CORRELATION OF FLAME SPEED WITH STRETCH IN TURBULENT PREMIXED METHANE/AIR FLAMES

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Direct numerical simulations of two-dimensional unsteady premixed methane/air flames are performed to determine the correlation of flame-speed with stretch over a wide range of curvatures and strain rates generated by intense two-dimensional turbulence. Lean and stoichiometric premixtures are considered with a detailed C1-mechanism for methane oxidation. The computed correlation shows the existence of two distinct stable branches. It further shows that exceedingly large negative values of stretch can be obtained solely through curvature effects, which give rise to an overall nonlinear correlation of the flame speed with stretch. Over a narrower stretch range, \(-1 \leq \kappa a \leq 1\), which includes 90% of the sample, the correlation is approximately linear, and, hence, the asymptotic theory for stretch is practically applicable. Overall, one-third of the sample has negative stretch. In this linear range, the Markstein number associated with the positive branch is determined for different initial turbulence intensities. For high turbulence intensity, the large eddy turnover time becomes shorter than a flame time, and the flame propagation becomes less responsive to unsteady straining. Reductions in strain Markstein numbers by as much as 37% from comparable steady counterflow computations are reported. In addition to the conventional positive branch, a negative-branch is identified. This negative branch occurs when a flame cusp, with a center of curvature in the burnt gases is subjected to intense compressive strain, resulting in a negative displacement speed. Negative flame speeds are also encountered for extensive tangential strain rates exceeding a Karlovitz number of unity, a value consistent with steady counterflow computations. In both situations, consistent with earlier findings, the source of the reduction in flame speed is attributed to an imbalance between diffusion and reaction.

Introduction

In the flamelet approach of turbulent premixed combustion, the flames are modeled as a wrinkled surface whose propagation speed, termed the displacement speed, is prescribed in terms of the local flowfield and flame geometry \([1]\). The response of the displacement speed, \(S_d\), to flame stretch, the combination of flow strain rate and flame curvature effects, can be characterized by a Markstein number. Theoretical studies \([2-4]\) suggest a linear relation between the flame speed and stretch for small values of stretch, \(S_d/S_L = 1 - \text{Ma} \kappa a\) \((1)\), where \(S_L\) is the laminar flame speed, \(\kappa a = \kappa \delta F/S_L\) is the nondimensional stretch, or the Karlovitz number, \(\text{Ma} = \frac{\text{Ma}}{S_L}\) is the Markstein number, and \(\Sigma\) is the Markstein length. The nominal flame thickness, \(\delta F\), is determined as the ratio of the mass diffusivity of the unburnt mixture to the laminar flame speed. Flame stretch, \(\kappa\), defined as the fractional rate-of-change of flame area, is expressed exactly as the sum of tangential strain rate, \(\alpha_T\), and a curvature term \([5-7]\):

\[\kappa = \alpha_T + S_T \nabla \cdot \mathbf{n}\] \(2\)

where \(\nabla \cdot \mathbf{n}\) is the flame curvature, and \(\mathbf{n}\) is the flame normal vector. The curvature is taken to be positive (negative) when the flame is convex (concave) to the unburnt gas.

In an actual implementation of a flamelet model in turbulent premixed flames, an accurate estimate of the Markstein number is crucial in predicting the turbulent flame speed, and thus the overall burning rate. The Markstein number is also required in flamefront tracking methods such as the G-equation formulation \([8]\) and relates the thermochemical state to the flowfield. More recently, a model G-equation has been developed for the thin reaction zone regime, a regime where turbulence intensity is large and the Kolmogorov scales penetrate the preheat zone \([9]\).

Experimental measurement of flame speed and stretch in turbulent flames, however, is extremely difficult. As a consequence, measurement of flame speed in a strained flow is often made in simple geometries \([10,11]\) for small values of stretch, where the effects of transients associated with unsteady strain and large flame curvatures are often ignored.
or not present. Recent direct numerical simulation (DNS) with constant Lewis number, along with experimental data obtained at the tip of a 2-D Bunsen flame, show a dependence of the displacement speed on stretch [12] due to negatively curved flames undergoing compressive strain. They show that the linear relation predicted by asymptotic methods applies to a much larger range of stretch values and that strain and curvature effects can be parameterized by stretch alone. However, their data are limited to steady flames that are curved convex to the burnt gases, and the computations do not account for differential diffusion of intermediate species that may be amplified at flame cusps.

