbulent premixed flames, Bray (1980) provides an excellent review and exposition of the fundamental issues. Useful material can also be found in the books of Kuo (1986), Williams (1985b), Strehlow (1968, 1985), Stambuleanu (1976), and Lewis & von Elbe (1961).

In the next section the fundamentals of turbulent premixed combustion are outlined. This includes a brief consideration of the governing equations, laminar premixed flames, and of the characterization of turbulence. Section 3 starts with a consideration of the important dimensionless parameters that are used to identify different regimes of turbulent premixed combustion. Then, for the important regimes, we examine the detailed structure and fundamental propagation processes and how probabilistic field theories succeed or fail in representing them. The effect of combustion on the turbulence is examined in Section 4. The primary effect is through the pressure field induced by the volume expansion. In the discussion, the major areas of uncertainty are identified and possible research approaches indicated.

2. FUNDAMENTALS

2.1 *Governing Equations*

A typical premixed flame may contain scores of species (mostly intermediates) that take part in hundreds of elementary reactions. Taking full account of this complexity, Warnatz has made useful and impressive computations of simple laminar flames (e.g. Warnatz 1984). But needless to say, sweeping simplifying assumptions are essential to progress in the analysis of laminar flames or in any approach to turbulent flames. The assumptions usually made fall into four categories:

1. General assumptions
2. Reaction scheme

3. Transport properties
4. Detailed assumptions.

The general assumptions, common to virtually all approaches, are single-phase (gaseous) flow, low Mach number, and negligible radiative heat transfer. The low-Mach-number assumption is particularly important: It implies that spatial differences in pressure Δp are much smaller than the absolute value of the pressure p_0. Hence the pressure enters the thermochemistry only through p_0, whereas only pressure differences affect the velocity field.

In most theories of laminar or turbulent premixed flames, the complex chemical reactions are modeled by a one-step overall reaction (for exceptions, see Williams 1985b). Such a sweeping assumption clearly has a limited range of validity. Clavin (1985) suggests that the assumption is generally satisfactory, but it is inadequate to describe chemical-kinetic extinction, pollutant formation, and sensitization or inhibition of the reaction by additives. In addition, a one-step mechanism is inadequate to describe ignition.

Equally sweeping assumptions are made concerning the molecular transport processes. In many laminar-flame studies, the diffusion coefficient of each species is assumed to be the same, Soret and Dufour effects are neglected, and the Lewis number is assumed constant. (The Lewis number Le is the ratio of the thermal to mass diffusivities.)

Finally, detailed assumptions are needed concerning the specific form of the reaction rate and the dependence of the density and diffusivity on temperature and species concentrations.

With all these assumptions, the thermochemistry of a premixed flame can be described by just two transport equations. The two dependent variables can be chosen to be a reaction progress variable $c(\mathbf{x}, t)$ and the enthalpy $h(\mathbf{x}, t)$. By definition, c is zero in the reactants and unity in the products. If the reactants were to burn homogeneously, then the enthalpy would remain constant: In particular, the enthalpy of the products is the same as that of the reactants. In a flame, the only mechanism by which the enthalpy changes is the differential diffusion of heat and mass. Consequently, in laminar-flame studies the Lewis number is of prime importance (see, e.g., Clavin 1985, Buckmaster & Ludford 1982).

For turbulent flames, it has generally been assumed (Bray & Moss 1974, Pope & Anand 1984) that the Lewis number is unity. Then the enthalpy is constant and uniform, and the thermochemistry is described by the single variable $c(\mathbf{x}, t)$. The assumption of unit Lewis number is clearly useful in reducing the number of dependent variables, but it must be borne in mind that it excludes phenomena that may be important—in particular, it excludes the diffusive-thermal instability (see, e.g., Williams 1985b).

With the above assumptions, the transport equation for the reaction progress variable $c(\mathbf{x}, t)$ is

$$\rho \frac{Dc}{Dt} = \rho\left(\frac{\partial}{\partial t} + \mathbf{U}\cdot\nabla\right)c = \nabla\cdot(\rho D\nabla c) + \rho S, \tag{1}$$

where $\mathbf{U}(\mathbf{x}, t)$ is the fluid velocity. The density ρ, the diffusivity D, and the reaction rate S are all given functions of c. Typically ρ may be given by

$$1/\rho(c) = 1/\rho_r + c(1/\rho_p - 1/\rho_r), \tag{2}$$

where ρ_r and ρ_p are the densities in the reactants and products, respectively. The ratio $R \equiv \rho_r/\rho_p$ is typically in the range 5–10. A typical reaction rate is (Pope & Anand 1984)

$$S(c) = S^*(c)/\tau_R, \tag{3}$$

where τ_R is the reaction time scale and

$$S^*(c) = 6.11 \times 10^7\, c(1-c)\exp\{-30{,}000/(300+1800c)\}. \tag{4}$$

This expression, which is plotted in Figure 1, corresponds to an activation temperature of 30,000 K and reactant and product temperatures of 300 K and 2100 K, respectively. The numerical constant is chosen so that the maximum of $S^*(c)$ is unity.

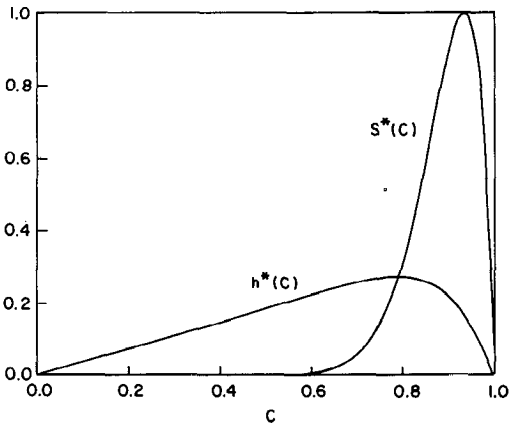

Figure 1 Normalized reaction rate $S^*(C)$ [Equation (4)] and laminar-flame function $h^*(C)$ [Equation (27)].

2.2 *Laminar Premixed Flames*

In some instances of premixed turbulent combustion, the flame surface behaves locally like a laminar flame. Studies of laminar flames have a bearing, therefore, on the turbulent case, especially those studies concerned with the effects of straining and curvature on the flame.

The simplest case is that of a plane laminar flame propagating steadily into quiescent reactants. The propagation speed (measured relative to the reactants) is the laminar-flame speed u_L, which is uniquely determined by the thermochemical state of the reactants. There are many experimental methods for determining u_L (Rallis & Garforth 1980), and there are abundant data in the literature (e.g. Metghalchi & Keck 1982). With appropriate boundary conditions, Equations (1–4) can be solved for a plane laminar flame, and u_L emerges as an eigenvalue. But, neglecting the variation of ρ and D with c, dimensional analysis suffices to yield the well-known result that u_L scales as $(D/\tau_R)^{1/2}$. Alternatively, this relation can be inverted to define a laminar-flame time scale

$$\tau_L \equiv D_r/u_L^2, \tag{5}$$

where D_r is the thermal diffusivity of the reactants. (Recall that with the unity-Lewis-number assumption, the thermal and mass diffusivities are equal.) Equation (5) is useful because, for a given fuel/oxidant mixture, D_r and u_L are usually known, whereas τ_R (even if well defined) is not generally known.

Figure 2 (adapted from Abraham et al. 1985) shows the temperature and heat-release profiles through a stoichiometric propane-air flame at

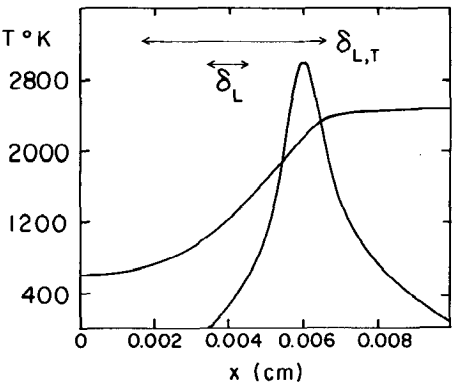

Figure 2 Temperature and heat-release (arbitrary scale) profiles for a propane-air laminar premixed flame, showing the thicknesses δ_L and $\delta_{L,T}$. Equivalence ratio = 1.0, reactant temperature = 600 K, pressure = 5 atm (after Abraham et al. 1985).

atmospheric pressure and an initial temperature of 600 K. In the preheat zone ($x < 0.004$ cm, say) the reaction rate is negligible, and so convection and diffusion are in balance. In the reaction zone (where heat release is significant), reaction and diffusion are the dominant processes.

