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Interactions between turbulence and flames in premixed reacting flows

Peter E. Hamlington,1,2,a) Alexei Y. Poludnenko,1 and Elaine S. Oran1
1Laboratories for Computational Physics and Fluid Dynamics, Naval Research Laboratory,
Washington, DC 20375, USA
2National Research Council Research Associateship Program

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The interactions between turbulence and flames in premixed reacting flows are studied for a broad range of turbulence intensities by analyzing scalar (reactant mass-fraction) gradient, vorticity, and strain rate fields. The analysis is based on fully compressible, three-dimensional numerical simulations of H2-air combustion in an unconfined domain. For low turbulence intensities, a flame reconstruction method based on the scalar gradient shows that the internal flame structure is similar to that of a laminar flame, while the magnitudes of the vorticity and strain rate are suppressed by heat release and there is substantial anisotropy in the orientation of intense vortical structures. As the turbulence intensity increases, the local flame orientation becomes increasingly isotropic, and the flame preheat zone is substantially broadened. There is, however, relatively little broadening of the reaction zone, even for high intensities. At high turbulence intensities, the vorticity and strain rate are only weakly affected by the flame, and their interactions with the scalar gradient are similar to those found in nonreacting turbulence. A decomposition of the total strain rate into components due to turbulence and the flame shows that vorticity suppression depends on the relative alignment between vorticity and the flame surface normal. This effect is used to explain the anisotropy of intense vortices at low intensities. The decomposition also reveals the separate effects of turbulent and dilatational straining on the flame width. © 2011 American Institute of Physics.
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I. INTRODUCTION

The interaction between a premixed flame and the turbulence in which it propagates is a fundamental problem in combustion theory. The ability to describe these interactions both qualitatively and quantitatively is required for practical problems ranging from the design of clean and efficient combustion engines to the prevention of gas explosions. Turbulence-flame interactions are also central to astrophysical problems, such as explosions of type Ia supernovae, which have many properties analogous to terrestrial gas-phase combustion.

In all of these applications, properties of both the turbulence and the flame depend on the relative strengths of chemical and turbulent processes, which are nonlinearly coupled.1,2 Chemical reactions result in heat release, which leads to changes in fluid properties such as the density and viscosity. These changes, in turn, affect the structure and dynamics of the turbulence. At the same time, turbulence transports the reactants and products and affects the structure of the flame.3 Combustion regime diagrams3,4 attempt to provide qualitative descriptions of the flame as the balance between chemical and turbulent processes varies, although questions remain about the quantitative characteristics of both the turbulence and the flame over a range of turbulence intensities. In the limit of high intensities, for example, turbulent diffusion is expected to significantly broaden the reaction zone in the flame. Prior studies5 have shown, however, that the reaction zone remains thin even at intensities where substantial broadening is expected to occur. Understanding this result requires consideration of the mutual interactions between the turbulence and the flame.

In this paper, we examine the interactions between turbulence and premixed flames using numerical simulations of stoichiometric H2-air combustion in an unconfined domain over a wide range of turbulence intensities, including very high intensities. The present study follows from previous simulations and analyses5,6 that have examined the details of turbulent flame acceleration and broadening for a single intensity. This study also substantially extends an earlier preliminary analysis7 of turbulence-flame interactions in premixed flames. Turbulence-flame interactions are studied here by analyzing the scalar (reactant mass fraction) gradient, vorticity, and strain rate fields, which, when taken together, allow the properties and interactions of the turbulence and the flame to be quantitatively characterized.

The scalar gradient, $\chi_i$, is defined in terms of the reactant mass fraction, $Y$, as

$$\chi_i \equiv \frac{\partial Y}{\partial x_i}, \quad (1)$$

where $Y = 1$ in the reactants and $Y = 0$ in the products. The magnitude and direction of $\chi_i$ determine the local flame width and orientation, respectively. Properties of the turbulence are characterized using the vorticity, $\omega_i$, and strain rate, $S_{ij}$, which are defined in terms of the velocity, $u_i$, as

$$\omega_i \equiv \epsilon_{ijk} \frac{\partial u_k}{\partial x_j}, \quad S_{ij} \equiv \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right). \quad (2)$$
where $\epsilon_{ijk}$ is the cyclic permutation tensor. Interactions between the turbulence and the flame can be understood from the coupled transport equations for $\chi_i$, $\omega_i$, and $S_{ij}$. Both $\omega_i$ and $S_{ij}$ appear explicitly in the equation for $\chi_i$, and all three quantities are affected by chemical reactions and heat release (as shown in Secs. III C and IV C).

