Direct numerical simulation of turbulent premixed flames and the response of flame speeds to intense turbulence

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Abstract

Direct numerical simulation of several three-dimensional spatially developing turbulent bunsen flames have been performed. The intensity of flow field turbulence is such that the flame structure is significantly different from a laminar flame. The data produced from the simulations were analyzed to understand the flame dynamics in the thin reaction zones (TRZ) regime. A simple global analysis of the burning velocity of the flame was performed to compare the different flames. Detailed statistical averages of the flame speed were also obtained to study the spatial dependence of displacement speed and its correlation to strain rate and curvature.

1 Introduction

Premixed combustion under intense turbulence is of fundamental interest due to its relevance to practical applications such as lean premixed stationary gas turbines. Premixed flames under lean conditions tend to be thicker, propagate slower and the flame structure is more susceptible to the influence of turbulence. Recently, Peters [1] has provided a model for flame propagation in the regime where the turbulence scales are capable of penetrating and influencing the preheat zone, but are incapable of penetrating the reaction zones. This regime is called the thin reaction zones (TRZ) regime.

The burning velocity of turbulent premixed flames remains one of the main quantities of interest, both from a fundamental understanding and a modeling perspective. One important question [2] encountered in premixed combustion is, "how fast can we burn?" In an attempt to quantify and model the influence of turbulence on premixed combustion, a premixed flame is treated as a surface separating the fresh reactants and burnt products. This allows the influence of turbulence on combustion to be distinguishable in to two important phenomena -(i) an increase in the flame surface area within the same volume through wrinkling and aerodynamic straining of the flame (ii) a change in the burning rate of the flame per unit surface area with respect to a laminar flame. Based on this concept, a model for the turbulent burning velocity has been suggested by Bray [3] and Candel and Poinsot [4]. The mean turbulent burning velocity can be written as,

$$S_{\rm T} = S_{\rm L} \cdot I_0 \cdot A' \tag{1}$$

where $S_{\rm L}$ is the laminar burning velocity, I_0 is the efficiency factor to account for change in burning velocity per unit area and A' accounts for the increase in surface area. Formulating

turbulent burning velocity in this manner allows models to be derived for these two contributing factors. For example, one can model the change in burning velocity per unit area of the flame based on a laminar strained flame and then account for the increase in flame surface area through a flame surface density model [5].

Here, 3D fully-resolved direct numerical simulations (DNS) of turbulent premixed combustion are performed in a spatiallydeveloping slot-burner Bunsen flame configuration with a detailed methane-air chemical mechanism. In this paper, three simulations in the TRZ regime at successively higher turbulence intensities have been investigated as part of a parametric study. The data is analyzed to obtain statistical measures of the influence of turbulence on the burning velocity of the flame. In particular the contribution to the burning rate due to wrinkling of the flame and the enhancement of burning rate per unit surface area are determined. Then, the response of the displacement speed of the flame surface to strain rate and curvature are studied.

2 Problem Configuration

The simulation was performed in a slot-burner Bunsen flame configuration. The slot-burner Bunsen configuration is especially interesting due to the presence of mean shear in the flow and is similar in configuration to the burner used in experimental studies, for example by Filatyev *et al.* [6]. This configuration consists of a central reactant jet through which premixed reactants are supplied. The central jet is surrounded on either side by a heated coflow, whose composition and temperature are those of the complete combustion products of the reactant jet. This arrangement is similar to the pilot flame surrounding slot burners commonly used in experiments [6]. The reactant jet was chosen to be a premixed methane-air jet at 800K and ϕ = 0.7. The unstrained laminar flame properties at these condi-

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tions computed using PREMIX [7] are as follows:

- 1. Flame speed, $S_{\rm L}$ = 1.8 m/s
- 2. Thermal thickness based on maximum temperature gradient, δ_L =0.3mm
- 3. Full width at half maximum (FWHM) of heat release rate, $\delta_{\rm H} = 0.14$ mm, and
- 4. Flame time scale, $\tau_{\rm f} = \delta_{\rm L} / S_{\rm L} = 0.17$ ms.

