The Influence of Lewis number and nonhomogeneous mixture on premixed turbulent flame structure

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The structure of a premixed flame front in two-dimensional turbulence is investigated using full numerical simulation including heat release, variable fluid properties, and one-step Arrhenius chemistry. Non-unity Lewis number (Le) effects are described by comparing the local instantaneous turbulent flame structure to the steady one-dimensional laminar flame structure for the same thermochemical parameters. Flame surface area, mean reactant consumption rate per unit area of flame (mean "flamelet speed"), turbulent flame speed, and statistical descriptions of the flame geometry (pdf’s of curvature and strain) also are reported. Principal findings are that the local flame structure correlates strongly with the local flame curvature, while global properties (e.g., turbulent flame speed) depend both on strain and on curvature.

Preliminary results for cases with nonhomogeneous reactant mixture strength are reported. Here the emphasis is on the ability of a propagating flame to recover after encountering a fuel-lean pocket in an otherwise homogeneous mixture. Both one-dimensional and two-dimensional cases are described.

1. Introduction

The structure of premixed flames in turbulent flows is an important fundamental and practical question in turbulent combustion. In applications such as reciprocating internal combustion engines, accurate modeling of turbulent premixed combustion is an essential step in formulating truly predictive multidimensional models that can be used to study in-cylinder processes and optimize engine designs.

Because flame structure information is difficult to obtain experimentally, numerical simulations have become an important tool in complementing experimental investigations of turbulent combustion. For the foreseeable future, numerical simulation of the full three-dimensional governing partial differential equations with variable density and transport properties and complex chemistry will remain intractable; thus various levels of simplification will remain necessary. On one hand, the requirement to simplify is not necessarily a handicap: numerical simulations allow the researcher a degree of control in isolating specific physical phenomena that is inaccessible in experiments. For example, one can "turn off" heat release to study...
the influence of turbulence on chemical reaction without the confounding effects of chemistry on the flow field through density and fluid property variations. On the other hand, the highly coupled nonlinear nature of the governing partial differential equations demands that one remains wary when extrapolating results obtained in such idealized modeled systems to practical turbulent premixed flames. A judicious balance of experiment and computation remains the most fruitful approach.

In the present study, the modeled system includes heat release, variable fluid properties, and simple chemistry in two-dimensional turbulence. While it is recognized that two-dimensional turbulence differs from three-dimensional turbulence (e.g., Herring et al., 1974; Lesieur, 1987), it is our feeling that the response of the physical flame structure to straining and curvature should be generic, even if detailed statistical correlations (especially of small-scale quantities) differ quantitatively from what would be found in three dimensions. Restricting the simulations to two dimensions also permits a wider dynamic range of scales to be computed, so that, for example, higher turbulence Reynolds numbers can be simulated while still resolving the flame structure. In any case, the present results can be compared with three-dimensional constant-density computations (e.g., Pope et al., 1989; Rutland, 1989; Yeung et al., 1990; Cant et al., 1990; Rutland & Trouvé, 1990) to better understand the limitations and similarities of the two approaches.

If chemical times are short enough compared to turbulence times, the flame zone is "thin" and may be treated, in the limit, as an interface separating fresh unburnt reactants from hot burnt products. This mode of combustion is called the flamelet regime. It has been invoked widely as a framework for the construction of turbulent combustion models (e.g., Bray & Libby, 1986; Candel et al., 1988; Pope & Cheng, 1988; Cant & Bray, 1988; El Tahry, 1990). Of primary importance for flamelet models are two quantities: 1) the total flame surface (the area of the interface between fresh and burnt gases); and, 2) the local structure of the individual flamelets. Although these flame elements are thin, their internal structure may be influenced by the flow characteristics and may have an influence on the global consumption rate of reactants.