The current understanding of how scalars and scalar gradients evolve in turbulent flows has been provided, in large part, by studies of the properties and coupled dynamics of $\chi_i$, $\omega_i$, and $S_{ij}$ in nonreacting turbulence,8–11 where $\chi_i$ in such flows represents the gradient of a passive, conserved scalar. In reacting flows, studies of non-premixed flames12–14 have shown that the properties of $\chi_i$, $\omega_i$, and $S_{ij}$ are substantially affected by chemical reactions and heat release. In particular, the scalar field is determined by a reaction-diffusion balance, and heat release affects the turbulence, causing, for example, changes in the nonlinear coupling between $\omega_i$ and $S_{ij}$ as well as the interactions between flames and coherent turbulent structures (including both vorticity22–24 and strain rate25,26 structures). Certain aspects of the dynamics and properties of $\chi_i$, $\omega_i$, and $S_{ij}$ in premixed reacting flows remain unclear; however, including the detailed effects of heat release on both $\omega_i$ and $S_{ij}$, and how all three fields—and, in particular, their coupling—vary with turbulence intensity and location in the flame.

Here, we examine these issues by studying the coupled dynamics and properties of $\chi_i$, $\omega_i$, and $S_{ij}$ over a wide range of intensities in premixed reacting flows. Conditional diagnostics based on the local, instantaneous values of $Y$ are used to examine the fields through the flame. Particular emphasis is placed on the internal structure of the flame; wrinkling is examined through distributions of the orientation of $\chi_i$, and the local flame width is connected to the magnitude of $\chi_i$ using an integral reconstruction method. Turbulence is characterized through the orientations and magnitudes of $\omega_i$ and $S_{ij}$, as well as through the characteristics of intense vortical structures. Turbulence-flame interactions are examined via the alignments of $\chi_i$, $\omega_i$, and the eigenvectors of $S_{ij}$, and by analyzing interaction terms in the transport equations for these quantities. Finally, a decomposition of the strain rate into turbulent and flame components is used to understand the variations in turbulence and flame properties with intensity and location in the flame.

II. NUMERICAL SIMULATIONS

The numerical simulations in this study solve the fully compressible, three-dimensional (3D) reactive flow equations5,6

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0, \quad (3)$$

$$\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} + \frac{\partial P}{\partial x_i} = 0, \quad (4)$$

$$\frac{\partial E}{\partial t} + \frac{\partial [(E + P) u_j]}{\partial x_j} - \frac{\partial}{\partial x_i} \left( K \frac{\partial T}{\partial x_i} \right) = -\rho q \dot{\omega}, \quad (5)$$

where $\rho$ is the density, $P$ is the pressure, $E$ is the energy density, $T$ is the temperature, $q$ is the chemical reaction rate, $Q$ is the chemical energy release, and $K$ and $D$ are the coefficients of thermal conductivity and molecular diffusion, respectively. The source term, $\dot{\omega}$, in Eqs. (5) and (6) is modeled using single-step, first-order Arrhenius kinetics as

$$\dot{\omega} = -ApY \exp \left(-\frac{Q}{RT} \right), \quad (7)$$

where $A$ is the pre-exponential factor, $Q$ is the activation energy, and $R$ is the universal gas constant. The molecular diffusion, $D$, and thermal conduction, $K$, are modeled as

$$D = D_0 \frac{T^n}{\rho}, \quad K = C_p \kappa_0 T^n, \quad (8)$$

where $D_0$, $\kappa_0$, and $n$ are constants and $C_p = \gamma R/M(\gamma - 1)$. The ideal gas equation of state is used for $P$, and the Lewis number, $Le = \kappa_0/D_0$, is unity for all simulations.