The laminar-flame thickness can be defined in many ways. Abraham et al. (1985) compared seven definitions, of which we consider two. A natural definition is $\delta_{L,T}$—the distance between the positions of 5% and 95% temperature rise. For the flame considered, $\delta_{L,T}$ is 0.0046 cm. But the determination of $\delta_{L,T}$ requires that the temperature profile be known. From Equations (1–4), again on dimensional grounds, it follows that the flame thickness (however defined) scales with $(D\tau_R)^{1/2}$ or, equivalently, with $(D_r\tau_L)^{1/2} = D_r/u_L$. Hence, we use the definition

$$\delta_L \equiv D_r/u_L. \tag{6}$$

For the flame considered, δ_L is 0.0011 cm or $\delta_L \approx \frac{1}{4}\delta_{L,T}$.

Above all it should be realized that premixed laminar flames are very thin: In the flame considered, $\delta_{L,T}$ is about 1/20 mm. Away from stoichiometric conditions, or with lower initial temperatures, the thickness increases. But, on the other hand, the thickness is inversely proportional to the pressure and hence can be yet smaller in spark-ignition engines.

Compared with the rudimentary description given here, Peters (1986) provides a more detailed account of the internal structure of premixed laminar flames.

2.3 *Characterization of Turbulence*

It is natural to suppose that a premixed flame is strongly influenced by the turbulence into which it is propagating. Hence, we need to characterize the turbulence field in the reactants ahead of the flame. This we do below, and we use the results subsequently. But it should be borne in mind that there is a two-way interaction between the flame and the turbulence; and the turbulence within the flame may be substantially different from that ahead of it. Indeed it may be possible for a turbulent flame to propagate into nonturbulent reactants (Wright & Zukoski 1962, Sivashinsky 1979).

In the reactants ahead of the flame, the density ρ_r and kinematic viscosity ν are uniform. At any location, the principal characteristics of the turbulence are the turbulence intensity u' and the dissipation rate ε. Let $\mathbf{u}(\mathbf{x}, t)$ be the fluctuating component of velocity, and let angled brackets denote means. Then we have

$$u' \equiv (\langle u_i u_i \rangle/3)^{1/2} \tag{7}$$

and

$$\varepsilon \equiv \nu \left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right\rangle. \tag{8}$$

In terms of these quantities we can further define length and time macroscales

$$l \equiv u'^3/\varepsilon \quad \text{and} \quad \tau \equiv u'^2/\varepsilon = l/u', \tag{9}$$

the Taylor (length) microscale

$$\lambda \equiv (15\nu u'^2/\varepsilon)^{1/2}, \tag{10}$$

and the Kolmogorov length and time microscales

$$\eta \equiv (\nu^3/\varepsilon)^{1/4} \quad \text{and} \quad \tau_k \equiv (\nu/\varepsilon)^{1/2}. \tag{11}$$

While the approximate significance of these scales is well known, some care is needed in providing more precise interpretations of them. In moderate-Reynolds-number grid turbulence, the longitudinal integral scale L is simply proportional to l. [$L = 1.2l$ can be deduced from the data of Comte-Bellot & Corrsin (1971).] Since the energy-containing scales are not universal, the constant of proportionality depends on the way the turbulence is produced. The Taylor scale has no clear physical significance (Tennekes & Lumley 1972), although it has been ascribed a significance in some theories of turbulence (Tennekes 1968) and turbulent combustion (Chomiak 1976, Tabaczynski et al. 1980).

According to the Kolmogorov hypotheses (see Monin & Yaglom 1975) the smallest turbulent motions are of size of order η. In order to be more precise, we need to define precisely a length scale l_s that characterizes the size of the smallest motions. A reasonable definition is that l_s is the wavelength corresponding to the centroid of the dissipation spectrum. Then, using a standard model of the energy spectrum in high-Reynolds-number turbulence (Tennekes & Lumley 1972, Equation 8.4.6), we obtain

$$l_s \approx 13\eta. \tag{12}$$

Thus, accepting l_s as a measure of the smallest scales, we see that η underestimates by an order of magnitude the size of the smallest motions.

The inverse of the Kolmogorov time scale τ_k is the root-mean-square (rms) velocity gradient: From Equations (8) and (11) we have

$$\tau_k^{-1} = \left\langle \frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} \right\rangle^{1/2}. \tag{13}$$

Both the symmetric part of $\partial u_i/\partial x_j$ (the rate of strain) and the antisymmetric

part (the vorticity) contribute to the right-hand side of Equation (13). While there are velocity gradients on all scales, the dominant contributions are from the smallest scales. Below, we use τ_k^{-1} as a measure of the rate of strain. But it should be borne in mind that this is the rms: At high Reynolds numbers, in view of internal intermittency, much higher strain rates can occur.

While the Taylor microscale has no clear physical significance, the inverse time scale u'/λ is a measure of the rms strain rate. Indeed, from Equations (10–11) we have

$$u'/\lambda = \tau_k^{-1}/(15)^{1/2}. \tag{14}$$

3. TURBULENT PREMIXED-FLAME STRUCTURE

3.1 *Regimes of Combustion*

Different conditions can give rise to qualitatively different regimes of combustion in which different physical processes occur. Some understanding of these regimes is provided by a consideration of the most important dimensionless groups.

Two dimensional quantities are needed to give a basic description of the thermochemistry. We choose the laminar-flame time scale τ_L and the diffusivity D_r. Since the Prandtl number $\mathrm{Pr} \equiv \nu/D_r$ is generally close to unity and has little effect on the combustion, we can replace D_r with ν. For the turbulence in the reactants, a basic characterization is provided by u', l, and ν. From the four dimensional quantities τ_L, ν, u', and l, two dimensionless groups can be formed, though their choice is not unique. Bray (1980) chose u'/u_L and the Reynolds number $\mathrm{R}_l \equiv u'l/\nu$; Williams (1985b) chose u'/u_L and η/δ_L. (Note that u_L, δ_L, and η can be expressed in terms of the four dimensional quantities.) Here we follow McNutt (1981) and Abraham et al. (1985) in choosing the Reynolds number R_l and the Damköhler number

$$\mathrm{Da} \equiv \tau/\tau_L. \tag{15}$$

This Damköhler number is the ratio of the (large-scale) turbulent time scale to the laminar-flame time scale.

Before examining the significance of different values of R_l and Da, we note that other quantities may also be important. Among these are the density ratio ρ_r/ρ_p, the Lewis number Le, and of course the geometry of the flame. In addition, a given flame may behave differently at different locations and times. Some of these additional effects are illustrated in Section 3.2.

Figure 3 shows the Reynolds-number/Damköhler-number plane. Given R_l and Da, any other dimensionless group can be determined. The loci on the plane where various ratios are unity are shown on the figure: Each of these ratios increases with Da (at fixed R_l). The open symbols correspond to conditions in particular spark-ignition engine experiments, and the dashed rectangle encloses all engine operating conditions (Abraham et al. 1985). We restrict our attention to moderate and high Reynolds numbers.

In the flame-sheet regime, the smallest turbulent motions are larger than the laminar-flame thickness ($\eta > \delta_L$), and the time scale of turbulent straining is large compared with the laminar-flame time scale ($\tau_k > \tau_L$). This suggests that combustion can, indeed, occur in thin ($\sim\delta_L$) flame sheets. If, on the other hand, η were significantly less than δ_L, then turbulent motions within the reaction sheet could disrupt the convective-diffusive balance in the preheat zone. Or if τ_k were less than τ_L, the straining might extinguish the flame, as originally suggested by Karlovitz et al. (1953). Such considerations led Kovasznay (1956), Klimov (1963), and Williams (1976) to suggest $\tau_k/\tau_L = 1$ or equivalently $\eta/\delta_L = 1$ as the boundary of the flame-sheet regime. In fact, as Abraham et al. (1985) observed, $\eta/\delta_L > 1$ is certainly a sufficient condition for flame-sheet combustion, but it may not be necessary: This is discussed further in Section 3.2.

Williams (1985b) and Abraham et al. (1985) refer to this as the "reaction-sheet" regime, but the term "flame-sheet" seems preferable, since the preheat zone as well as the reaction zone is contained in the sheet. These

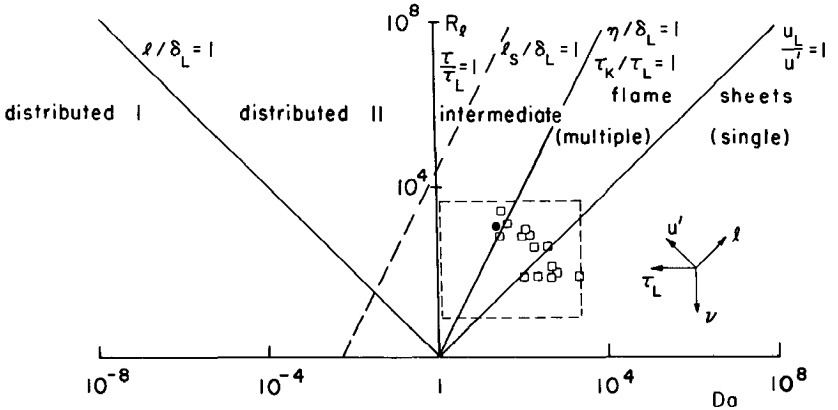

Figure 3 Reynolds-number/Damköhler-number plane, showing regimes of turbulent premixed combustion. Arrows indicate effect of changing one variable while holding the other three fixed. Hainsworth's (1985) experiment ●; engine experiments □ (from Abraham et al. 1985; rectangle encloses engine operating conditions).

authors also suggest a subdivision of the regime into single sheets ($u_L/u' > 1$) and multiple sheets ($u_L/u' < 1$).