One of the reasons for choosing a preheated inflow condition is that the cost of computation is inversely proportional to the Mach number at the inflow. Preheating the reactants leads to a higher flame speed and allows a higher inflow velocity without blowing out the flame. Also, many practical devices such as internal combustion engines, gas turbines and recirculating furnaces operate at highly preheated conditions. One important consequence of preheating is that the reaction zone is broadened at 800K ($\delta_L/\delta_H=2$) compared to 300K ($\delta_L/\delta_H=3$).

A parametric study was performed to investigate the effect of increasing turbulence intensity on lean premixed combustion. The problem configuration, mixture equivalence ratio and temperature are the same for all three simulations. However, they differ in the domain sizes and inflow turbulence conditions. The simulation parameters are given in Table 1. A uniform grid mpacing of 20μ m was used in the streamwise, x, and spanwise, z, directions, while an algebraically stretched mesh in the transverse, y, direction was obtained from $y(s) = f(s) \times L_y/2$, where s is the equi-spaced computational grid and $0 \le s \le 1$. The stretching function is given by,

$$f(s) = \beta s + \frac{1}{2} \left(1 + \tanh \frac{s - s^*}{\sigma} \right) \left(e^{ks} - \beta s \right), \quad (2)$$

where $k = \ln(\beta s^*)/(s^* - 1)$. The resultant mesh was mirrored across the jet centerline (y = s = 0) to obtain a symmetric mesh. The form of the stretching function along with the choice of constants, $\beta = 0.55$, $s^* = 0.75$ and $\sigma = 1/16$, yields a mesh that has a uniform spacing of 20μ m in the center of the domain over a region 5h in width. Here h denotes the slot width. The increase in grid spacing, ($\Delta_{i+1}/\Delta_i - 1$), in the outer part of the domain does not exceed 2%. While the uniform grid spacing at the center of the jet ensures numerical fidelity and flexibility in post-processing, the boundaries are pushed farther away to reduce their influence on the flame.

3 Numerical Method

A reduced chemical mechanism for lean premixed methaneair flames was derived, specifically tailored to minimize temporal stiffness while maintaining accuracy. The reduction was accomplished through the sequential application of directed relation graph (DRG), sensitivity analysis and computational singular perturbation (CSP) over the GRI-1.2 detailed mechanism. Details on the reduction methodology and validation of the reduced mechanism can be found in Ref. [8, 9]. A notable aspect of the reduced mechanism is that the quasi-steady

state (QSS) species concentrations were obtained through explicit analytical expressions without the need for expensive iterations. Consequently, overall convergence was obtained at a lower cost.

The simulations were performed using the DNS code S3D, which solves the fully compressible Navier Stokes, species and energy equations with a fourth-order Runge-Kutta method for time integration and an eighth-order explicit spatial differencing scheme [10, 11]. A tenth-order filter was used periodically to damp any spurious high-wave number oscillations. The mixture specific heat is determined locally as a function of mixture composition; that is, $C_p = \sum_k C_{p,k} Y_k$, where each $C_{p,k}$ is curve-fitted as a function of temperature using the Chemkin thermodynamic database [12]. The molecular viscosity is also temperature dependent and constant Lewis numbers for individual species are used.

The flame is anchored at the inflow plane by specifying the species mass fractions and temperature from an unstrained laminar flame solution using a progress variable lookup. A hyperbolic tangent function was used to obtain a smooth variation of progress variable between the unburned and burned conditions. A turbulent velocity field was synthesized by specifying the length scale, magnitude of velocity fluctuations and spectral energy density. The resultant velocity field was added to the mean inflow velocity profile and used as the velocity inflow boundary condition based on Taylor's hypothesis.

Navier-Stokes characteristic boundary conditions (NSCBC) [13–16] were used to prescribe the boundary conditions. The boundary conditions were periodic in the spanwise direction (z), non-reflecting inflow and outflow in the streamwise direction (x), and non-reflecting outflow [13] in the transverse direction (y). Based on the jet inlet velocity and the streamwise domain length, a flow-through time is 0.24ms. The solution was advanced at a constant 2ns time-step for three flow through times for case A and two flow through times for cases B and C. The first flow through time was neglected to account for initial transients when performing analysis. Data from 61 equally spaced time instants from the remainder of the simulation was used to obtain the statistical results presented in the next section. Averaging is performed in the homogeneous direction (z) and time. Symmetry across the centerline is exploited where feasible.