Equations (3)–(8) are solved with Athena-RFX,5 a reactive-flow version of the magnetohydrodynamic code Athena,27,28 using a high-order fully conservative Godunov-type method based on the unsplit, corner-transport upwind algorithm.29–30 Small-scale kinetic energy dissipation is provided by numerical viscosity, an approach which has been shown3 to extend the inertial range without placing prohibitive demands on computational resources.

Turbulence is generated and sustained in the simulations by injecting velocity perturbations at the largest scale of the flow. The imposed perturbations are isotropic and do not introduce any net momentum or artificial compressions/rarefactions (they are divergence-free).5 The perturbations are continued even after ignition of the flame, in contrast to prior studies2 of premixed flames in freely decaying turbulence. The intensity of the resulting turbulence is determined by the energy-injection rate of the driving, which is maintained at a constant value per unit volume throughout the simulation domain. This forcing procedure represents a situation in which energy is injected by motions on scales much larger than the characteristic scales of local variations in fluid properties. Examples of such systems include turbulence produced in the course of a type Ia supernova explosion by large-scale Rayleigh-Taylor-unstable plumes of hot product rising in the gravitational field of a star, or in terrestrial applications where reacting flows are driven by pistons or other machinery. The random velocity perturbation field is regenerated at time intervals of approximately $\tau_{ed}/40$ for all simulations, where $\tau_{ed} = U/L$ is the eddy turnover time and $U$ is the turbulent velocity at the scale of the domain width, $L$.

The simulations represent premixed, stoichiometric H$_2$-air combustion in an unconfined domain,5 with parameters in Eqs. (3)–(8) based on the reaction model of Gamezo et al.31 (as summarized in Table 1). Simulations at five different turbulence intensities, $I_T \equiv U/\beta S_L$, have been performed, where $U_l$ is the integral turbulent velocity in the reactants and $S_L$ is the speed of
the corresponding laminar H₂-air flame. The intensities vary
from $I_T = 2.45$ to 30.6, denoted F1–F5 in Table II, and are
shown on the combustion regime diagram in Fig. 1. The present
simulations are extensions of those carried out previously,5 in
which the turbulent flame properties were examined in detail
for a single intensity (F4 in the present study). In all cases, the
turbulence integral scale is $l = 1.90 \delta_L$, where $\delta_L \equiv (T_b - T_0)/
(\partial T/\partial x)_{L,max}$ is the thermal width of the laminar flame. This
value of $l$ makes it computationally feasible to survey a relatively
wide range of combustion regimes, as shown in Fig. 1,
while at the same time allowing the development of a realistic
turbulent flame with a complex, highly convoluted structure (the
flame brush width is $\gtrsim 10 \delta_L$, see also Ref. 5). As shown in Table
II, this range of simulation parameters corresponds to Dam-
köhler numbers $Da \equiv (l/U_L)/(l_f/\delta_L) = 0.39 - 0.03$, where
$l_f = D/\delta_L \approx 2 \delta_L$ is the full width of the laminar flame. The
corresponding range of Karlovitz numbers $Ka \equiv (l_f/l)^{1/2}(U/L)\delta_L^{3/2}$
is approximately $3.9 - 174.2$.32

For all computations, the domain has a physical width
$L = 0.259$ cm, with a length-to-width ratio of $L_x/(L_y, L_z) = 16:1$. The size of the computational grid in all cases is
$N_x \times N_y \times N_z = 2048 \times 128 \times 128$, giving 16 computational
cells per $\delta_L$. Both lower (8 cells per $\delta_L$) and higher (32 cells per $\delta_L$) resolutions have been examined5 for F4, and it was
found that the present resolution accurately captures properties
of the flame. At this resolution, the inertial range of the
turbulent cascade extends to scales $\approx \delta_L$ (see Fig. 2). It was
shown in Ref. 5 that further increases in the resolution,