The objective of this work is to investigate the dependence of these two quantities on the Lewis number $Le$ (ratio of thermal to species diffusivities) and on the spatial distribution of reactant mass fraction. The Lewis number has been identified in asymptotic analyses of laminar flames as an important parameter influencing premixed flame structure and stability; we wish to assess its importance in determining the local and global structure of turbulent flames. Nonhomogeneous combustion is an important mode of burning in practical devices including direct-injection or stratified-charge internal combustion engines. There is, however, relatively little analysis or experimental results to guide the modeling of this mode of combustion with turbulence. Most of the discussion will focus on Lewis number effects; only preliminary results for nonhomogeneous cases will be given.
2. Numerical method

We consider a compressible viscous reacting flow. The chemical reaction is represented by a single–step mechanism,

\[ R \ (\text{reactants}) \rightarrow P \ (\text{products}), \]

and the reaction rate \( \dot{w}_R \) is expressed as,

\[ \dot{w}_R = B \rho Y_R \exp \left( \frac{-T_a}{T} \right). \]

This can be interpreted as a binary reaction where one of the reactants \( (Y_R) \) is always deficient. It is convenient to follow Williams (1985) and cast this expression in the form,

\[ \dot{w}_R = B \rho Y_R \exp \left( \frac{-\beta(1-\Theta)}{1-\alpha(1-\Theta)} \right). \]

Here \( \Theta \) is the reduced temperature, \( \Theta = (T - T_1)/(T_2 - T_1) \), where \( T_1 \) is the fresh gas temperature and \( T_2 \) is the adiabatic flame temperature for unity Lewis number. The activation energy is \( T_a \), and the coefficients \( B, \alpha, \) and \( \beta \) are, respectively, the reduced pre-exponential factor, the temperature factor and the reduced activation energy,

\[ B = B \exp(-\beta/\alpha), \quad \alpha = (T_2 - T_1)/T_2, \quad \text{and} \quad \beta = \alpha T_a/T_2. \]

The mass fraction of the reactants \( Y_R \) may be conveniently nondimensionalized by the initial mass fraction of reactants \( Y_R^0 \) in the fresh gases, \( \tilde{Y} = Y_R/Y_R^0 \), so that \( \tilde{Y} \) varies from 1 in the fresh gases to 0 in the burnt gases. Fluid properties follow the equations of state,

\[ \rho = \rho_1(pT_1/p_1T), \quad \mu = \mu_1(T/T_1)^b, \]

\[ Le = \lambda/\rho Dc_p = \text{constant}, \quad Pr = \mu c_p/\lambda = \text{constant}, \]

where \( \mu, \lambda, \) and \( D \) are molecular diffusivities of momentum, internal energy, and species, respectively. Here a subscript 1 refers to reference properties in the fresh gases. Heat losses can be included in the energy equation: a dimensionless heat loss coefficient \( c \) expresses the magnitude of the heat loss (Poinsoet et al., 1990). For the homogeneous runs, \( c = 0 \) (adiabatic).

Using these assumptions and a Cartesian frame of reference, the conservation equations for compressible flows are solved using a high–order finite difference scheme. The numerical accuracy is sixth–order in space and third–order in time (Lele, 1990). Spatial derivatives are computed using a compact scheme and the time advancement is produced by a minimal–storage third–order Runge–Kutta method (Wray, 1990). Boundary conditions are specified using the NSCBC method (Poinso
Details concerning the system of equations solved and the numerical methods can be found in these papers. Typical grids contain 160000 points.

A schematic of the computational configuration is given in Figure 1. The calculations are initialized with reactants on one side of the computational domain and products on the other; these are separated by a laminar premixed flame. The initial velocity field (turbulence spectrum) and spatial distribution of reactant mass fraction is specified at $t = 0$: the system is then allowed to evolve in time. The initially planar flame is convected and strained by the turbulence while the combustion influences the fluid mechanics through dilatation and temperature-dependent properties (Eq. 5). Typical contours of temperature, reactant mass fraction, reaction rate, and vorticity are shown in Figure 2 for a homogeneous reactant, $Le = 1.2$ case. There it can be seen that the initially planar flame has been strongly distorted and stretched by the turbulence. There is very little vorticity behind the flame in the hot products: the high viscosity there (Eq. 5) suppresses most turbulent velocity fluctuations.