4 Results and Discussion

4.1 Turbulence characteristics

Due to the presence of mean shear in the configuration, the turbulence scales continue to evolve downstream. The development of favre-averaged turbulence intensity along the jet centerline is shown in Fig. 1. It is seen that u' quickly decays from the imposed inflow conditions close to the inlet and varies less drastically at further downstream locations. Similarly the turbulence length scales were also observed to re-adjust quickly from those of the synthesized field injected at the inlet. Therefore, the simulations are characterized by the turbulence levels at the 1/4th downstream location ($x = 1/4L_x$) instead of those at the inlet. Table 1 lists the various turbulence characteristics of the flow-field obtained from aver-

	Case A	Case B	Case C
slot width (<i>h</i>)	1.2 mm	1.2 mm	1.8 mm
Domain size, $L_x \times L_y \times L_z$	$12h \times 12h \times 3h$	$20h \times 12h \times 3h$	$13h \times 12h \times 3h$
Mesh size, $N_x \times N_y \times N_z$	$720 \times 400 \times 180$	$1200 \times 400 \times 180$	$1200 \times 600 \times 270$
Number of grid points	52 Million	86 Million	195 Million
Turbulent jet velocity (\overline{U})	60m/s	100m/s	100m/s
Laminar coflow velocity	15 m/s	25 m/s	25 m/s
Turbulence intensity ⁴ $(u'/S_{\rm L})$	3	6	10
Turbulence length scale ^{2,4} (l_t/δ_L)	0.7	1	1.5
Integral length scale ^{3,4} $(l_{33}/\delta_{\rm L})$	2	2	4
Jet Reynolds no ($\operatorname{Re}_{\operatorname{jet}} = \overline{U}h/\nu$)	840	1400	2100
Turbulence Reynolds no ($\operatorname{Re}_{t} = u' l_{33} / \nu$)	40	75	250
Karlovitz no $(\delta_{\rm L}/l_{\rm k})^2$	100	100	225
Damkohler no $(S_{\rm L} l_{33}/u' \delta_{\rm L})$	0.7	0.3	0.4

Table 1: Simulation parameters

 1 Kinematic viscosity at the inflow conditions, $\nu=8.5e-5m^2/s,$ is used to compute Reynolds number.

² Turbulence length scale l_t is estimated as $l_t = u'^3 / \tilde{\epsilon}$, where $\tilde{\epsilon}$ is the average turbulent kinetic energy dissipation rate.

 3 Integral length scale l_{33} is defined as the integral of the auto- correlation of the spanwise component of velocity in the spanwise direction.

⁴ The turbulence scales evolve from the synthetic turbulence specified at the inflow. The u', l_t and l_{33} values reported here are at the 1/4th streamwise location along the jet centerline.



Figure 1: Favre-averaged turbulence intensity (u'/S_L) along the jet centerline.

aging the flow-field over multiple times. Based on the turbulence parameters the three flames are in the thin reaction zones (TRZ) regime [1] of combustion, progressively moving from the boundary with the flamelets regime (case A) towards the boundary with the broken reaction zones regime (case C).

4.2 Definition of progress variable (c)

A reaction progress variable, c, is defined based on the mass fraction of O₂. While c is usually defined based on the deficient reactant, in this case CH₄, such a definition here will omit a significant portion of the oxidation layer, since the heat release is only 66% complete where CH₄ is completely consumed. Therefore, c is defined using O₂ mass fraction. The reaction progress variable varies from 0 in the reactants to 1 in

the products. Also, based on the laminar flame solution at the chosen reactant conditions, the heat release is a maximum at c = 0.65.

4.3 Treatment of flame as an iso-surface

The progress variable iso-surface, c=0.65, is taken as representative of the instantaneous flame front and is used to study the characteristics of flame propagation. The iso-surface is extracted from volume data through triangulation. A local unit normal to the flame surface is obtained from $\hat{n} = -\nabla c/|\nabla c|$. \hat{n} is first computed on the cartesian mesh and interpolated to the vertices of the iso-surface. The negative sign in the definition of \hat{n} points the normal in the direction of unburnt mixture (c=0). \hat{n} also yields a curvature tensor, whose eigen values are the two principal curvatures of the surface [17]. The curvature is positive when the center of curvature lies in the burnt gas (c=1). The arithmetic mean of the two principal curvatures is known to be equal to $0.5\nabla \cdot \hat{n}$.