In this study, results of DNS of unsteady two-dimensional flames with detailed methane/air chemistry provide an alternative method of obtaining flame structure and propagation statistics. Although the two-dimensional configuration commands a limited view of realistic turbulence due to the absence of vortex stretching, turbulent flame curvature statistics [13] suggest that the local flame geometry is most likely to be two-dimensional. Because flame propagation depends locally on a balance between reaction and diffusion influenced by the local flame geometry, determining the flame response to two-dimensional unsteady vortical flowfields is relevant to turbulent situations. The primary objective, then, is to determine the correlation between the displacement speed and flame stretch over a broad range of Karlovitz numbers, both positive and negative, and the distribution of stretch over the flame. The sensitivity of the location of evaluation of the displacement speed is determined using unburnt methane as a marker of the flame front. The observed response of the displacement speed is then interpreted in terms of unsteady tangential strain rate and curvature effects.

**Numerical Method**

The numerical scheme is based on the solution of the Navier–Stokes, species and energy equations for a compressible gas mixture. The explicit finite difference algorithm uses a fourth-order low-storage Runge–Kutta method for time advancement [14] and an eighth-order centered finite difference scheme for spatial differencing [15]. The chemical mechanism is based on a detailed $C_1$-mechanism for methane–air oxidation [16] with 17 species and 68 reversible reactions. The species mass diffusion is determined by prescribing the Lewis numbers of individual species [17]. The molecular viscosity of the mixture is temperature dependent [18], whereas the thermodynamic properties (enthalpy, specific heat) are temperature and composition dependent. The Prandtl number is taken to be 0.708 for air.

The computations are initialized with a 1-D steady laminar flame profile. Fuel-lean to stoichiometric mixtures (equivalence ratios of 0.7 and 1.0) of methane/air are preheated to 800 K in the reactant free stream. The profiles are obtained from a one-dimensional steady code PREMIX [19], and the solution is allowed to adjust to the simplified transport in a one-dimensional DNS.

The turbulence is prescribed by an initial 2-D turbulent kinetic energy spectrum function [20] that is superimposed on the laminar flame. The ratio of the turbulence intensity to the laminar flame speed, $u' / S_{fl}$, is taken to be 4.0 and 10.0, and the ratio of the integral eddy scale to the thermal flame thickness, $L_{11}/\delta_t$, is 4.05 and 2.90. The large eddy turnover time, $\tau_w$, is defined as the ratio $L_{11}/u'$ and the flame time, $\tau_f$, as $\delta_t/L_{11}$. The turbulence Reynolds number based on $L_{11}$ and the unburned gas properties at 800 K is 181. The initial transients associated with the superposition of the turbulence on the laminar flame subside by one eddy turnover time based on monitoring pressure fluctuations in the computational domain. The computational domain size is 0.67 cm, or 21.6 $\delta_t$ in the directions parallel and perpendicular to the laminar flame. The boundary conditions are nonreflecting [18], and periodic in the directions parallel and perpendicular to the initial vertical laminar flame, respectively. The thermal thickness, $\delta_t$, is 4.48 times the nominal flame thickness, $\delta_t$. The domain is discretized into 750 uniform grid points in each direction.

**The Displacement Speed: Location of Evaluation and Definition**

The DNS results are used to evaluate the flame speed in terms of the displacement speed of an isoline representing the flame front. Because the theoretical formulation is based on asymptotically thin flames, for finite-thickness flames described by multistep chemical kinetics, the choice of location of $S_d$ evaluation in the flame is somewhat ambiguous. Experiments in steady laminar flames [21,22], however, indicate that the burning velocity is most likely to be reproducible and independent of variations in local geometry and flame curvature when measured in the thin primary reaction zone. Elsewhere in the flame, the measurements are subjected to cross-stream diffusion and lateral flow expansion effects by the flame.