### Table I. Input model parameters and resulting laminar flame properties common to all numerical simulations.5

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_0$ (K)</td>
<td>293</td>
</tr>
<tr>
<td>$P_0$ (Pa)</td>
<td>$1.01 \times 10^6$</td>
</tr>
<tr>
<td>$\mu_0$ (kg/m s)</td>
<td>$8.73 \times 10^{-4}$</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>1.17</td>
</tr>
<tr>
<td>$M$ (g/mol)</td>
<td>21</td>
</tr>
<tr>
<td>$A$ (cm$^{-5}$ K$^{-1}$ s)</td>
<td>$6.85 \times 10^{-12}$</td>
</tr>
<tr>
<td>$Q$ (kJ/kg)</td>
<td>$46.37 RT_0$</td>
</tr>
<tr>
<td>$q$ (kJ/kg)</td>
<td>$43.28 RT_0$</td>
</tr>
<tr>
<td>$\kappa_0$ (g/(s·cm K))</td>
<td>$2.9 \times 10^{-5}$</td>
</tr>
<tr>
<td>$D_0$ (g/(s·cm K))</td>
<td>$2.9 \times 10^{-5}$</td>
</tr>
<tr>
<td>$n$</td>
<td>0.7</td>
</tr>
<tr>
<td>$T_f$ (K)</td>
<td>2135</td>
</tr>
<tr>
<td>$\rho_f$ (kg/m$^3$)</td>
<td>$1.2 \times 10^{-5}$</td>
</tr>
<tr>
<td>$\delta_L$ (cm)</td>
<td>0.032</td>
</tr>
<tr>
<td>$S_L$ (cm/s)</td>
<td>302</td>
</tr>
</tbody>
</table>

### Table II. Initial turbulent-to-laminar flame speed ratio $I_T \equiv U/L_S$, Damköhler number, $Da \equiv (l/U_L)/(l_f/\delta_L)$, Karlovitz number $Ka \equiv (l_f/l)^{1/2}(U/L)\delta_L^{3/2}$, and eddy turnover time, $\tau_{ed} = L/U_L$, in the unburned mixture at ignition for the five simulations, denoted F1–F5. The number of temporal snapshots, $N_t$, used in the analysis of each case is shown in the last column.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>$I_T$ (U/$L_S$)</th>
<th>$Da$</th>
<th>$Ka$</th>
<th>$\tau_{ed}$ (s)</th>
<th>$N_t$</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1</td>
<td>2.45</td>
<td>0.39</td>
<td>3.9</td>
<td>$2.14 \times 10^{-4}$</td>
<td>540</td>
</tr>
<tr>
<td>F2</td>
<td>4.90</td>
<td>0.19</td>
<td>11.1</td>
<td>$1.07 \times 10^{-4}$</td>
<td>600</td>
</tr>
<tr>
<td>F3</td>
<td>9.81</td>
<td>0.10</td>
<td>31.5</td>
<td>$5.36 \times 10^{-5}$</td>
<td>630</td>
</tr>
<tr>
<td>F4</td>
<td>18.4</td>
<td>0.05</td>
<td>81.0</td>
<td>$2.86 \times 10^{-5}$</td>
<td>600</td>
</tr>
<tr>
<td>F5</td>
<td>30.6</td>
<td>0.03</td>
<td>174.2</td>
<td>$1.71 \times 10^{-5}$</td>
<td>600</td>
</tr>
</tbody>
</table>

### FIG. 1. (Color online) Combustion regime diagram4 showing the location of simulations F1–F5 (red squares). Here, $Re = (l/U_L)/(\nu L_S)$ is the Reynolds number, $Do$ is the Damköhler number, $Ka$ is the Karlovitz number, and $Ma_F$ is the turbulent Mach number in cold H₂-air fuel at atmospheric conditions.

Extending the inertial range to even smaller scales, do not affect either the internal structure of the flame or its dynamics. This is particularly important, since fully resolving the Kolmogorov scale, $\eta_K$, in the reactants using a realistic value of the physical viscosity of H₂-air for high $I_T$ would be computationally prohibitive. Periodic boundary conditions are used in the spanwise directions, resulting in a statistically planar flame in the $y-z$ plane, with a mean flow in the $x$-direction. The $x$-boundaries are periodic prior to ignition, at which time they are switched to zero-order extrapolation boundary conditions to prevent pressure build-up inside the domain.