The mean flame profile and instantaneous flame surface were presented in the last U.S. combustion meeting [18]. They are repeated here for reference in further analysis and to give an intuitive picture that would allow the reader to visualize the configuration and nature of the flame studied. Figure 2 shows an instantaneous flame surface for the three cases. In all three cases the flame is initially planar at the inlet, but is wrinkled within a short distance in the downstream direction. Also the scale of wrinkling increases in the downstream direction. Comparing the three cases, it is seen that the amount of wrinkling increases from case A to case C. The mean progress variable computed by favre-averaging is shown in figure 3.



Figure 2: Instantaneous iso-contour of the progress variable (c = 0.65) representing flame surface for cases A, B and C.



Figure 3: Favre averaged mean progress variable (\tilde{c}) is shown as a pseudocolor plot. The color scale varies from blue (0) to red (1). The iso-contour of $\tilde{c} = 0.65$ is shown as a solid line.

4.4 Strain rate

The tangential strain rate on a flame surface has a significant effect on the burning rate of the flame and surface area generation. The tangential strain rate is computed on two progress variable iso-surface, one corresponding to the fresh mixture (c = 0.2) and the other corresponding to the approximate location of the heat release layer (c = 0.65). Figure 4 shows the evolution of conditional mean strain rate on these two iso-surfaces as a function of the axial distance. The strain rate is higher in cases B and C than case A due to the larger jet velocity and the higher mean shear. It is also seen that the mean strain rate decays with distance due to a widening of the shear layer. An important observation is that, in the first, roughly, 1/4th of the domain, the strain rate at $c^* = 0.2$ is higher than at 0.65. But this difference disappears at the downstream locations and the mean strain rate is the same at $c^* = 0.2$ and 0.65. This is because, the inflow boundary condition was set up such that the flame is anchored outside the shear layer at the inflow. But as the flow develops in the downstream direction, the flame moves inside the shear layer as the jet widens and the flame tip closes [9].



Figure 4: Mean strain rate, conditional on $c = c^*$, as a function of the axial distance. In (a) $c^* = 0.2$ and in (b) $c^* = 0.65$.

4.5 Global burning velocity

Here, we define and measure a global burning velocity of the flame similar to Filatyev et al. [6]. As a first step, we treat the mean turbulent flame as the surface defined by $\tilde{c} = 0.65$ as shown in figure 3. In our simulations, the domain was large enough that almost all the reactants that entered the domain were consumed by combustion before exiting the computational domain. A mass flux analysis to measure the mass of fuel entering through the inlet and leaving unburnt from the outflow boundaries showed that 15%, 5% and 9% of the reactants leave the boundary unburnt in cases A, B and C, respectively. Flame pinch-off, which causes a portion of the flame surface to detach and to be swept downstream due to advection is the main source of unburnt fuel leaving the computational domain. The domain length required to compute the complete combustion of the fuel will make the simulation prohibitively expensive. Since the mean flame brush defined by $\tilde{c} = 0.65$ is well within the domain, the mass efflux of reactants can be ignored for the purpose of estimating the global burning velocity.

The mass inflow of the reactants is computed by integrating over the inflow plane as,

$$\dot{m}_{in} = \int\limits_{A} \rho u_1 c \, dA \tag{3}$$

A turbulent burning velocity $S_{\rm T}$ can be defined such that, the reactants are consumed at this rate, uniformly, over the area of the mean flame brush defined by $\tilde{c} = 0.65$. Let *P* denote the length of this iso-contour line as measured from Figure 3. Then the area of this unwrinkled flame is $A_{\rm flat} = PL_z$, where L_z is the domain length in the spanwise direction. Through mass balance,

$$\rho_{\rm u} S_{\rm T} A_{\rm flat} = \dot{m}_{in}. \tag{4}$$

Table 2 shows the $S_{\rm T}$ computed using the relation 4 along with the observed flame heights for the three cases. It is seen that the ratio of the turbulent burning velocity ($S_{\rm T}$) to the laminar burning velocity progressively increases from case A to C. This is evident from comparing the flame heights alone for cases B and C. Although the jet in case C was 1.5 times wider than case B, the flame heights were the same. The burning velocity had to be much larger in order to combust the higher mass flux within the same flame height.