At the other end of the Damköhler-number range there is distributed combustion. The criterion $l/\delta_L < 1$ proposed by Damköhler (1940) defines a region of distributed combustion, denoted "distributed I" on Figure 3. (This region is somewhat unnatural, in that for a turbulent flame to exist, the flow field must be much larger than the integral length scale and must endure for many time scales.) In this regime the structure of the flame is similar to that of the laminar flame, but with a turbulent viscosity ν_T (of order $u'l$) replacing ν. Hence the turbulent-flame speed u_T is of order $(\nu_T/\tau_L)^{1/2} \sim u'\mathrm{Da}^{1/2} \ll u'$; and the turbulent-flame thickness δ_T is of order $(\nu_T\tau_L)^{1/2} \sim l\mathrm{Da}^{-1/2} \gg l$. Note that the time scale δ_T/u_T is simply τ_L, which is greater than τ by a factor of $\mathrm{Da}^{-1} \gg 1$. As a consequence, fluctuations in thermochemical quantities (e.g. c) are very small: Their dissipation rate ($\sim\tau^{-1}$) is much greater than their production rate ($u'l/\delta_T^2$).

The above physical arguments used to justify the existence of distributed combustion rely only on the criteria $u_T \ll u'$ and $\delta_T \gg l$. These criteria are satisfied provided that $\mathrm{Da} \ll 1$. Hence, the region denoted "distributed II" on Figure 3 also corresponds to distributed combustion, and there is no transition across the line $l/\delta_L = 1$. McNutt (1981) made calculations, based on a modeled transport equation for the pdf of c, that support this extended region of distributed combustion: For all Damköhler numbers less than 0.1 the calculated turbulent-flame speed and thickness agree with Damköhler's theory, and the fluctuations in c are less than 1%.

About the remaining intermediate regime (defined by $0.1 < \mathrm{Da} < \mathrm{R}_l^{1/2}$), little is known with certainty. And as Williams (1985b) observes, there may be more than one regime of combustion within the region. One possibility is that (for $1 \ll \mathrm{Da} \ll \mathrm{R}_l^{1/2}$) there is a region of distributed preheating but localized reaction. This possibility is discussed further in Section 3.4.

3.2 *Flame-Sheet Regime*

There is little doubt that spark-ignition engines and most laboratory experiments operate in the flame-sheet regime. In order to study the fundamental processes in this regime and the types of theory that are applicable, we examine one flame in some detail.

Hainsworth (1985) performed an experiment on a statistically spherical methane-air flame propagating into (nominally) homogeneous isotropic turbulence. The experimental conditions are given in Table 1, and the corresponding (R_l, Da) point is plotted on Figure 3.

It is observed (by Schlieren photography) that the initial flame kernel is a smooth sphere of radius 1.5 mm. The subsequent evolution of the flame-

Table 1 Conditions at the time of ignition in Hainsworth's (1985) experiment[a]

$u' = 1.93$ m s^{-1}	$\tau = 4.23$ ms
$u_L = 0.29$ m s^{-1}	$\tau_k = 0.13$ ms
$l = 8.16$ mm	$\tau_L = 0.18$ ms
$\eta = 0.044$ mm	$R = 5.3$
$\delta_L = 0.052$ mm	$R_l = 1070$
	Da = 24

[a] Methane-air mixture, equivalence ratio 0.8, atmospheric temperature and pressure.

ball radius $R_f(t)$ is shown in Figure 4. For the first millisecond (about 7 Kolmogorov time scales) the rate of change of radius $\dot{R}_f$ is just the same as for a laminar flame ball, strongly suggesting that the flame sheet propagates at the laminar-flame speed and remains approximately spherical. While the flame ball as a whole is convected by the large-scale velocity fluctuations (of order $u' \approx 7u_L$), the structure of the flame is affected only by the turbulent motions of size $R_f(t)$ or less. It is these less energetic, smaller-scale motions that initially wrinkle the flame.

It is possible that the initial wrinkling of the surface is not due to turbulence, but instead is due to the thermal-diffusive instability

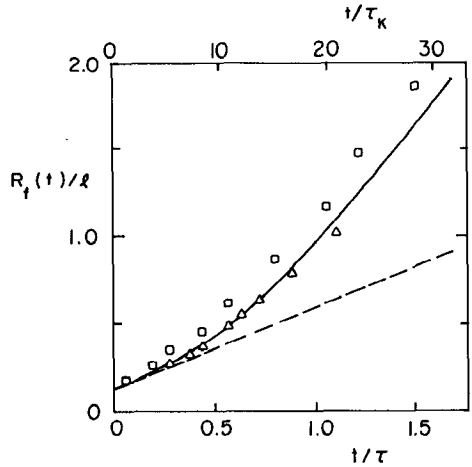

Figure 4 Flame-ball radius $R_f(t)$ versus time t. Solid line, pdf calculation (Pope & Cheng 1986); dashed line, laminar-flame-ball radius; symbols, two experimental realizations (Hainsworth 1985). Normalizing variables (l, τ, τ_k) are evaluated at $t = 0$.

(Strehlow 1968, Sivashinsky 1983). However, for most fuel-air mixtures, thermal-diffusive effects (Le $\neq 1$) are likely to be stabilizing (Abraham et al. 1985).

For some time the surface, although it is convected, bent, and strained by the turbulence, remains regular and singly connected. (This observation illustrates the limitations of representing regimes of combustion in terms of R_l and Da alone.) Several theoretical approaches have been based on the representation of the flame as a propagating surface. Most of these are *global* in that they attempt to describe the evolution of the surface as a whole (e.g. Matalon & Matkowsky 1982, Clavin & Williams 1979, 1982, Clavin 1985). Pope (1986) has developed a *local* description of propagating surfaces in which the evolution of surface-element properties is studied. These properties are the principal curvatures, principal directions, and fractional area increase of the surface element. In global theories, with a complete description of the surface, the effect of surface shape, etc., on the propagation speed w can be accounted for more accurately. But the simpler local description leads to a tractable probabilistic approach (Pope 1986). Neither approach has been used to make detailed calculations of turbulent flames. (The propagation speed w, which may vary over the surface, is defined relative to the reactants just ahead of the flame.)

In Hainsworth's (1985) experiment the reaction sheet propagates (initially) with the laminar-flame speed (i.e. $w = u_L$), even though the turbulent strain rates τ_k^{-1} are comparable to τ_L^{-1}. In other experiments (notably Fox & Weinberg 1962) it is found that the propagation speed is significantly different from u_L. Clearly, for theories based explicitly on reaction sheets it is essential to know the dependence of propagation speed on straining, curvature, and other relevant parameters.

In the reactants just ahead of a point on the flame, let γ be the rate of strain in the plane of the flame. Then $\gamma\tau_L$ is a nondimensional measure of the straining. Let H be the mean curvature of the surface, with H positive if the surface is concave to the reactants. Then $H\delta_L$ is a nondimensional measure of curvature. The fractional rate of area increase of the surface is called the flame stretch K (see Karlovitz et al. 1953, Matalon 1983, Chung & Law 1984). In terms of γ, H, and the propagation speed w, the flame stretch is (Pope 1986)

$$K = \gamma - 2Hw, \tag{16}$$

and a nondimensional measure of flame stretch is

$$\kappa \equiv K\tau_L. \tag{17}$$

The many analytical studies of laminar flames with strain and curvature have been reviewed by Clavin (1985) and Williams (1985b). A general

conclusion of these studies is that when both strain ($\gamma\tau_L$) and curvature ($H\delta_L$) are small (compared with unity), then the propagation speed is

$$w/u_L = 1 + A\kappa + O(\kappa^2), \tag{18}$$

where A (which is of order unity) depends on the thermochemistry. Experiments on strained laminar flames (Mendes-Lopes & Daneshyar 1985, Wu & Law 1984, Law et al. 1986) support this linear, order-one dependence on strain rate.