Relevant dimensionless parameters in the homogeneous reactant simulations are:
- ratio of rms turbulence intensity $u'$ to the undisturbed laminar flame speed $s^0_l$;
- ratio of turbulence integral length scale $l$ to laminar flame thickness $\delta_{l1}$, where $\delta_{l1} = (T_2 - T_1)/(dT/dx)_{\text{max}}$;
- turbulence Reynolds number $Re_t = u'l/\nu$;
- ratio of turbulence time scale $\tau = l/u'$ to flame time scale $\tau_f = \delta_{l1}/s^0_l$;
- strain Karlovitz number $K a_{st} \equiv \langle s_t \rangle \cdot \tau_f$, where $\langle s_t \rangle$ is the area-averaged mean strain rate tangent to the flame;
- ratio of turbulence micro-length-scale $l_\eta$ to laminar flame thickness $\delta_{l1}$; and,
- ratio of turbulence micro-time-scale $\tau_\eta$ to flame time scale $\tau_f$.

The values of these parameters as functions of time for three cases are given in Table I ($\tau_0$ is the initial value of the turbulence time scale $\tau$). Table II contains the fixed parameters for the homogeneous reactants cases. Initial turbulence specification is (statistically) the same for all three cases in Table I; runs made with
different initial spectra have been made, but are not reported here.

The microscales $l_\eta$ and $\tau_\eta$ are based on the dissipation rate of enstrophy; presumably, this is the most appropriate definition of the scales of the smallest motions in two-dimensional turbulence (Herring et al., 1974; Lesieur, 1987). The enstrophy $\Omega$ (mean-square vorticity) and its dissipation rate $\eta$ are given by,

$$\Omega = .5 \left| \nabla \times \mathbf{v} \right|^2, \quad (6)$$

$$\eta = \nu \left| \nabla \times (\nabla \times \mathbf{v}) \right|^2, \quad (7)$$
where the overbar denotes a spatial average. The ratios of the enstrophy-based microscales \( l_\eta = (\nu^3/\eta)^{1/6}, \tau_\eta = \eta^{-1/3} \), to the more conventional Kolmogorov microscales appropriate for three-dimensional turbulence \( l_k = (\nu^3/\epsilon)^{1/4}, \tau_k = (\nu/\epsilon)^{1/2} \), where \( \epsilon \) is the dissipation rate of turbulence kinetic energy) are also given in Table I. There it can be seen that the length microscales differ by 50%-60%, while the time microscales differ by up to nearly a factor of three. It should be noted that all turbulence scales \( (u', l, \tau, l_\eta, \tau_\eta, l_k, \text{and} \tau_k) \) are volume-averaged mean quantities conditional on being in the fresh gases in front of the flame.

Table I. Dimensionless parameters for three homogeneous mixture cases.

First row for each Lewis number is the initial condition \((t = 0)\), second row is at normalized time \( t/\tau_0 \approx 1.8 \).

<table>
<thead>
<tr>
<th>( Le )</th>
<th>( t/\tau_0 )</th>
<th>( u'/s_1^0 )</th>
<th>( l/\delta_{11} )</th>
<th>( Re_i )</th>
<th>( \tau/\tau_f )</th>
<th>( \text{Kao}_{st} )</th>
<th>( \eta/\delta_{11} )</th>
<th>( \tau_\eta/\tau_f )</th>
<th>( l_\eta/l_k )</th>
<th>( \eta/\tau_k )</th>
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<tr>
<td>0.8</td>
<td>0.00</td>
<td>6.44</td>
<td>2.57</td>
<td>81</td>
<td>0.40</td>
<td>0.00</td>
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<td></td>
<td>1.83</td>
<td>4.82</td>
<td>5.29</td>
<td>126</td>
<td>1.10</td>
<td>1.47</td>
<td>0.24</td>
<td>0.28</td>
<td>1.49</td>
<td>2.23</td>
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<td>6.11</td>
<td>2.68</td>
<td>81</td>
<td>0.44</td>
<td>0.00</td>
<td>0.20</td>
<td>0.20</td>
<td>1.64</td>
<td>2.69</td>
</tr>
<tr>
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<td>4.68</td>
<td>5.80</td>
<td>132</td>
<td>1.24</td>
<td>1.25</td>
<td>0.25</td>
<td>0.30</td>
<td>1.48</td>
<td>2.20</td>
</tr>
<tr>
<td>1.2</td>
<td>0.00</td>
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<td>2.91</td>
<td>77</td>
<td>0.52</td>
<td>0.00</td>
<td>0.22</td>
<td>0.23</td>
<td>1.64</td>
<td>2.68</td>
</tr>
<tr>
<td></td>
<td>1.84</td>
<td>4.32</td>
<td>6.46</td>
<td>124</td>
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<td>1.09</td>
<td>0.27</td>
<td>0.37</td>
<td>1.48</td>
<td>2.34</td>
</tr>
</tbody>
</table>