Equation 4 was useful to obtain a global burning velocity estimate for the three flames. It is possible to further extend this simple analysis to determine the contributions from increase in flame surface area and from the increase in burning rate per unit area of the flame, as described in the introduction. Rewriting equation 4 as,

$$\rho_{\rm u} S_{\rm L} I_0 A_{\rm wrinkled} = \dot{m}_{in}.$$
(5)

Let $A' = A_{\text{wrinkled}} / A_{\text{flat}}$. Then,

$$\frac{S_{\rm T}}{S_{\rm L}} = I_0 A' \tag{6}$$

The area of the wrinkled flame surface A_{wrinkled} is obtained by triangulation, as in figure 2 and then used to compute

 I_0 using the above relation. The results are reported in table 2. It is seen from the area ratios that the extent of wrinkling increases progressively going from case A to case C. However, I_0 decreases from case A to case B, but is relatively constant between cases B and C.

	Case A	Case B	Case C
Flame height (H)	13.3 mm	18.1 mm	18.7 mm
$S_{ m T}/S_{ m L}$	1.47	1.9	2.67
A'	1.5	2.2	3.0
I_0	0.98	0.86	0.89

Table 2: Global burning velocity of the turbulent flame.

4.6 Local burning velocity

In this section, we perform a more local analysis of the burning velocity and use it to compute I_0 and A' at various downstream locations. To obtain a relation for the local burning velocity, eq. 5 is rewritten as,

$$\rho_{\rm u} S_{\rm L} I_0 A_{\rm wrinkled} = \int_0^{L_x} \int_0^{L_y} \int_0^{L_z} \dot{\omega}_{\rm c} \, dz \, dy \, dx \tag{7}$$

where the mass influx of reactants has been replaced by the volume integrated consumption rate of reactant. For the purpose of this analysis, the domain is decomposed into thin slices perpendicular to the streamwise (x) direction. A local balance between the consumption of reactants and turbulent flame propagation is assumed in each slice. Then, eq. 7 is assumed to be valid locally in each y-z slice.

$$\rho_{\rm u} S_{\rm L} I_0(x) A_{\rm wrinkled}(x) = \int_x^{x+\Delta} \int_0^{L_y} \int_0^{L_z} \dot{\omega}_{\rm c} \, dz \, dy \, dx \qquad (8)$$

where $A_{\text{wrinkled}}(x)$ is the flame surface area within a local slab of thickness Δ at location x. Taking the unwrinkled flat flame area to be $2\Delta L_z$, we then obtain statistical averages for $A'(x) = A_{\text{wrinkled}}/A_{\text{flat}}$ and $I_0(x)$. The results are shown in fig. 5 and the following observations are made. The flame surface area trends seen in fig. 5 are consistent with the qualitative observations made based on fig. 2. The flame area increases when going from case A to case C, in that order. Beginning from an initial flat laminar flame profile (A' = 1) specified at the inflow boundary, the flame area quickly increases to a high value and stays fairly constant and then rapidly decreases near the outflow. The decrease in surface area at the downstream locations is due to two reasons. Firstly the flame annihilation events have a higher incidence at the downstream locations and lead to destruction of flame area. Secondly, the probability of finding a c = 0.65 surface is non-unity at the far downstream locations due to complete combustion at upstream locations.

 I_0 is found to be lower near the inflow and increase in the downstream direction. It is known that lean methane-air flames have a positive Markstein length and hence the burning velocity decreases with stretch. The very high strain rates near the inflow due to imposed mean shear are responsible for the low I_0 near the inflow. As the strain rate relaxes, I_0 increases in the downstream direction. The spurious values of I_0 greater than unity close to the outflow are due to vanishing flame surface areas close to the outflow (see eq. 8).



Figure 5: Flame area and burning velocity variation along the axial direction.