### FIG. 2. (Color online) Instantaneous kinetic energy spectra in the full simulation domain immediately prior to ignition for F1–F5. Inertial ($k^{-5/3}$) and dissipation ($k^{-5}$) range scalings are shown by black dash-dot lines, and wavenumbers corresponding to $\delta_L$ and $2\delta_L$ are shown by vertical dashed lines.
Homogeneous isotropic turbulence is allowed to develop for $2\tau_{ed}$ before the flame is initialized in the domain. Instantaneous kinetic energy spectra immediately prior to ignition are shown in Fig. 2 for F1–F5. In all cases, the spectra follow an $E(k) \sim k^{-5/3}$ scaling (where $k$ is the wavenumber) to scales approximately equal to $\delta_L$, which is indicative of fully developed turbulence. After $2\tau_{ed}$, a planar flame is ignited near the center of the $x$-axis using the exact laminar profile characterized by the parameters in Table I. The analysis of the numerical data begins approximately $2\tau_{ed}$ after ignition ($4\tau_{ed}$ from the start of the simulation). Data snapshots are output approximately every $0.05\tau_{ed}$.

Dissipation of the turbulent kinetic energy causes gradual heating of the reactants. The relative temperature increase per $\tau_{ed}$ is $\Delta T/T = \Delta K_\text{ed} (\gamma - 1) \text{Ma}_F^2$, where $\Delta K_\text{ed} = 0.5$, $\text{Ma}_F = U/c_s$ is the turbulent Mach number in the reactants, and $c_s$ is the sound speed. Since $\text{Ma}_F$ increases with $I_F$ ($\text{Ma}_F = 0.033$ for F1 and $\text{Ma}_F = 0.41$ for F5), dissipative fuel heating becomes non-negligible for the highest $I_F$ examined here (1.8 K per $\tau_{ed}$ for F4 and 4.9 K per $\tau_{ed}$ for F5). This temperature increase causes $S_L$ to gradually grow and $\delta_L$ to decrease, thus affecting the overall turbulence-flame interaction. In order to avoid such systematic effects and to maintain statistical stationarity, the analysis of the data extends for a period of up to $1.5\tau_{ed}$ (over the range $4-5.5\tau_{ed}$ from the start of the simulation). During this time, properties of the flow are essentially stationary, as evidenced by the flame-brush averages of $\bar{f} \equiv \langle f \rangle_{t,x}^{1/2}$, $\omega \equiv \langle \omega_x \rangle_{t,x}^{1/2}$, $S \equiv \langle S_{y,z} \rangle_{t,x}^{1/2}$, and $\psi$ in Fig. 3. In order to achieve adequate statistical convergence while limiting the dissipative fuel-heating effects, the simulations were repeated multiple times from the beginning of the analysis period ($2\tau_{ed}$ after ignition or $4\tau_{ed}$ from the start of the run), ensuring nondeterministic system evolution on each iteration. This has allowed us to obtain between 540 and 630 snapshots for each value of $I_F$ (see Table II).

In addition to the reacting-flow cases, simulations of nonreacting, passive scalar evolution in homogeneous isotropic turbulence (with fluid properties identical to those of the reactants) were also carried out. The values of $I_F$ correspond to those used in F1–F5 (Table II), and the resolution is the same as that used for the reacting cases, with computational meshes of size $N_x \times N_y \times N_z = 128 \times 128 \times 128$ and periodic boundaries in all directions. Equations (3)–(6) are solved with $D$ and $K$ again given by Eq. (8) and with $\psi = 0$, so that, for these cases, the scalar is passive and conserved. Comparisons of the nonreacting and reacting simulations are used in the following to understand the effects introduced by exothermic reactions in premixed flames.

**III. TURBULENT FLAME PROPERTIES**

The instantaneous 3D isosurfaces of $Y$ in Fig. 4 show the structure of the flame folded inside the flame brush for simulations F1, F3, and F5. For a laminar flame, the isosurfaces are parallel at all $Y$. For turbulent flames as in Fig. 4, this is no longer necessarily the case, as wrinkling may occur over a broad range of scales. Figure 4 shows that for all $I_F$, there is less small-scale wrinkling near the products than the reactants, consistent with previous results for F4. As $I_F$ increases, the degree of small-scale wrinkling on both sides of the flame increases. The internal width of the turbulent flame is given by the separation between consecutive isosurfaces of $Y$, and Fig. 4 indicates that this separation is larger near the reactants than the products, and that it increases at most values of $Y$ with increasing $I_F$.