In the flame-sheet regime, since τ_k^{-1} is smaller than τ_L^{-1}, straining is generally weak, and it certainly is so in the regime of single sheets: It is generally assumed that the curvature is small also. In particular, Klimov (1975) assumes that the mean curvature H is of order η^{-1}, which is small compared with δ_L^{-1} (in this regime). If strain and curvature are small, then so also is κ, and to a good approximation the propagation speed is simply

$$w = u_L(1 + A\kappa). \tag{19}$$

This expression emerges from global theories of flame surfaces and can readily be incorporated in local theories.

The support for the assumption that the curvature ($H\delta_L$) is small is not clear. Even for the simpler case of a material surface, it has not been proved or demonstrated that the curvature is no greater than of order η^{-1}. The most that can be stated with confidence is that the curvature of a material surface cannot increase more than exponentially with time (Pope 1986). The principal curvature k_1 of a propagating surface increases at a rate wk_1^2 as a result of propagation. Hence, a singularity ($k_1 = \infty$), such as a cusp, can form in finite time. Schlieren photographs of some turbulent flames clearly show cusplike regions (Fox & Weinberg 1962, Keck 1982).

Returning to the statistically spherical flame, as time progresses the wrinkling increases, cusps are possibly formed, and eventually the flame sheet collides with itself. If the flow were two dimensional, then as the flame sheet collided with itself, an island of reactants would form. In three dimensions, contrary to some authors' assertions, islands do not form once a collision has taken place. Rather, just after the first collision, the reactants, the products, and the surface remain connected, but they are each doubly connected. Disconnected regions of reactants can form subsequently, but, in the absence of extinction, the products remain connected.

Given the geometric complexity of multiply connected flame sheets, it would be difficult to construct a quantitative theory based on the explicit representation of the flame surface.

In Hainsworth's (1985) flame, the initial turbulent-flame speed u_T is equal to the laminar-flame speed u_L and subsequently increases. But at large times, does the turbulent-flame speed depend on u_L? The observable

times in the experiment are too short to answer this question. In a different (double-kernel) experiment, at the highest Reynolds numbers measured ($R_l = 3000$–4000), Abdel-Gayed & Bradley (1981) observed $u_T \approx 2u'$ independent of u_L for u_L/u' as small as 1/35. Since in this regime combustion depends on the propagation of the flame sheet, can such a result (i.e. $u_T \approx 2u'$) be valid in the limit $(u_L/u') \to 0$? This important question was addressed by Klimov (1975), who obtained an expression of the form

$$u_T/u' \sim (u_L/u')^{0.3}, \tag{20}$$

which suggests that u_T/u' tends to zero in the limit.

Klimov's (1975) analysis pertains to notional turbulence of a single length and time scale. The above result stems from the claim that the time required for combustion to take place (τ_c) tends to infinity as u_L tends to zero. (We can define τ_c as the inverse of the mean reaction rate.) In fact, using the same physical arguments as Klimov but taking account of the different scales of turbulence, we now show that the appropriately normalized combustion time τ_c/τ is of order unity as u_L/u' tends to zero. First, we observe from the relations $u_L/u' = \mathrm{Da}/R_l$ and (in the flame-sheet regime) $R_l^{1/2} < \mathrm{Da} < R_l$ that the limit $(u_L/u') \to 0$ corresponds to $R_l \to \infty$.

For simplicity we consider a constant-density, statistically homogeneous flow. Initially ($t = 0$) the surface area of the flame sheet per unit volume, Σ_0, is of order l^{-1}. The effect of straining on the sheet is assumed to be the same as on a material surface—that is, the area increases exponentially with time on the Kolmogorov time scale (see Monin & Yaglom 1975). Hence the surface-to-volume ratio at time t is

$$\Sigma(t) = \Sigma_0 \exp(at/\tau_k), \tag{21}$$

where a is of order unity. Assuming that the propagation speed is $w = u_L$ and for the moment neglecting collisions of the surface, we find that the fraction of the volume burnt in time t is

$$B(t) = \int_0^t u_L \Sigma(t')\, dt' = \frac{u_L \Sigma_0 \tau_k}{a} [\exp(at/\tau_k) - 1]. \tag{22}$$

A characteristic combustion time τ_c' is obtained by solving the equation $B(\tau_c') = 1$:

$$\tau_c' = \frac{\tau_k}{a} \ln\left(1 + \frac{a}{\Sigma_0 \tau_k u_L}\right). \tag{23}$$

(This equation is the same as Klimov's Equation (3), with τ_k/a being his

time scale.) When nondimensionalized, Equation (23) becomes

$$\tau_c'/\tau = \frac{R_l^{-1/2}}{a} \ln(1 + aR_l Da^{-1/2}). \tag{24}$$

Given the inequality $R_l^{1/2} < Da < R_l$ in the flame-sheet regime, it may be seen that according to Equation (24), τ_c'/τ tends to zero as R_l tends to infinity.

This analysis is an oversimplification because of the neglect of collisions, which is equivalent to the assumption that the surface fills the space uniformly. While the rate of area increase scales with τ_k^{-1}, the rate of dispersion of the surface throughout the volume scales with τ^{-1} [note that $\tau^{-1} \ll (\tau_c')^{-1} \ll \tau_k^{-1}$]. This, then, is the rate-controlling process, and τ—not τ_c'—is the appropriate estimate of the mean reaction time τ_c.

The observation that τ_c/τ is of order unity is far from a proof that u_T/u' is independent of u_L/u' as R_l tends to infinity. It does, however, invalidate Klimov's (1975) claim that u_T must depend on u_L for $u_L/u' \ll 1$. Experiments have not provided a clear answer to the question. Klimov cites Russian experiments in support of Equation (20), while other experiments (e.g. Abdel-Gayed & Bradley 1981) suggest $u_T/u' \approx 2$, independent of u_L/u'. The more recent data of Abdel-Gayed et al. (1984) show that u_T/u' is constant for moderate values of u'/u_L but that it decreases for large values. However, this decrease is associated with the experimental conditions approaching the intermediate regime (τ_L/τ_k approaching unity).

We now examine in more detail the Klimov-Williams criterion $\delta_L/\eta < 1$ (or equivalently $\tau_L < \tau_k$) for flame-sheet combustion. As the boundary $\delta_L/\eta = 1$ is approached from the flame-sheet regime, the flame stretch κ becomes of order unity and Equation (19) is no longer valid. At this boundary, or perhaps further into the intermediate regime, two qualitative changes could also occur. First, the thermochemical fields in the flame sheets could cease to be essentially one dimensional (i.e. no longer varying appreciably only normal to the sheet) because of velocity variations (on a scale δ_L or less) within the flame. Second, because of large strain rates $\gamma\tau_L \gtrsim 1$, the flame sheet could be extinguished locally.

In Section 2.3 it was suggested that rather than η, the length scale $l_s \approx 13\eta$ more precisely measures the size of the small-scale motions. Thus $\delta_L/l_s = 1$ may be a better criterion for the breakdown of essentially one-dimensional flame sheets. (The line $l_s/\delta_L = 1$ is shown on Figure 3.) Several factors cloud the picture, however: Because of strain, the flame-sheet thickness may be less than δ_L; since the kinematic viscosity in the flame may be 10 times that of the reactants, even l_s may underestimate the size of the small-scale motions; and because of the intermittent nature of the small scales, some motions may be much smaller than l_s. At moderate

Reynolds number, the third point may not be important: The first two suggest that the breakdown of flame sheets occurs to the left of the line $l_s/\delta_L = 1$ on Figure 3.

It has long been speculated (Karlovitz et al. 1953) that extinction occurs when a flame sheet is strained sufficiently rapidly ($\gamma\tau_L > 1$). The evidence has to be examined carefully. One flow that has been extensively analyzed is an infinite, plane, strained laminar flame between semi-infinite bodies of reactants and products, the products being at the adiabatic flame temperature. The analyses—recently reviewed by Williams (1985b)—indicate that the flame cannot be extinguished by straining except if the Lewis number is unusually large. But these analyses are almost all based on one-step kinetics that may be inadequate to study extinction. Numerical calculations by Warnatz & Peters (1984) incorporating detailed kinetics show that a rich hydrogen-air flame (Le $\approx$ 3) can be extinguished, and the calculations of Rogg (reported by Peters 1986) based on a four-step scheme show that a stoichiometric methane-air flame can also be extinguished by straining.

A second relevant flow is a pair of infinite, plane laminar flames between two semi-infinite, counterflowing reactant streams. As the flow rate (and hence the strain rate) increases, the two flames move closer together. If the Lewis number is greater than unity, extinction can occur before the flames merge on the plane of symmetry: For Le $<$ 1, extinction occurs as the flames merge. Both analyses and experiments support this picture [see Williams (1985b) for references].

These observations suggest that straining can cause extinction locally in a turbulent flame sheet. There is also direct experimental evidence (Abdel-Gayed et al. 1984) that turbulent straining ($\gamma\tau_L \approx 1$) can cause global extinction of the flame. As theory suggests, flames with large Lewis numbers are most susceptible to extinction (Abdel-Gayed & Bradley 1985).