4.7 Displacement speed

In numerical studies with finite rate chemistry, a mathematically rigorous definition of the flame burning velocity, known as the displacement speed (S_d), is well suited. The displacement speed is defined as the velocity of the flame isosurface with respect to the local fluid medium [19] and is given by

$$S_{\rm d} = -\frac{Dc}{Dt} \frac{1}{|\nabla c|} \tag{9}$$

where the negative sign ensures that the displacement speed is positive when a reactant that is consumed in combustion is used to evaluate S_d , as is the case here. S_d can be decomposed in to three components [20] as,

$$S_{\rm d} = S_{\rm d,r} + S_{\rm d,n} + S_{\rm d,c}$$
 (10)

where the three terms on the right hand side are the reaction, normal diffusion and tangential diffusion terms respectively. Further, a density weighted displacement speed is defined as $S_{\rm d}^* = \rho S_{\rm d} / \rho_{\rm u}$ where $\rho_{\rm u}$ is the unburnt mixture density.

Weighting by the local density allows the displacement speed to be measured with respect to the unburnt mixture conditions as is customary for other definitions of flame speed.

Here, a conditional average of S_d^* is computed on the c = 0.65 iso-surface and plotted as a function of axial distance in figure 6. It is seen that the mean displacement speed increases with downstream direction for all 3 cases, similar to the trend shown by I_0 in fig. 5. It is also seen that mean S_d^* is negative close to the inlet for cases B and C. Premixed flames are known to have a negative displacement speed at large strain rates. This has been observed in opposed flow experiments with a reactant and burnt product stream opposed to each other. Under high strain rates, It has been observed that the premixed flame can move from the reactant side past the stagnation plane in to the product stream and exhibit a negative displacement speed. Here too, the negative displacement speed can be attributed to the very high strain rates observed close to the inlet.



Figure 6: Mean $S_{\rm d}^*$, conditional on c = 0.65, as a function of the axial distance.

This is confirmed by analyzing the displacement speed statistics together with the local strain rate. Figure 7 shows the pdf of strain rate and the conditional means (conditioned on c = 0.65) of displacement speed (S_d^*). The results are shown at three different axial locations. $x/L_x=1/4$, 1/2 and 3/4. Also the response of a laminar strained flame in a opposed flow configuration with a reactant streams opposed to a burnt product stream was computed using OPPDIF [21] and is shown in fig. 7 for reference.

The pdfs of strain rate, show that the width of strain rate distribution decreases in the downstream direction for all 3 cases, presumably due to the jet development. It is also seen that cases B and C have a much larger distribution of strain rates compared to case A. S_d^*/S_L averages conditional on strain rate show that the slope of its response to strain rate, also known as Markstein length, is lower in the turbulent flames compared to the laminar strained flame. It is also seen that the displacement speed has a positive slope to negative strain rates.

Further, the correlation of displacement speed and its components to curvature is analyzed. Figure 8 shows the distribution of curvatures on the c = 0.65 iso-surface at the $x = 1/2L_x$



Figure 8: PDF of curvature conditional on c=0.65 at the 1/2 downstream location.

location. It is seen that the curvature distribution for all 3 cases look similar with only minor differences. It is seen that the curvature distribution is not symmetric and the distribution has a longer tail towards the positive curvature side. This shows that flames with very high positive curvatures (center of curvature is in the burnt gas) are more likely than those with very high negative curvatures. This quantitatively confirms the observation made based on fig. 2.

The average of $S_{\rm d}^*$ conditional on curvature and C=0.65is shown in figure 9 for all three cases. Also, the correlation of the components of S_d^* namely reaction, normal diffusion and curvature or tangential diffusion is shown in fig. 10 for case C (cases A and B had a similar correlation as case C and hence omitted). All three cases show a similar response to curvature with very little variation between the 3 cases. It is also seen that S_d^* shows a non-linear response to curvature with two distinct slopes - a higher slope on the negative curvature side and a lower slope on the positive curvature side. There are some similarities and differences with previously observed results by Echekki et al. [20]. It is seen that the curvature term has a low contribution towards the net displacement speed. The reaction term shows a two-slope correlation to curvature with a negative slope at negative curvatures and zero slope at positive curvatures. The non-linearity in the correlation of net S_d^* can be mainly attributed to the reaction term. Interestingly, it is seen that the normal diffusion component has a negative correlation to curvature and is not independent of curvature as was observed earlier [20]. Finally, it is confirmed that negative displacement speeds (flame receding) are possible at large positive curvatures.