Following the suggestion by Fristrom [21] and Dixon-Lewis and Islam [22], the isoline chosen in the present DNS is the 10% value of the unburnt methane mass fraction, which is within the primary reaction zone in the flame. This isoline is plotted for the high turbulence intensity lean case in Fig. 1 to indicate the degree of flame corrugation after 3.76 eddy turnover time. Here, the local release isocountours are overlaid on the isoline, confirming the adequacy of the particular choice of isoline for tracking
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Fig. 1. Isocontours of heat release rate after 3.76 eddy turnover time in a lean premixed methane/air flame, $d = 0.7$, $u'/S_L = 10.0$. The black line corresponds to 10% of unburnt CH$_4$ mass fraction. The coordinates are normalized by the flame thermal thickness, $Y$, where $Y = 4.48$. 

Fig. 2. Displacement speed along selected flame normals as a function of methane mass fraction. — — — lines correspond to high $\omega$ and low $\nabla \cdot n$; — — — — line corresponds to large negative $\nabla \cdot n$; — — — — — line corresponds to large positive $\nabla \cdot n$. The shaded band, between 5% and 30% of the unburnt mass fraction of methane, denotes the region in which most of the heat release occurs.

The density-weighted displacement speed of the flame relative to the local gas velocity is defined as:

$$S_{\|} = \frac{\rho S_{\|}}{\rho_o} = - \frac{\omega_a}{\rho_o \nabla Y_a} \cdot \frac{\partial}{\partial Y_a} \left( \frac{\rho D_a}{\rho_o} \frac{\partial Y_a}{\partial Y_a} \right)$$

$$- \frac{\rho D_a}{\rho_o} (\nabla \cdot n)$$ (3)

where $\rho_o$ denotes the density in the unburned state of the mixture, and $\eta$ is the direction normal to the flame. The density-weighted formulation minimizes thermal expansion effects on the displacement speed and has been shown, for low turbulence intensity, to yield a relatively constant value across the reaction zone [18]. Here, the subscript $a$ is the index of the species that defines the mass fraction isocontour.

The Markstein number and flame stretch given by equations 1 and 2 in terms of density-weighted values of $S_{\|}$ are

$$S_{\|}^3/S_L = 1 - MaKa$$

where

$$Ka = Ka_t + Ka_c = \delta_p/S_L (\alpha_t + S_{\|} \nabla \cdot n)$$ (6)

Results and Discussion

We first examine the correlation of displacement speed with the Karlovitz number, $Ka$, the sum of the
Fig. 3. Correlation of displacement speed with Karlovitz number, based on nominal flame thickness, \( \delta_f = D_f/S_L \), for a premixed methane/air flame, \( \phi = 0.7 \), \( u'/S_L = 10.0 \), at 3.76 eddy turnover time.

Fig. 4. Probability density function of normalized stretch rate, \( K_a \) (solid line) and tangential strain rate, \( K_{at} \) (dashed line) evaluated at the flame surface, 10% unburnt CH\(_4\), \( \phi = 0.7 \), \( u'/S_L = 10.0 \), at 3.76 eddy turnover time.

tangential strain and curvature components, \( K_a \) and \( K_{ac} \). The correlation is obtained by plotting sequential points along a given species mass fraction isoline. Based on the previous discussion, the 10% unburnt methane mass fraction isoline is used to represent the flame front, and all values used in the correlation (e.g., tangential strain rate, density, \( S_i^p \), curvature) are evaluated locally along this isoline. Three DNS simulations were performed: two lean cases at \( \phi = 0.7 \) for \( u'/S_L = 4.0 \) and 10.0, and one stoichiometric case for \( u'/S_L = 10.0 \). Because the correlation of flame speed with stretch is qualitatively similar for the three cases, only the statistics for the lean case at higher turbulence intensity will be presented. However, where appropriate, a comparison of the cases will be made.