3.3 *Calculations of Flame-Sheet Combustion*

Standard turbulence models—mean-flow or second-order closures—experience severe difficulties when applied to premixed flames (except in the least important case Da $\ll$ 1). A major problem is that the mean reaction rate $\langle S(c)\rangle$ (recall Equations 1–4) cannot be approximated in terms of a few moments of c, because $S(c)$ is highly nonlinear (Figure 1).

Two approaches have proved more successful. The first is the Bray-Moss-Libby model, which is a second-order closure with special closure approximations appropriate to flame-sheet combustion. Libby (1985) provides a recent review of the model and calculations based on it. The second approach is the pdf method, in which a modeled transport equation is solved for the joint probability density function (pdf) of the velocities and

the reaction progress variable. Pope (1985) provides a comprehensive review of the theory and modeling involved in pdf methods.

The structure of thin, multiply connected flame sheets presents a challenge to any probabilistic field theory. In this section we describe how this challenge is met in pdf methods, first in the limit $R_l \to \infty$ (Pope & Anand 1984). Then the application of the pdf method to Hainsworth's (1985) flame is described (Pope & Cheng 1986). (Consideration of the effect of combustion on the turbulence is postponed to Section 4.)

Pope & Anand (1984) considered the idealized case of a statistically one-dimensional and stationary constant-density flame in nondecaying homogeneous turbulence. The appropriate joint pdf is $f(\mathbf{V}, C; x)$—the joint probability density of $\mathbf{u}(\mathbf{x}, t) = \mathbf{V}$, $c(\mathbf{x}, t) = C$ at $x_1 = x$, where $\mathbf{u}$ is the velocity fluctuation. The derivation, modeling, and solution of pdf transport equations are fully described by Pope (1985). Here we consider just the modeling concerned with flame sheets.

Pope & Anand (1984) considered "flamelet combustion" defined by $1 \ll R_l^{1/2} \ll Da \ll R_l$, which is essentially the case discussed at the end of the previous subsection (i.e. $R_l \to \infty$, $u_L/u' \to 0$). Since the flame sheets are thin ($\delta_L/\eta \ll 1$) and the straining is weak ($\tau_k^{-1}/\tau_L^{-1} \ll 1$), it is assumed that locally (i.e. on a scale δ_L) the flame-sheet structure is the same as that of a plane, unstrained laminar flame. [Implicitly, it is assumed that regions of high curvature ($H\delta_L \gtrsim 1$) and regions of flame-sheet collision account for a negligible fraction of the total sheet area.]

In the pdf method, the relevant term that has to be modeled is the conditional expectation of the right-hand side of Equation (1):

$$\hat{h}(C, \mathbf{x}, t) \equiv \langle \nabla \cdot (\rho D \nabla c) + \rho S | c(\mathbf{x}, t) = C \rangle. \tag{25}$$

As is now shown, the assumption made about the flamelet structure is sufficient to determine $\hat{h}$.

In a plane, unstrained laminar flame, the scalar quantity $[\nabla \cdot (\rho D \nabla c) + \rho S]$ is uniquely related to c (since c increases monotonically through the flame). That is, there is a function h (that can be determined from the laminar-flame solution) such that

$$[\nabla \cdot (\rho D \nabla c) + \rho S]_{c=C} = h(C). \tag{26}$$

The nondimensional function

$$h^*(C) \equiv \tau_L h(C), \tag{27}$$

obtained from the solution of Equations (1–4) (with constant ρ and D), is shown on Figure 1. With the assumption that the turbulent flamelets have

the laminar structure, we obtain simply

$$\hat{h}(C, \mathbf{x}, t) = h(C), \tag{28}$$

a known quantity. The striking conclusion is that with the flamelet assumption, the reaction and diffusion terms in the pdf equation are closed without ad hoc or empirical modeling assumptions.

Unfortunately, this closure is flawed because, for somewhat subtle reasons, the flamelet assumption is too strong. An examination of the resulting modeled pdf equation shows that if a fluid element is initially specified to be pure reactants ($c = 0$), it will never burn, irrespective of the state of the surrounding fluid. This problem arises because the flamelet assumption breaks down in the far preheat zone. At a distance $\Delta \gg \delta_L$ from the flamelet (on the reactants side), according to the laminar-flame assumption, the reaction progress variable and its gradient are

$$c = \exp(-\Delta/\delta_L) \tag{29}$$

and

$$|\nabla c| = \exp(-\Delta/\delta_L)/\delta_L. \tag{30}$$

From Equation (29) we see that the specification $c = 0$ implies that the fluid element in question is infinity far from a flamelet ($\Delta = \infty$) and hence will not burn in finite time. In fact, the fate of any fluid element is predetermined by its initial condition through the ordinary differential equation

$$\frac{dc}{dt} = h(c) \tag{31}$$

(see Pope 1985). Strictly, c is greater than zero at all finite distances from the flame, and hence the initial condition $c = 0$ is incorrect: But a model that requires initial and boundary conditions to be specified to such precision is not useful.

In the regime considered, δ_L is much smaller than η. Consequently, from Equation (30) it may be seen that at a distance η from a flamelet the gradient is small compared with η^{-1}. At such distances it is no longer reasonable to assume, therefore, that the progress-variable field is uniquely determined by the laminar-flame structure independent of the turbulence. To account for the additional effect of turbulent mixing remote from flamelets, Pope & Anand (1984) added a standard mixing model to the modeled pdf equation. This causes pure reactants ($c = 0$) to be preheated to some extent ($c > 0$) at a rate proportional to τ^{-1}.

Subsequent reaction takes place rapidly. Equation (31) can be rewritten

$$\tau \frac{dc}{dt} = \mathrm{Da}\, h^*(c), \tag{32}$$

where $h^*(c)$ (Figure 1) is of order unity. Once mixing has increased c just slightly ($c \gtrsim \mathrm{Da}^{-1} \ll 1$), reaction takes place ($c \to 1$) in a short time of order $\tau\ \mathrm{Da}^{-1}$. Consequently, there is only a small probability (of order Da^{-1}) of c adopting intermediate values ($\mathrm{Da}^{-1} < c < 1 - \mathrm{Da}^{-1}$). That is, to a good approximation, the pdf of c adopts a double-delta-function distribution, as assumed in the Bray-Moss-Libby model and as an inevitable consequence of the assumption that the flame sheets occupy a small fraction of the volume.

In summary, the virtues of the rigorous closure Equation (28) are eclipsed by the necessity to add a mixing model, which is rate controlling. The details of the function $h^*(c)$ are unimportant, since they only affect intermediate values of c that have negligible probability. Pope & Anand's (1984) result that the turbulent-flame speed scales with u' (specifically $u_T = 2.1u'$) is a direct consequence of the assumption that the mixing rate is proportional to τ^{-1} independent of u_L/u'.

Even though the rate-controlling combustion process is not modeled in a fundamental way, nevertheless the modeled joint pdf equation appears to yield solutions in accord with observations. For example, Pope & Cheng (1986) applied the method (with some refinements) to Hainsworth's (1985) statistically spherical flame. The flame radius R_f as a function of time is calculated quite accurately (see Figure 4). This is not an easy flow for a model to deal with: the initial flame radius (1.5 mm) is small compared with the turbulence scale ($l \approx 8$ mm), and initially the flame is convected a significant distance compared with its radius.

In Pope & Anand's analysis the laminar-flame speed is assumed to be small ($u_L/u' \ll 1$). Even though in Hainsworth's flame this ratio is quite small ($u_L/u' \approx 1/7$), nevertheless at early times laminar propagation is the dominant process. Pope & Cheng (1986) accounted for this in an ad hoc way. It may be possible to construct a better probabilistic model, valid for all u_L/u', based on local flame-surface properties (Pope 1986).

3.4 *Intermediate Regime*

For spark-ignition engines, it may be seen from Figure 3 that higher speeds (increased u') and leaner mixtures (increased τ_1) drive the combustion from the flame-sheet regime into the intermediate regime. Similarly, while a rod-stabilized V-flame may be in the flame-sheet regime, the higher velocities used in ducted stabilized flames may result in combustion in the intermediate regime.

There is no consensus on the nature of combustion in this regime, and indeed there may be several regimes. Here we discuss the idealized limiting case $1 \ll \mathrm{Da} \ll \mathrm{R}_l^{1/2}$.

The limit $1 \ll \mathrm{Da} \ll \mathrm{R}_l^{1/2}$ corresponds to high Reynolds numbers and conditions remote from both the distributed-reaction and flame-sheet regimes. We have the strong inequalities $u_L/u' \ll 1$, $\delta_L/\eta \gg 1$, and most importantly $\tau_\eta^{-1} \gg \tau_L^{-1} \gg \tau^{-1}$. That τ_L^{-1} is much greater than τ^{-1} suggests that reaction is not the rate-limiting process: that τ_η^{-1} is much greater than τ_L^{-1} suggests that on the small scales, turbulent straining—not reaction—causes the steepest gradients of the reaction progress variable c.