Table II. Fixed parameters for homogeneous reactant cases.

<table>
<thead>
<tr>
<th>( \alpha )</th>
<th>( \beta )</th>
<th>( \Lambda )</th>
<th>( b )</th>
<th>( Pr )</th>
<th>( c )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.75</td>
<td>8.00</td>
<td>146.</td>
<td>0.76</td>
<td>0.75</td>
<td>0.00</td>
</tr>
</tbody>
</table>

3. Diagnostics

For homogeneous cases, postprocessing of the two-dimensional computed fields (snapshots at fixed times) begins by defining a flame front as an isocontour of either temperature \( T \) or of reactant mass fraction \( Y_R \). The choice of dependent variable and the value of isocontour selected to identify the flame have been seen to have little influence on the results. Unless otherwise specified, the \( Y_R = 0.3 \) isocontour has been used to define the flame in the results that follow; this contour lies slightly in front of the reaction zone towards the fresh gases.
Once the flame front has been located, the local normal and local flame curvature are readily computed: curvatures concave towards the hot products are assigned positive values. One-dimensional cuts normal to the flame are taken; it is these profiles that define the local "structure" of the turbulent flame. We compare the local turbulent flame profiles with the steady one-dimensional laminar flame profile for the same chemistry and fluid properties. Of particular interest is the distribution along the flame of the normalized local flame speed ("flamelet speed") \( s_n \) defined by,

\[
s_n = \int \dot{w} \, dn / s^0_f,
\]

that is, the integral of the reaction rate profile in a direction locally normal to the isocontour defining the turbulent flame, normalized by the undisturbed laminar flame speed. If the local turbulent reaction rate profile is identical to that of an undisturbed laminar flame, then \( s_n = 1 \). The isocontour curvature and the components of the strain rate normal to \( (\nabla_n \cdot \dot{\gamma}) \) and tangent to \( (\nabla_t \cdot \dot{\gamma}) \) the flame contour are also computed along the flame front. Area-weighted (arc-length-weighted in two dimensions) statistics of \( s_n \), curvature, and components of the strain rate are calculated. The mean consumption rate of reactants per unit area of flame surface ("mean flamelet speed"), normalized by the laminar flame value, is computed as,

\[
\langle s_n \rangle = \int s_n \, dA / \int dA.
\]

For nonhomogeneous reactant cases, appropriate diagnostics are still being developed.

4. Non-unity Lewis number effects in turbulent premixed flames

Results for \( Le = 0.8, 1.0, \) and \( 1.2 \) are reported (see Table I). We begin in Section 4.1 with a brief review of analytic and earlier computational results for nonunity Lewis numbers in premixed flames. Next, we describe the local flame structures found in the present simulations. In Section 4.3, global quantities of interest are discussed. And finally, in Section 4.4, statistics of flame front curvature and strain rate are given; these are compared with results obtained in three-dimensional uniform-property simulations.