The correlation of the displacement speed with Karlovitz number at 3.76 eddy turnover time is shown in Fig. 3. Three features are immediately evident: first, that there exists two distinct stable branches depending upon the sign of the displacement speed; second, that the correlation between flame speed and stretch is nonlinear, and, third, that exceedingly large negative values of flame stretch are rare. The range of stretch rates experienced by the flame is \( -11 \leq K_a \leq 1.2 \).

To substantiate the statistical significance of various portions of the data shown in Fig. 3, the probability density function (PDF) of the stretch rate is shown in Fig. 4. Although not shown, the range of flame curvature is \( -1 \leq \nabla \cdot \mathbf{U}_f \leq 3 \), with a mean of zero. The overall shape of the stretch and curvature PDFs are consistent with DNS results using simple chemistry [25].

We also find in Fig. 4 that over 90% of the flames are between \( -1 \leq K_a \leq 1 \), and the proportion of flames undergoing compression, or negative stretch, is 30%. This represents a significant fraction of the overall flame area and suggests a need to better understand how flames propagate in the presence of both compression and curvature. Incidentally, this result supports the recent study [26] based on statistical results of propagating surfaces from constant-density DNS data, in which the model assumes that approximately one-third of the flames are undergoing compression.

Figure 4 further shows the PDF of the tangential strain rate, \( K_{at} \). By comparing the stretch and strain PDFs, it is evident that the long negative tail in the stretch PDF is attributed solely to the curvature term, \( K_{ac} \), and not to tangential strain. Therefore, it appears that only a few regions of large negative stretch exist, even when the flame is subjected to high intensity turbulence. Although not shown in Fig. 4, a comparison of the PDF of \( K_{at} \) for the two different turbulence intensities at an earlier time, \( \tau = 0.7 \), shows that, as expected, a larger mean value and a broader range of strain rates is experienced by the higher turbulence intensity case. The mean value of \( K_{at} \) is 0.45 and 0.30 for \( u'/S_L \) of 10.0 and 4.0, respectively. We note that the mean value of \( u'/S_L \) is inversely correlated with the mean value of \( K_{at} \).

At \( \tau = 0.7 \), the mean value of \( S_i^p/S_L \) is 0.58 and 0.70, for \( u'/S_L \) of 10.0 and 4.0, respectively.

Given the statistical importance of flame stretch within the range \( -1 \leq K_a \leq 1 \), we first determine the displacement speed correlation of those points with stretch. The data in Fig. 3, replotted over a narrower range of stretch are shown in Fig. 5. The
upper branch shows that the displacement speed decreases with an increase in $Ka$ (and therefore positive $Ma$ from the definition in equation 1), which is consistent with theoretical results for thermodiffusively stable flames ($Le \approx 1$). The data further show, within the limitation of the observed scatter, that the dependency on stretch in this range is nearly linear. This demonstrates that the asymptotic theory, formally applicable to small values of stretch, ($Ka \ll O(1)$) can be applied over a broader range of strain rates and curvatures, ($Ka \sim O(1)$).

A least-squares linear fit over the data in Fig. 5 yields a Markstein number based on total stretch, $Ka$. Similarly, a linear fit over $S_L^*$ versus $Ka_s$ data, conditioned on curvature magnitudes less than 0.2, yields a Markstein number based on tangential strain, $Ma_s$. A comparison of the two Markstein numbers, and with a Markstein number obtained from comparable fresh-to-burnt steady counterflow computations, is summarized in Table 1 for lean to stoichiometric methane/air mixtures. In this table, Markstein numbers for both moderate and high initial turbulence intensities are reported for linear fits obtained over two ranges of $Ka$ over which most of the data lie. Also reported in the table are the time of evaluation and the percentage reduction in kinetic energy, $AQ$, at the time of evaluation. Two interesting observations can be made from the comparison in Table 1. First, for both initial turbulence intensities considered, $Ma$ is attributed primarily to tangential strain, and not to curvature/propagation effects. The differences between $Ma$ and $Ma_s$ are less than 20%. Second, a comparison of $Ma$ for different ratios of eddy turnover to flame time, $u'/S_L$, ranging from infinity (steady counterflow case) to one-third ($u'/S_L = 10$), reveals that, as the turbulence time becomes short relative to the flame time, the flames become less responsive to unsteady straining. For $u'/S_L = 10$ and $\phi = 0.7$, $Ma$ is only 63% of the steady laminar value. A similar decrease in $Ma$, is also observed for the stoichiometric case. The decrease in strain Markstein number with an increase in turbulence frequency for the range of finite amplitude strain rates obtained in the DNS is consistent with the theory regarding the high-frequency response of laminar premixed flames to weak fluctuations in velocity gradients [27].