In this regime it is highly likely that the mean time for combustion τ_c scales with τ. One reason is that τ is the longest relevant time scale; another is that plausible models of distributed combustion (McNutt 1981) and of flame-sheet combustion (Pope & Anand 1984) yield $\tau_c \sim \tau$ as the intermediate regime is approached from each side.

It follows immediately from the scaling $\tau_c \sim \tau$ that reaction cannot be distributed but must be localized in space or time—or both. We can define a space-time point in the flame as "reactive" or not depending on whether the reaction rate is greater than one tenth (say) of the maximum reaction rate. Then the fraction F of space-time that is "reactive" is

$$F = \mathrm{Prob}\{S(c) > 0.1/\tau_R\}, \tag{33}$$

where $S(c)$ is the reaction rate with maximum value τ_R^{-1} (see Figure 1). The mean reaction rate τ_c^{-1} then scales as F/τ_R. (This assumes that the dominant contribution to the mean reaction comes from the "reactive" regions. An order-of-magnitude analysis of the pdf equation for c confirms the validity of this assumption.) The two scaling relations for τ_c combine to yield

$$F \sim 1/\mathrm{Da} \ll 1. \tag{34}$$

Reaction is not the rate-limiting process, since in reactive regions the reaction rate is larger than τ^{-1} by order Da. The rate-limiting process is the mixing process by which reactants ($c = 0$) are preheated to such an extent ($c \geq c_r$) that reaction becomes rapid [$S(c_r) = 10/\tau$, say].

The structure of combustion in this regime and the precise nature of the rate-limiting mixing process are unknown. It is likely that a satisfactory description must take account of the intermittent nature of the smaller turbulent scales (Klimov 1975). Possibly an important process is the turbulent mixing that occurs when a region of high dissipation rate intersects the boundary between regions of reactants and products. Since the local mixing rate (τ_η^{-1}) is large compared with the reaction rate (τ_R^{-1}), well-

mixed reactive regions (of unknown shape and size) can form and subsequently burn.

The idea that turbulent mixing is the rate-controlling process is central to the eddy breakup model of Spalding (1971). It is also an inevitable consequence of Pope & Anand's (1984) modeling of the joint pdf equation for this regime (which they, perhaps inappropriately, referred to as the distributed-combustion regime). In the pdf method, as in the flame-sheet regime, the relevant term to be modeled is the conditional expectation $\langle \nabla \cdot (\rho D \nabla c) + \rho S | c(\mathbf{x}, t) = C \rangle$. The part involving the reaction rate is in closed form [i.e. $\rho(C)S(C)$], while Pope & Anand argue that a standard mixing model that ignores the presence of reaction is appropriate to the first term, since (locally) mixing is rapid compared with reaction ($\tau_\eta^{-1} \gg \tau_R^{-1}$).

Pope & Anand's (1984) pdf calculations in this regime are for an idealized, one-dimensional, constant-density flame. Figure 5 shows $f_c(C)$, the calculated pdf of c at the location where $\langle c \rangle = 1/2$, for Da $= 10^4$. There are spikes (with probabilities 0.10 and 0.42) at zero and unity corresponding to pure reactants and products, respectively. Where the reaction rate $S(c)$ is large compared with τ^{-1} ($c_r = 0.55 < c < 0.99$) there is negligible probability. (In fact, here the pdf of c is of order [Da $S^*(C)]^{-1}$.) But where the reaction rate is relatively small ($c < 0.45$) there is significant probability of partially preheated reactants. Thus, unlike in the flame-sheet regime, the pdf of the reaction progress variable is not a double-delta function.

The value of c at which reaction becomes rapid, c_r, decreases weakly with Damköhler number. Consequently, as Da increases, the amount of preheating needed before reaction takes place decreases. For this reason, although turbulent mixing is the rate-controlling process, Pope & Anand (1984) found a weak dependence of the turbulent-flame speed on Da. Specifically, over the range studied ($1 \leq$ Da $\leq 10^4$) they obtained

$$u_T/u' = 0.25 + 1.25 \log_{10} \text{Da}. \tag{35}$$

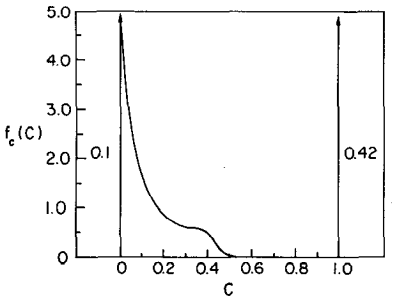

Figure 5 Progress variable pdf in the center of the flame ($\langle c \rangle = 1/2$). From joint pdf calculations (Pope & Anand 1984) in the intermediate regime for Da $= 10^4$.

The conclusions that there is significant probability of partially preheated reactants and that u_T/u' depends (albeit weakly) on Da rest on the details of the mixing model. They are, therefore, subject to confirmation.

4. EFFECTS OF COMBUSTION ON TURBULENCE

Combustion affects the turbulent velocity field through the large increases in specific volume and viscosity resulting (mainly) from the large temperature rise. Typically the ratios ρ_r/ρ_p and ν_p/ν_r are 7 and 10, respectively.

The main effects of the increase in viscosity with temperature are on the small scales of turbulence. At the moderate (cold) Reynolds numbers often encountered in turbulent premixed flames, these effects could be significant. With few exceptions (e.g. Wu et al. 1985) these effects have not been studied.

To an extent, the effects of density variations have been successfully accounted for both in the Bray-Moss-Libby model and in the pdf approach. As is described in the following subsection, the models yield countergradient diffusion and large turbulence-energy production in accord with experimental observations. But the neglect of the fluctuating pressure field (associated with density variations) is a weakness in the modeling. We return to this point in Section 4.2

4.1 *Countergradient Diffusion and Energy Production*

The original Bray-Moss model (Bray & Moss 1974, 1977) assumed gradient diffusion. But an improved version was developed by Libby & Bray (1981) and applied by Bray et al. (1981). The improved version, reviewed by Libby (1985), is a second-order closure that avoids gradient-diffusion assumptions, not only for the second moments, but for the third moments as well. An extension of the model from one-dimensional flames to the general case is presented by Bray et al. (1985).

The Bray-Moss-Libby model calculations of Bray et al. (1981) and Libby (1985) and the pdf calculations of Anand & Pope (1986) pertain to a statistically stationary and one-dimensional flame in the flame-sheet regime with $u_L/u' \ll 1$. The reactants and products have densities ρ_r and ρ_p, and their ratio $R \equiv \rho_r/\rho_p$ is the dominant parameter in the problem. In this regime the pdf of the reaction progress variable adopts a double-delta-function distribution—there is negligible probability of partial reactedness.

From the Euler equations

$$\frac{D\mathbf{U}}{Dt} = -\frac{1}{\rho}\nabla p, \tag{36}$$

it is readily seen that a given pressure gradient accelerates the light products more than the heavier reactants. This mechanism is responsible both for countergradient diffusion and for turbulent energy production. For a model to represent these processes accurately it must, therefore, take proper account of the effects of density variations on convection and on the pressure field.

In the velocity-composition joint pdf equation, the convective term is in closed form even in variable-density flows (Pope 1985). In second-order closures—such as the Bray-Moss-Libby model—this is not the case. But the closure problem is greatly alleviated by the use of density-weighted (or Favre) averaging (see, e.g., Libby & Williams 1980). For the reaction progress variable $c(\mathbf{x}, t)$, the Favre mean and fluctuation are

$$\tilde{c} \equiv \langle \rho c \rangle / \langle \rho \rangle \quad \text{and} \quad c'' \equiv c - \tilde{c}. \tag{37}$$

Libby (1985) neglects the effects of pressure fluctuations completely, while Anand & Pope (1986) retain a model appropriate to constant-density flow. (This modeled term is found to have little effect on the calculations.) Thus in both models it is the mean pressure gradient that is responsible for the differential acceleration of reactants and products. For a statistically stationary one-dimensional flame, the reactants flow into the flame at the turbulent-flame speed u_T. In view of mass conservation the products leave at speed $u_T \rho_r / \rho_p = R u_T$; and momentum conservation shows that there is a pressure drop of magnitude $\rho_r u_T^2 (R-1)$.