4.1. Review of Lewis number influence in premixed flames

Textbook discussions of thermodiffusive effects for premixed flames with nonunity Lewis numbers reveal the following behavior (e.g., Williams, 1985). For \( Le = 1 \) (and subject to other assumptions consistent with those made here in Section 2), only one of \( Y_R \) or \( T \) is independent (\( \bar{Y} + \theta = 1 \) everywhere), and the reaction rate is a unique function of the reactant mass fraction or temperature. Flame curvature is not expected to influence the local flame structure. Straining can thin the flame (for positive, or extensive, straining in the tangent plane) or thicken the flame (for negative, or compressive, straining in the tangent plane), but the maximum reaction rate remains unaffected. Thus the local flamelet speed (Eq. 8) is expected
to (slightly) decrease/increase for a flame element subjected to positive/negative tangential strain.

For Lewis numbers other than unity, differential diffusion between heat and species leads to richer possibilities in flame structure. In particular, flame front curvature influences the local burning rate. For \( Le > 1 \), elements of flame surface that are concave towards the reactants are expected to burn faster, while elements that are concave towards the products are expected to have a lower burning rate compared to that of a planar flame. Positive (extensive) tangential strain will decrease the flamelet speed relative to that of an undisturbed laminar flame for \( Le > 1 \). On the other hand, Lewis numbers less than unity are expected to display the opposite behavior: lower burning rate for elements concave towards reactants; higher burning rates for elements concave towards products; and, increasing flamelet speed with extensive strain.

Ashurst et al. (1987) reported two-dimensional numerical simulations of premixed flames with nonunity Lewis numbers in the limit of zero heat release. The thermodiffusive effects described above for nonunity Lewis number were observed in their simulations. Results were expressed in terms of the excess enthalpy relative to an undisturbed laminar flame; a correlation between strain rate and excess enthalpy was reported. Here, we calculate cases with higher turbulence intensity (Table I), variable properties, and heat release. The local flame structure is found to correlate more strongly with the local flame curvature than with strain rate, while global flame behavior depends on both strain and curvature.

### 4.2. Simulation results: local flame structure

The local flame structure, as illustrated through one-dimensional cuts of reaction rate, is shown in Figure 3 for each of the three Lewis numbers simulated. There, it is clear that the local flame structure is everywhere nearly identical to that of an undisturbed laminar flame for \( Le = 1 \) (Figure 3b), while for nonunity Lewis numbers, there is no collapse of the local turbulent flame profiles onto the one-dimensional undisturbed laminar flame profile (Figures 3a and 3c). From the discussion given in Section 4.1 above and the sample reaction rate contours shown in Figure 2, we expect to see a correlation between local flame curvature and the local flamelet speed; indeed, this is the case. Figures 4a, 4b, and 4c illustrate this correlation for each of the three Lewis numbers computed. For \( Le = 0.8 \) (Figure 4a), flame elements concave towards reactants tend to have lower local flamelet speeds, and conversely for elements concave towards products; for \( Le = 1.0 \) (Figure 4b), there is no apparent correlation between local curvature and local flame structure; and, for \( Le = 1.2 \) (Figure 4c), the correlation is opposite to that shown in Figure 4a.

If instead, we attempt to correlate the local flamelet speed in the turbulent flame with the strain rate tangent to the flame, then the scatter plots of Figure 5 result. There is no apparent systematic correlation evident for the nonunity Lewis number cases. For \( Le = 1 \), a small negative slope can be seen. This presumably is a reflection of flame thickening/thinning resulting from compressive/extensive tangential straining. The strain Karlovitz number \( Ka_{st} \) at this time is greater than unity (Table I) so that it is reasonable to expect that turbulent straining could affect the
Lewis number and nonhomogeneous mixture

FIGURE 3. Local reaction rate profiles normal to the turbulent flame (lines) and laminar reaction rate profile (symbols) for three Lewis numbers at normalized time $t/r_0 = 1.8$: a) $Le = 0.8$; b) $Le = 1.0$; c) $Le = 1.2$.