Changes in the flame width with $I_F$ are further illustrated by the two-dimensional (2D) instantaneous fields of $Y$ in Fig. 5. The $Y = 0.6$ contour in this figure denotes the approximate boundary between the preheat and reaction zones. In the following, the preheat zone is defined as the region where $0.6 < Y < 0.9$ while the reaction zone is the region where $0.1 < Y < 0.6$. Comparison with the laminar flame in Fig. 5(a) shows that the internal structures of the turbulent flames are broadened for F3 and F5 (Figs. 5(c) and 5(d)) in the preheat zone. This is evident from the greater separation between the $Y = 0.6$ and $Y = 0.9$ contours for these cases, as compared to the laminar flame contours in Fig. 5(a). The separation between these contours for F1 (Fig. 5(b)), however, is similar to that of the laminar flame, indicating that the preheat zone is only weakly broadened for low $I_F$. In the reaction zone, the separation between the $Y = 0.1$ and $Y = 0.6$
contours is close to the laminar case for all $I_T$. This indicates that the reaction zone is broadened substantially less than the preheat zone for the values of $I_T$ examined here, again consistent with prior results for F4. Both Figs. 4 and 5 show that the width of the flame brush, denoted $\delta_T$, is larger for F5 than F1, where $\delta_T$ is defined as the width of the region bounded by the minimum and maximum $x$ coordinates where $Y \geq 0.95$ and $Y \leq 0.05$ at all points with larger and smaller $x$, respectively.

A. Flame orientation and wrinkling

The turbulent flame structures in Figs. 4 and 5 can be analyzed quantitatively by examining the properties of $\gamma_i$, defined in Eq. (1). Here, we focus on flame wrinkling, which can be quantitatively described using the variations in the local normal to isosurfaces of $Y$. The orientation of this normal is given by $ni = \gamma_i / \tilde{\gamma}$, where $\tilde{\gamma} = (|\tilde{\gamma}_i| |\tilde{\gamma}|)^{1/2}$ is the scalar gradient magnitude. By definition, the normal points in the direction of increasing $Y$. Distributions of $ni$ along a particular isosurface can be used to determine the most probable orientation of the flame and the overall degree of flame wrinkling. Establishing the characteristic scales of wrinkling, however, requires additional analyses of spatial correlations in $ni$ along each $Y$ isosurface, which is not examined here.

Figure 6 shows conditional probability density functions (pdfs), $P(n_\|Y)$, of the component of $ni$ along the $x$-axis. Due to the periodic boundary conditions in the spanwise directions, $n_y$ and $n_z$ are approximately isotropically distributed for all $Y$ and $I_T$, and, hence, the corresponding pdfs are not shown here. The pdfs are conditioned on the local,.
instantaneous values of \(Y\) in the flame brush, which effectively allows variations in flow properties to be examined through the internal structure of the flame. The values of \(Y\) included in the conditional statistics are restricted to 0.002 \(\leq Y \leq 0.998\), since \(Y = 0\) and \(Y = 1\) (i.e., pure products and pure reactants, respectively) may occur in the flame brush at locations far from the flame itself. Following Kim and Pitsch, spatial variations of conditional statistics are neglected, since the inhomogeneity associated with these statistics is expected to be weaker than for the unconditional statistics. In a one-dimensional, planar laminar flame (e.g., Fig. 5(a)), \(n_i\) is oriented along the positive \(x\)-axis, giving a \(\delta\)-function pdf at \(n_i = 1\) for all \(Y\). Conversely, for a completely isotropic flame (namely, one that is equally likely to be oriented in any direction), \(P(n_i | Y)\) is given by a uniform distribution between \(n_i = -1\) and 1. Figure 6 shows that, for all \(I_f\) and \(Y\), \(P(n_i | Y)\) is greater than the isotropic profile for \(n_i \geq 0\) and smaller for \(n_i \leq 0\). This is indicative of a preferential orientation of the flame normal in the positive \(x\) direction (i.e., towards the reactants in Fig. 5). This orientation is most pronounced for low \(I_f\), and as \(I_f\) increases, \(P(n_i | Y)\) becomes increasingly similar to the isotropic pdfs, particularly for F4 and F5. This is consistent with the increased flame wrinkling observed in Figs. 4 and 5 for increasing \(I_f\). The pdfs in Fig. 6 further show that deviations from isotropy are generally larger in the reaction zone (\(Y < 0.6\)) than in the preheat zone (\(Y > 0.6\)), again consistent with the observation (Figs. 4 and 5) that the flame is less wrinkled near the products than the reactants.