The negative branch in Fig. 5 may seem counterintuitive, as it appears that for some portion of the flame, the displacement speed increases with the Karlovitz number. However, by conditioning the correlation in Fig. 5 on local curvature, it is found that this branch occurs in a region of large positive curvature, where the center of curvature is located in the burnt gases. In this case, the flame is convectively pulled upstream by strong turbulent eddies, such that the magnitude of the diffusive flux tangential to the flame front exceeds that of the adverse convective flux [23]. As a result, the flame retreats.

**TABLE 1**

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$u'/S_L$</th>
<th>$\tau_f/\tau_F$</th>
<th>$\tau_F$</th>
<th>$% AQ$</th>
<th>$Ma$</th>
<th>$Ma_s$</th>
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</thead>
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<td>0.7</td>
<td>1-D steady CF</td>
<td>$\infty$</td>
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<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>0.7</td>
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<td>1.0</td>
<td>0.73</td>
<td>9.0</td>
<td>1.06</td>
<td>0.91</td>
</tr>
<tr>
<td>0.7</td>
<td>10.0</td>
<td>0.29</td>
<td>0.70</td>
<td>14.0</td>
<td>0.51</td>
<td>0.74</td>
</tr>
<tr>
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<td>0.29</td>
<td>1.1</td>
<td>25.0</td>
<td>0.71</td>
<td>0.92</td>
</tr>
<tr>
<td>1.0</td>
<td>1-D steady CF</td>
<td>$\infty$</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>1.0</td>
<td>10.0</td>
<td>0.35</td>
<td>1.1</td>
<td>23.0</td>
<td>0.93</td>
<td>0.90</td>
</tr>
</tbody>
</table>
Fig. 6. Correlation of displacement speed with stretch rate for a premixed methane/air flame, $\phi = 0.7$, $u'/S_L = 10.0$, at 1.0 eddy turnover time. Note the linear segment showing negative flame speed for $Ka \approx 1$.

Fig. 7. Correlation of displacement speed with normalized strain rate, $Ka_s$, for 1-D steady counterflow computation in a fresh-to-burnt configuration. For methane-air flame, $\phi = 0.7$.

results, when the turbulence intensity is the highest, negative displacement speed was observed for positive Karlovitz number in excess of unity as shown by the extension of the linear segment for $Ka > 1$ in Fig. 6. This is consistent with planar premixed counterflow computations in a fresh-to-burnt configuration shown in Fig. 7, where, at 10% unburnt methane, the crossover point to negative speeds occurs at $Ka = 0.722$. Note that isoconcentration lines of methane evaluated at the location corresponding to the half maximum of the heat release on the upstream side do not exhibit negative speeds; only isolines downstream of this location in the reaction zone cross over to the product gases. This is also consistent with the DNS results; the crossover to negative speeds occurs at a value of methane mass fraction equal to 20% of the unburnt value.