4.3. Simulation results: global quantities

The mean reaction rate along the turbulent flame (mean flamelet speed) and the flame surface area are quantities of interest in constructing flamelet models for turbulent premixed combustion. In Figure 6, probability density functions (pdf’s) of the normalized local flamelet speed in the turbulent flame are shown for each of the three Lewis numbers at time $t/r_0 = 1.8$. For nonunity Lewis numbers, it can be seen that the pdf of flamelet speed is broadened and shifted relative to $Le = 1.0$. The unity Lewis number case shows a small spread about the undisturbed laminar flame speed, presumably reflecting the influence of tangential strain. The area–averaged mean flamelet speeds, referred to that of an undisturbed laminar flame at the same Lewis number, are $1.14$ ($Le = 0.8$); $1.00$ ($Le = 1.0$); and, $0.86$ ($Le = 1.2$).

Figure 7 illustrates the Lewis number effects in a different way. There, the variation with time of the turbulent flame speed (computed from the volume–averaged mean reaction rate over the entire two–dimensional computational domain), normalized by the laminar flame speed, is shown for each of the three cases. Superimposed on this is the flame area (or length, in two dimensions), normalized by the initially planar flame length. The turbulent flame speed is (normalizations aside) the product of the mean flamelet speed and the flame area. The interesting finding is that
the turbulent flame speed increases more rapidly than the flame area for $Le = 0.8$; that for $Le = 1.0$, these two quantities evolve identically; and, that for $Le = 1.2$, the flame surface increase exceeds the turbulent flame speed augmentation. Figure 7d repeats the turbulent flame speed curves for the three Lewis numbers to emphasize the decrease in turbulent flame speed with increasing Lewis number.

Comparison of Figures 7a–7c reveals that, for $Le = 0.8$, the turbulence creates more flame surface than for $Le = 1.0$. This results from the interaction between flame curvature and thermodiffusive effects for nonunity Lewis numbers. Thus the higher turbulent flame speed relative to flame area for $Le = 0.8$ can be seen to result from two complementary effects: more flame surface, plus higher mean flamelet speed (Figure 6). Similarly, for $Le = 1.2$, the lower turbulent flame speed is a consequence of less flame area being generated, coupled with a lower mean flamelet speed.

4.4. Simulation results: flame curvature and strain rate

Typical pdf's of flame curvature (normalized by the laminar flame thickness $\delta_{11}$) are shown in Figure 8. It may be seen that the pdf is nearly symmetric, with a mean value near zero, and with few curvatures exceeding one over the laminar flame thickness. The smallest radii of curvature are equal to about one-half of $\delta_{11}$. The
Lewis number and nonhomogeneous mixture

Figure 5. Scatter plots of normalized local flamelet speed in the turbulent flame (Eq. 8) versus local flame tangential strain rate (normalized by the laminar flame timescale $\tau_f = \delta t / \delta^0$) for three Lewis numbers at normalized time $t/\tau_0 = 1.8$: a) $Le = 0.8$; b) $Le = 1.0$; c) $Le = 1.2$.

Near symmetry of the pdf suggests that the differences in mean flamelet speed with Lewis number seen in Figure 6 are primarily attributable to strain.

For simulations with heat release and variable properties, it is important to distinguish between the normal and tangential components of the strain rate on the flame. Here the normal component is dominated by the velocity divergence through the flame resulting from the change in fluid density. Pdf's of tangential strain rate are given in Figure 9. There it can be seen that extensive strain rates are dominant—that is, the flame aligns preferentially with extensive strains; there is no apparent systematic dependence on $Le$. This is again consistent with the notion that the differences in normalized mean flamelet speeds for the three Lewis numbers is principally a strain effect. The dominance of extensive strain rates is also seen in three-dimensional simulations (Yeung et al., 1990—for material surfaces; Rutland, 1989; Cant et al., 1990; Rutland & Trouvé, 1990). The mean tangential strain rate in Figure 9 has been scaled with the flame time $\tau_f$ to emphasize interactions between chemistry and turbulence. If, instead, we scale the mean tangential strain rate with the enstrophy micro–time–scale $\tau_\eta$ as,

$$\langle \nabla_t \cdot \vec{v} \rangle = C_\eta / \tau_\eta,$$

then it is found that the value of $C_\eta$ varies from a zero value at the beginning of
FIGURE 6. Pdf's of normalized local flamelet speed $s_n$ (Eq. 8) for three Lewis numbers at normalized time $t/\tau_0 = 1.8$.