Figure 6 shows Anand & Pope's calculations of the turbulent flux of products $\widetilde{u''c''}$ plotted against $\tilde{c}$ (which of course increases monotonically with x—the distance through the flame). For the constant-density case ($R = 1$) it may be seen that this flux is negative everywhere, which indicates gradient diffusion (i.e. $\widetilde{u''c''}\, d\tilde{c}/dx < 0$). But for density ratios of 4 and above, the favorable pressure gradient preferentially accelerates the lighter products in the flow direction, thus yielding a positive flux of products nearly everywhere. At the cold boundary there is, of necessity, a region of gradient diffusion (Libby 1985).

According to the calculations for $R = 10$, the variance of the axial velocity $\widetilde{u''^2}$ increases by a factor of 17 through the flame, while the variances of the other two components increase by just 50%. Figure 7 shows the budget of $\langle \rho \rangle \widetilde{u''^2}$ through the flame. The large source, it may be seen, is due to the mean-pressure-gradient term $-2\langle u'' \rangle d\langle p \rangle / dx$. Since $\langle u'' \rangle$ is proportional to $\widetilde{u''c''}$ (Libby 1985), countergradient diffusion and energy production go hand in hand. At small density ratios ($R < 4$) there is gradient diffusion and the pressure-gradient term is a sink. For all density ratios the dilatation term $-2\langle \rho \rangle \widetilde{u''^2}\, d\tilde{U}/dx$ is a sink.

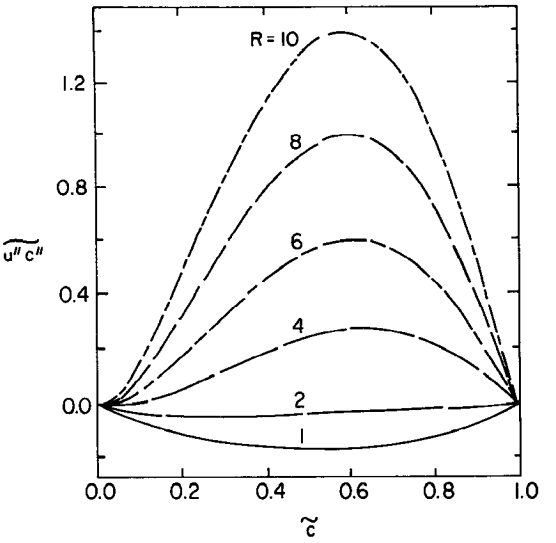

Figure 6 Scalar flux $\widetilde{u''c''}$ versus $\tilde{c}$ as a function of density ratio R. From joint pdf calculations (Anand & Pope 1986) in the flame-sheet regime. (Here u'' is normalized with the upstream turbulence intensity.)

Compared with the Bray-Moss-Libby model, the pdf method has the advantages that fewer processes have to be modeled and more information can be extracted from the solution. But for this flame, the two methods give similar results.

A statistically stationary and one-dimensional flame has not been realized experimentally, and so the calculations cannot be compared directly with data. Although it involves some uncertainty, Bray et al. (1981) and Libby (1985) compared their calculations with the data of Moss (1980) obtained in a conical flame. In general there is good agreement. But in order to provide an unambiguous, quantitative test of the modeling, more accurate data are needed, and the calculations should correspond more closely to the experimental configuration.

4.2 *Pressure Field in Flame-Sheet Combustion*

In turbulent combustion in general, our knowledge of the statistics of the pressure field and of their effect on the turbulence is slight. The experimental problems are severe: The pressure has to be measured on the smallest length and time scales of turbulence; and, rather than the pressure itself, its gradients and their correlation with the velocity are the prime quantities of importance. Though some progress has been made

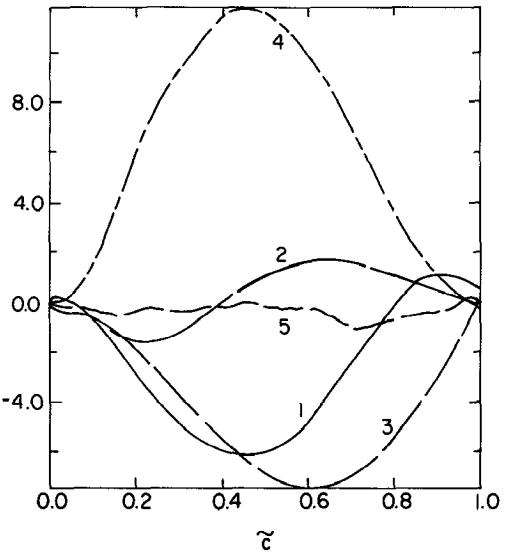

Figure 7 Budget of axial component $\langle\rho\rangle\widetilde{u''^2}$ of turbulence energy versus $\tilde{c}$. From joint pdf calculations (Anand & Pope 1986) in the flame-sheet regime for $R = 10$. (1) Convection: $-\langle\rho\rangle\tilde{U}\, d\widetilde{u''^2}/dx$; (2) diffusion: $-d(\langle\rho\rangle\widetilde{u''^3})/dx$; (3) dilatation: $-2\langle\rho\rangle\widetilde{u''^2}d\tilde{U}/dx$; (4) mean pressure gradient: $-2\langle u''\rangle d\langle p\rangle/dx$; (5) remainder: modeled redistribution term and statistical error. (All quantities are normalized with the upstream density, intensity, and length scale.)

(Komerath & Strahle 1983), accurate measurements of the velocity–pressure-gradient correlation are not in sight.

In constant-density flows, the usual theoretical approach is to relate one-point pressure statistics to two-point velocity statistics through the Poisson equation for pressure. But for variable-density reactive flows, the Poisson equation contains additional source terms that, in general, make this approach intractable. A different approach has been explored by Strahle (1982).

First, we present an argument that suggests that the neglect of pressure fluctuations in the model calculations is a serious omission. Then we show that because of the special structure of the density field in flame-sheet combustion, useful information can be obtained from the Poisson equation. Specifically, one-point pressure statistics can be related to two-point velocity-velocity and velocity–flame-front statistics.

A direct implication of the neglect of pressure fluctuations is that the pressure field accelerates an element of products more by a factor of $R = \rho_r/\rho_p$ than it accelerates an element of reactants (at the same position

and time but in a different realization). Simply, the instantaneous Euler equation becomes

$$D\mathbf{U}/Dt = -\rho^{-1}\nabla\langle p\rangle. \tag{38}$$

The differential acceleration results in countergradient diffusion and energy production in accord with experimental observations. But the factor of R is too large, since it ignores acceleration reaction[1] (see, e.g., Batchelor 1967). That is, an acceleration of the light products is accompanied by a proportionate acceleration of the displaced heavier reactants. Part of the work done by the applied force goes to accelerate the reactants, and hence the acceleration of the products is less than that implied by Equation (38).

The magnitude of the overestimate of the differential acceleration could be large. By analogy, consider Equation (38) applied to an initially stationary, spherical air bubble randomly located within a quiescent body of water. According to Equation (38) the bubble will accelerate vertically at the rate $g(R'-1)$, where g is the gravitational acceleration and $R' \approx 1000$ is the density ratio (water to air). But taking due account of acceleration reaction, we find that the true acceleration of the bubble is just $2g(R'-1)/(R'+2) \approx 2g$ (see Batchelor 1967).

Although the errors resulting from the neglect of pressure fluctuations may be large, the calculations reported in Section 4.1 appear to be in agreement with the data of Moss (1980). This apparent conflict emphasizes the need for more direct comparisons between model calculations and experimental data.

In the development of models for constant-density flows, the fluctuating pressure is eliminated by use of the Poisson equation $\nabla^2 p = -\rho(\partial U_i/\partial x_j)(\partial U_j/\partial x_i)$. This approach, introduced by Chou (1945), has been used to deduce both the form of pressure correlations and some exact results (see, e.g., Rotta 1951, Launder et al. 1975, Pope 1981). For a general variable-density turbulent reacting flow, the Poisson equation contains additional source terms that, to date, have nullified the usefulness of this approach. But for turbulent premixed flames in the flame-sheet regime, the density field has a special structure that allows the Poisson equation to be expressed in a useful form. This is demonstrated for a simple case.

Figure 8 shows a sketch of the flame sheet at an instant in an unbounded, statistically spherical turbulent flame, such as that of Hainsworth (1985). Provided that the flame-sheet thickness ($\sim\delta_L$) is much smaller than other relevant length scales, the flame sheet can be regarded as a mathematical surface separating constant-density regions of reactants and products (see, e.g., Markstein 1964, Matalon & Matkowsky 1982, Pope 1986). The flame

[1] I am indebted to Dr. J. C. R. Hunt for this observation.