As a further remark regarding the curvature portion of stretch, we observe that large negative values of Karlovitz number are found to be due to the effect of strong curvature; and in these cases, the correlation shows nonlinear behavior. The form of the nonlinearity can be determined by recasting equation 5 in terms of the Markstein number as

$$Ma = \frac{1 - S_S/S_L}{\delta (\nabla \cdot \mathbf{n})}$$

and in the limit when $S_S/S_L \gg 1$ and $S_S \nabla \cdot \mathbf{n} \gg \alpha_T$, we obtain

$$Ma \sim -\frac{1}{\delta \nabla \cdot \mathbf{n}}$$

Therefore, at large magnitude of $\nabla \cdot \mathbf{n}$, we expect to obtain small $Ma$. In Fig. 8 a scatter plot of $S_S^2$ versus curvature clearly shows that the first criterion,
found to be inversely proportional to the local flame curvature. The nonlinear dependence is linear, with the source of nonlinearity derived from the curvature term. The nonlinear dependence is found to be inversely proportional to the local flame curvature in the limit of large curvature. The large magnitudes of the displacement speed encountered at the cusps serve as a stabilizing mechanism to counter the effect of the intense turbulence and should result in a reduction in the overall turbulent flame area. For intense compressive strain at positive cusps, a second stable branch in the correlation arises due to negative flame propagation brought on explicitly by the positive local curvature.

The contribution of the tangential strain rate is found to be linear and continuous going from positive to negative values. We find it remarkable that the linear relation (equation 1) is an excellent approximation for stretch rates far larger (Ka ~ O(1)) than what it was formally derived for (Ka < O(1)). For the given turbulence parameters considered in this study, we note that, over the statistically relevant stretch range, the flame propagation response to tangential strain is much larger than the response to curvature. We further find that the flame response to unsteady straining decreases for large turbulence intensities, where the turbulent eddy turnover time is short relative to the flame time, and over a positive stretch range, 0 < Ka < 1. This result is consistent with theoretical results showing a marked decrease in Markstein number for strain at high frequencies with theoretical results showing a marked decrease in Markstein number for strain at high frequencies. The contribution of the tangential strain rate is found to be linear and continuous going from positive to negative values. We find it remarkable that the linear relation (equation 1) is an excellent approximation for stretch rates far larger (Ka ~ O(1)) than what it was formally derived for (Ka < O(1)). For the given turbulence parameters considered in this study, we note that, over the statistically relevant stretch range, the flame propagation response to tangential strain is much larger than the response to curvature. We further find that the flame response to unsteady straining decreases for large turbulence intensities, where the turbulent eddy turnover time is short relative to the flame time, and over a positive stretch range, 0 < Ka < 1. This result is consistent with theoretical results showing a marked decrease in Markstein number for strain at high frequencies with theoretical results showing a marked decrease in Markstein number for strain at high frequencies.

For large negative curvatures (upper branch in Fig. 3), the displacement speed is enhanced, not only by differential diffusion and focusing of mobile radicals, but also by upstream flame–flame interactions. Local flame curvatures in excess of four thermal thicknesses are observed as a result of the intense turbulence. For a radius of curvature less than one thermal flame thickness, the flame starts to undergo mutual annihilation with neighboring flames as their respective thermodynamic and reactive layers start to merge. This interaction leads to further acceleration of the flames due to vanishing species gradients and shifts in balance between chemical reaction and normal diffusion as the cusp retreats [30]. On the other hand, when the flame is positively curved, in the limit of large curvature, the displacement speed becomes linearly proportional to the local curvature, or diffusion tangential to the flame surface [23]. The contributions from normal diffusion and reaction in this configuration are minimal.

Concluding Remarks

Two-dimensional unsteady DNS data for lean and stoichiometric premixed methane–air flames have been used to determine the correlation of displacement speed with flame stretch. It was observed that for the high turbulence intensity encountered by the flame, the correlation exhibits two distinct stable branches. The overall correlation is found to be nonlinear, with the source of nonlinearity derived from the curvature term. The nonlinear dependence is found to be inversely proportional to the local flame curvature. The large magnitudes of the displacement speed encountered at the cusps serve as a stabilizing mechanism to counter the effect of the intense turbulence and should result in a reduction in the overall turbulent flame area. For intense compressive strain at positive cusps, a second stable branch in the correlation arises due to negative flame propagation brought on explicitly by the positive local curvature.

Acknowledgments

This research was supported by the United States Department of Energy, Office of Basic Energy Sciences, Chemical Sciences Division. The authors thank Dr. Tarek Echekki for many insightful discussions.

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