FIGURE 7. Normalized turbulent flame speed (lines) and flame area (symbols) for three Lewis numbers as a function of time. Both quantities are normalized by their $t = 0$ values: a) $Le = 0.8$; b) $Le = 1.0$; c) $Le = 1.2$; d) turbulent flame speeds for all three Lewis numbers.
5. Nonhomogeneous reactants

As a first step towards understanding and modeling the behavior of turbulent flames in nonuniform mixtures, we have modeled the case of a laminar flame propagating through a "hole" or pocket of lean ($Y_R = 0$) reactants in an otherwise homogeneous ($Y_R = 1$) mixture. We first briefly review related previous work concerning nonhomogeneous combustion, then show preliminary results for the cases that we have calculated.

5.1. Background

Several configurations of laminar combustion in nonhomogeneous mixtures have been investigated analytically using high-energy asymptotics. These include cases of one-dimensional laminar flames propagating into gradients in reactant mass fraction normal to the flame (e.g., Bissett & Reuss, 1986; Mikolaitis, 1984), and cases

\[
\langle \nabla_t \cdot \nu \rangle = C_k / \tau_k = C_k (\epsilon / \nu)^{1/2}.
\]  

In this case, values of $C_k$ range from 0.15 to 0.20 once the flame has become sufficiently wrinkled ($t / \tau_0 > \approx 1$). In three-dimensional simulations, $C_k$ is found to be 0.25 – 0.28 (Yeung et al., 1990 – for material surfaces; Cant et al., 1990). It should be emphasized that $\tau_k$ is probably not a physically meaningful scale for two-dimensional turbulence; it is shown here only for comparison with three-dimensional results.

FIGURE 8. Normalized pdf's of flame curvature for three Lewis numbers at normalized time $t / \tau_0 = 1.8$.
where there is a gradient in reactant concentration parallel to the premixed flame front (Buckmaster & Matalon, 1988). In these analyses, it is principally the mass consumption rate of the transient flame compared to that of an undisturbed steady laminar flame at the same local mixture strength that is of interest.

Nonhomogeneous mixtures also have been incorporated into models for turbulent combustion by Veynante et al. (1989) within the framework of the modified coherent flame model of Marble and Broadwell (1977). This model uses two modeled equations for flame surface-to-volume ratio, one for premixed burning and the other for post-flame diffusion burning.

Here, nonhomogeneous combustion is addressed in two simple configurations. The single-step Arrhenius chemistry of Eqs. (1)–(4) is retained, but heat losses are allowed \((c > 0)\) so that extinction effects can be modeled. The Lewis number is unity, and all chemistry parameters are as in Table II. Since we monitor a single reactant mass fraction, we are restricting our attention to cases where one of the reactants is always deficient (i.e., the mixture is everywhere rich or lean). This precludes some interesting behavior that can be expected when equivalence ratios on both sides of stoichiometric are present (Buckmaster & Matalon, 1988). A planar laminar flame propagating in a homogeneous mixture \((Y_R = 1)\) encounters a pocket of zero fuel mass fraction \((Y_R = 0)\). As a first step, we seek to quantify the parameters that govern whether the flame will reignite or extinguish following its encounter with the hole. The governing parameter is expected to be a ratio of a length scale characteristic of the post-flame temperature gradient resulting from the heat loss to a characteristic hole size.

### 5.2. One-dimensional laminar calculations

Typical initial profiles of reactant mass fraction and temperature are shown in
5. Lewis number and nonhomogeneous mixture

1. Lewis number and nonhomogeneous mixture

**FIGURE 10.** Initial profiles of reactant mass fraction and temperature for a one-dimensional laminar case with a reactant “hole.”

**FIGURE 11.** Normalized total reaction rate versus time as a function of hole half-width \( R \) for two values of the heat loss coefficient \( c \): a) \( c = 5 \cdot 10^{-5} \); b) \( c = 1 \cdot 10^{-4} \).

Figure 10. As the flame propagates, the reaction rate drops as the flame encounters the hole. The half-width of the hole, \( R \), is taken as a characteristic dimension of the disturbance.