5 Concluding Remarks

Three-dimensional direct numerical simulation of a spatiallydeveloping slot Bunsen flame was simulated at three successively higher turbulence intensities. The data was analyzed to compute the turbulent burning velocity. The statistics of the displacement speed of the flame surface was computed and its dependence on strain rate and curvature were studied. A budget of the displacement speed was computed and the correla-



Figure 7: PDF of strain rate conditional on c = 0.65 at the 1/2 downstream location.



Figure 9: Curvature conditional mean $S_{\rm d}^*$ on c=0.65 at the 1/2 downstream location.



Figure 10: Curvature conditional mean S_d^* components on c=0.65 at the 1/2 downstream location for case C.

tion of the constituent terms to curvature was analyzed. The results confirm several behavior that have been previous observed in simpler calculations. There are also some differences from previous two-dimensional simulations. Further work is necessary to fully analyze the data and obtain a thorough understanding of the dependence of the flame velocity on parameters of interest to the modelling community.

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References

- N. Peters. Journal of Fluid Mechanics, 384 (1999) 107– 132.
- D. Bradley. Proceedings of the Combustion Institute, 24 (1992) 247–262.
- K. N. C. Bray. Proceedings of the Royal Society of London, Series A, 431 (1990) 313–323.
- S. M. Candel and T. J. Poinsot. Combustion Science and Technology, 70 (1990) 1–15.
- R. S. Cant, B. Rogg, and K. N. C. Bray. Combustion Science and Technology, 69 (1990) 1–3.
- S. A. Filatyev, J. F. Driscoll, C. D. Carter, and J. M. Donbar. *Combustion and Flame*, 141 (2005) 1–21.
- R. J. Kee, J. F. Grcar, M. D. Smooke, and J. A. Miller. PREMIX: A fortran program for modeling steady laminar one-dimensional premixed flames. Technical Report SAND85-8240, Sandia National Laboratories, 1985.
- R. Sankaran, E. R. Hawkes, J. H. Chen, T. Lu, and C. K. Law. Study of turbulent premixed flame thickness using direct numerical simulations in a slot burner configuration. In *Proceedings of the 44nd Aerospace Sciences Meeting and Exhibit, Reno, USA*, 2006. AIAA Paper 2006-0165.
- R. Sankaran, E. R. Hawkes, J. H. Chen, T. Lu, and C. K. Law. *Proceedings of the Combustion Institute*, 31 (2007) 1291–1298.
- C. A. Kennedy and M. H. Carpenter. *Applied Numerical Mathematics*, 14 (1994) 367–458.
- 11. C. A. Kennedy, M. H. Carpenter, and R. M. Lewis. *Applied Numerical Mathematics*, 35 (2000) 177–264.
- R. J. Kee, F. M. Rupley, and J. A. Miller. Chemkin-II: A fortran chemical kinetics package for the analysis of gas-phase chemical kinetics. Technical Report SAND89-8009B, Sandia National Laboratories, 1991.
- T. J. Poinsot and S. K. Lele. Journal of Computational Physics, 101 (1992) 104–129.
- 14. J. C. Sutherland and C. A. Kennedy. *Journal of Computational Physics*, 191 (2003) 502–524.
- 15. C. S. Yoo, Y. Wang, A. Trouve, and H. G. Im. *Combustion Theory and Modelling*, 9 (2005) 617–646.
- C. S. Yoo and H. G. Im. Combustion Theory and Modelling, 11 (2007) 259–286.
- 17. S. B. Pope. Int J Eng Science, 26 (1988) 445-469.

- R. Sankaran, E. R. Hawkes, C. S. Yoo, J. H. Chen, T. Lu, and C. K. Law. Direct numerical simulation of stationary lean premixed methane-air flames under intense turbulence. In *Proceedings of the Fifth US Combustion Meeting*, 2007. Paper No. B09.
- T. Echekki and J. H. Chen. *Combustion and Flame*, 106 (1996) 184–202.
- 20. T. Echekki and J. H. Chen. *Combustion and Flame*, 118 (1999) 308–311.
- A. E. Lutz, R. J. Kee, J. F. Grcar, and F. M. Rupley. OP-PDIF: A fortran program for computing opposed-flow diffusion flames. Technical Report SAND96-8243, Sandia National Laboratories, 1997.