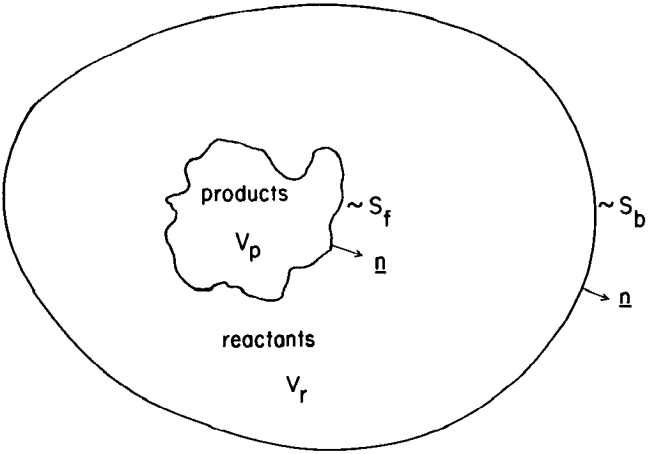

Figure 8 Sketch of closed flame sheet S_f.

surface S_f is assumed to be regular and has local normal $\mathbf{n}$ (pointing into the reactants) and propagates at the local speed w (in the direction of $\mathbf{n}$, relative to the reactants just ahead). Enclosed by the surface S_f is the volume V_p of constant-density (ρ_p) products. For mathematical convenience we define a closed surface S_b remote from S_f. Between S_f and S_b is the volume V_r of constant-density (ρ_r) reactants.

With this construction it follows from Green's third identity (Kellogg 1967, pp. 219–21) that the pressure at any point $\mathbf{x}$ in V_r or V_p can be decomposed into five contributions,

$$p(\mathbf{x}) = p_r(\mathbf{x}) + p_p(\mathbf{x}) + p_{fw}(\mathbf{x}) + p_{fa}(\mathbf{x}) + p_b(\mathbf{x}), \tag{39}$$

corresponding, respectively, to integrals over V_r, V_p, S_f, S_f, and S_b.

The first two integrals are

$$4\pi p_{r,p}(\mathbf{x}) = -\iiint_{V_{r,p}} r^{-1} \nabla^2 p \, dV = \rho_{r,p} \iiint_{V_{r,p}} r^{-1} \frac{\partial U_i}{\partial x_j} \frac{\partial U_j}{\partial x_i} \, dV, \tag{40}$$

where integration is over all points $\mathbf{y}$ in V_r or V_p, r is the distance $|\mathbf{y}-\mathbf{x}|$, and the integrands are evaluated at $\mathbf{y}$. The right-hand expression in Equation (40) follows from the momentum equation with the assumption of uniform density and Newtonian viscosity. These terms are familiar from constant-density studies.

The first integral over the flame surface is

$$4\pi p_{\mathrm{fw}}(\mathbf{x}) = \iint_{S_\mathrm{f}} [p] \frac{\partial r^{-1}}{\partial n}\, dS = \rho_\mathrm{r}(R-1) \iint_{S_\mathrm{f}} w^2 \frac{\partial r^{-1}}{\partial n}\, dS, \tag{41}$$

where integration is over all points $\mathbf{y}$ in S_f, square brackets denote the jump across the surface (reactant-side value minus product-side value), n is the coordinate in the direction of $\mathbf{n}$, and the integrands are evaluated at $\mathbf{y}$.

The right-hand expression in Equation (41) follows from the known jump conditions across the surface (Markstein 1964) with the neglect of viscous terms. Thus the contribution p_{fw} arises from the motion of the surface relative to the fluid. [For a material surface ($w = 0$), p_{fw} is zero.]

It is interesting to note that in the products, if w is constant ($w = u_\mathrm{L}$, say) then p_{fw} is a constant and hence causes no acceleration. Let $d\Omega$ be the solid angle subtended at $\mathbf{x}$ by the surface element dS at $\mathbf{y}$ and having the sign of $\mathbf{n}\cdot(\mathbf{y}-\mathbf{x})$. Then, from Equation (41) we obtain

$$p_{\mathrm{fw}}(\mathbf{x}) = -\frac{\rho_\mathrm{r}(R-1)}{4\pi} \iint_{S_\mathrm{f}} w^2\, d\Omega = -\rho_\mathrm{r}(R-1)\, u_\mathrm{L}^2, \tag{42}$$

the integral expression holding in general (Kellogg 1967, p. 67), the right-hand expression for points in V_p for the case $w = u_\mathrm{L}$.

The second contribution from S_f is

$$4\pi p_{\mathrm{fa}}(\mathbf{x}) = -\iint_{S_\mathrm{f}} \left[\frac{\partial p}{\partial n}\right] r^{-1}\, dS = \rho_\mathrm{r}(1-R^{-1}) \iint_{S_\mathrm{f}} r^{-1} a_n\, dS, \tag{43}$$

where again integration is over all points $\mathbf{y}$ in S_f and the integrands are evaluated at $\mathbf{y}$. The jump in $\partial p/\partial n$ is related to the acceleration of the surface (again neglecting viscous terms): a_n is the component of the acceleration of a surface point in the direction of $\mathbf{n}$.

The final contribution,

$$4\pi p_\mathrm{b}(\mathbf{x}) = \iint_{S_b} r^{-1} \frac{\partial p}{\partial n} - p \frac{\partial r^{-1}}{\partial n}\, dS, \tag{44}$$

need not be considered in detail, at least for unbounded flows. The surface S_b can be chosen to be remote from $\mathbf{x}$ (i.e. many integral scales away), and then p_b makes a negligible contribution to quantities of interest such as $\langle u_i'(\mathbf{x}) p(\mathbf{x})\rangle$. (This is because $\langle u_i'(\mathbf{x}) p(\mathbf{x}+\mathbf{r})\rangle$ and its derivatives are negligible at large $|\mathbf{r}|$.)

It may be seen then that for the case considered, a useful formal solution for the pressure $p(\mathbf{x})$ is obtained. One-point statistics of p and its derivatives can be expressed in terms of two-point statistics of the velocity field and of the flame surface. Beyond the case considered, the solution is valid for multiple, open or closed, nonintersecting surfaces (Kellogg 1967).

5. DISCUSSION AND CONCLUSION

Over the past 10 years significant progress has been made in the development of probabilistic field theories for turbulent premixed flames. Both the Bray-Moss-Libby model and the pdf approach are able to account for countergradient diffusion and energy production. As far as can be deduced from the imperfect comparison with experimental data, both approaches yield quantitatively plausible results. Nevertheless, there remain two major areas of uncertainty: the nature of combustion in the intermediate regime, and the effect of combustion-induced pressure fluctuations.

In spite of the advances over the past decade, our predictive abilities for turbulent premixed flames are modest and uncertain compared with our abilities for turbulent-diffusion flames. In 1975 models were capable of calculating, reasonably accurately, the basic features of simple jet diffusion flames (Lockwood & Naguib 1975, Kent & Bilger 1976). Now, for these simple flames, more refined calculations with multistep kinetics have been performed (e.g. Correa et al. 1984, Pope & Correa 1986, Jones & Kollmann 1986). And the basic model has been applied to the three-dimensional flow in a gas-turbine combustion chamber (Coupland & Priddin 1986).

From a theoretical viewpoint, turbulent diffusion flames are inherently simpler than premixed flames. But four other reasons can be identified for the relatively rapid progress for diffusion flames:

1. There is a simple canonical flow—a fuel jet in a coflowing airstream—for which there is a good data base (Bilger 1980).
2. Standard turbulence models (incorporating gradient diffusion) can be applied.
3. The boundary-layer approximations can be applied to mean equations.
4. Laser diagnostics have been extensively applied to the flows (e.g. Correa et al. 1984).

In contrast, for turbulent premixed flames, the canonical one-dimensional stationary flame considered in theories has not been realized in practice. Laser diagnostics are now being applied to premixed flames (e.g. Dandekar & Gouldin 1982, Cheng 1984, Gulati & Driscoll 1986a,b), but the configurations being studied have drawbacks. In particular, for stationary, unconfined, stabilized flames the boundary-layer approximations are not valid because of the rapid volume expansion. Thus the

computationally more demanding elliptic equations are appropriate. Nevertheless, because direct quantititative comparison of calculations with experiments is vital to the development of theories, it appears that model calculations of these (elliptic) flows is an unavoidable step toward significant progress. This conclusion is reinforced by the numerous recent experiments on these flames. To the same end, further experiments on the computationally simpler statistically spherical flames would be valuable.

The theories described here are in some ways quite limited: They apply only to homogeneously premixed reactants; different modeling is required in the flame-sheet and intermediate regimes; and without ad hoc modifications, they are valid only for $u_L/u' \ll 1$. Consequently, further developments are needed before the models can be used in some important applications—stratified-charge spark-ignition engines, for example.

As in the past, it can be expected that laminar-flame analyses and experiments will contribute to our understanding of flame-sheet turbulence. It can also be expected that Full Turbulence Simulations (Rogallo & Moin 1984) will play an expanding role in elucidating the structure and mechanisms of combustion in both the flame-sheet and intermediate regimes.

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