Figure 11 shows the transient behavior of the flame (normalized total reaction rate versus time) as it passes through the hole as a function of \( R \) for two values of the heat loss coefficient \( c \). There is a critical value of \( R \), \( R_{\text{crit}} = R_{\text{crit}}(c) \), such that for \( R > R_{\text{crit}} \), the flame extinguishes and for \( R < R_{\text{crit}} \), the flame reignites. For \( c = 5 \cdot 10^{-5} \), Figure 11 shows that \( R_{\text{crit}} \approx 0.05 \); and, for \( c = 1 \cdot 10^{-4} \), \( R_{\text{crit}} \approx 0.014 \). In the limit of zero heat loss (\( c = 0 \)), the flame will always reignite.

5.2 Two-dimensional laminar calculations

Similar calculations have been repeated in two spatial dimensions for a round hole of lean \((Y_R = 0)\) reactants embedded in a \(Y_R = 1\) mixture. Compared to the one-dimensional case, the flame now can travel around the hole to reignite on the other side. An example of a case where the flame failed to reignite after passing the hole is shown in Figure 12.
6. Summary and conclusions

Calculations of premixed turbulent flame structure in two–dimensional turbulence have been reported. Quantitative results have been presented illustrating the effect of Lewis number on the local and global flame structure. Pdf's of flame strain rate and curvature have also been shown. Conclusions are that: 1) the local flamelet speed in the $Le = 1$ flame is everywhere nearly identical to that of an undisturbed laminar flame; 2) for $Le \neq 1$, the local flamelet speed differs from that of the undisturbed laminar flame and correlates strongly with local flame curvature; 3) flame strain results in a mean flamelet speed that is higher than the laminar value for $Le < 1$, is identical to the laminar value for $Le = 1$, and is lower than the laminar value for $Le > 1$; 4) straining and curvature effects result in more flame surface for $Le < 1$ than for $Le > 1$ – this, combined with the dependence of mean flamelet speed on $Le$, results in a strong dependence of turbulent flame speed on $Le$; 5) pdf's of flame curvature are nearly symmetric with a near-zero mean value – the maximum curvatures found are of the order of one over the laminar flame thickness; and, 6) pdf's of strain rate tangent to the flame are skewed towards positive (extensive) strains with a mean strain rate of the order of the inverse of the time scale of the smallest turbulent motions. These results imply that, for the range of parameters investigated, curvature is more important than strain rate in determining the local flame structure. Turbulent flame speed, however, is influenced both by curvature (through the flame surface area) and by strain (through the flame surface area and mean flamelet speed), and is strongly Lewis number dependent.

These results may have implications for the implementation of flamelet models of turbulent premixed combustion. The prototype laminar configuration for which

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**Figure 12.** Contours of temperature for a two–dimensional laminar calculation with a lean hole in the reactants. The flame has failed to reignite after passing through the hole.
flamelet libraries have been generated is generally that of a one-dimensional laminar stagnation-point burner. This configuration accounts, in some sense, for the effect of tangential strain, but does not account for flame front curvature. A second important result for modeling is that the flame surface area, the mean flamelet speed, and the turbulent flame speed all are functions of Lewis number: this dependence has been neglected in most models.

Questions remaining to be addressed include: further comparisons between two-dimensional and three-dimensional calculations to quantify the limitations and virtues of each; relative contributions of straining versus curvature to the total flame stretch; and, quantitative correlations between global quantities such as turbulent flame speed, turbulent rms velocity, and Lewis number.

For nonhomogeneous mixture cases, the bulk of the data reduction remains to be done. Here, we need to: quantify the recovery limits for flames propagating through lean holes, add at least one additional species so that both fuel-rich and fuel-lean regions can be modeled, include turbulence in the calculations, and try more complex (random) initial spatial distributions of the reactants.

REFERENCES


CANDEL, S., MAISTRET, E., DARABIHA, N., POINSOT, T., VEYNANTE, D., & LACAS, F. 1988 Experimental and numerical studies of turbulent ducted flames. Marble Symposium. CALTECH.