It should be noted that the most probable value of \(n_i\) at \(Y = 0.1\) and 0.6 for F1 is \(n_i \approx 0.5\). The prevalence of this direction may be due to the combination of large-scale flame wrinkling and the periodic boundary conditions, which “buckle” the flame near the center of the domain (see, for example, Figs. 4(a) and 5(b)).

B. Flame width and reconstruction

The internal widths of the flame in Figs. 4 and 5 are given by the distance between isosurfaces of \(Y\), which can, in turn, be connected to the scalar gradient magnitude, \(\tilde{Y}\). Prior studies have noted that the local flame width can be inferred from the inverse of \(\tilde{Y}\), where large \(\tilde{Y}\) indicates a thin flame and small \(\tilde{Y}\) a broad flame. The connection between the local flame width and \(\tilde{Y}\) can be formalized by defining the instantaneous separation between two isosurfaces \(Y = Y_a\) and \(Y = Y_b\) as the average length of scalar gradient trajectories beginning from points on the \(Y_a\) isosurface and ending at points on the \(Y_b\) isosurface. By definition, scalar gradient trajectories follow the local value of \(n_i\) at each location in the flame, and we assume that \(Y \) is strictly increasing along the trajectories, with \(Y_a \leq Y \leq Y_b\). We also assume that trajectories do not cross, and that every trajectory beginning on the \(Y_a\) isosurface passes through the \(Y_b\) isosurface, and vice versa. This last condition is assumed to be true even if the \(Y_a\) and \(Y_b\) surfaces have different areas. These assumptions are valid if \(\tilde{Y} \neq 0\) for all \(0 < Y < 1\) in the flame brush, and if isolated pockets of partially burned reactants are neglected. In this framework, \(\tilde{Y} = 0\) for only \(Y = 0\) and \(Y = 1\), and all trajectories can be extended to cover the full range \(Y = [0, 1]\). Similar requirements were imposed on the flame reconstruction method outlined in Poludnenko and Oran, where it was noted that isolated pockets of unburned reactants are relatively rare in the simulations, even for high \(I_f\).

With these assumptions and conditions, the position along a scalar gradient trajectory can be parameterized using \(Y\), and the instantaneous length of one such trajectory between \(Y_a\) and \(Y_b\) is given by

\[
\delta(Y_a, Y_b) = \int_{Y_a}^{Y_b} \left(\frac{\partial Y}{\partial n} \right)^{-1} dY = \int_{Y_a}^{Y_b} \tilde{Y}^{-1}(Y) dY, \tag{9}
\]

where \(\partial n / \partial Y = (\partial Y / \partial n)^{-1} = \tilde{Y}^{-1}\) and \(\partial \| \partial x = n_i \partial / \partial x_i\) is the derivative along \(n_i\). For a laminar flame, where isosurfaces are parallel, all lengths given by Eq. (9) are equal, regardless of the starting location on the \(Y_a\) isosurface. For turbulent flames, however, the trajectory lengths may vary from one starting location to another. We can thus define an average width as

\[
\langle \delta(Y_a, Y_b) \rangle = \int_{Y_a}^{Y_b} \langle \tilde{Y}^{-1} \rangle dY, \tag{10}
\]

where \(\langle \cdot \rangle\) denotes an average over all space, time, and ensembles, and \(\langle \cdot | Y \rangle\) is a conditional average based on the local, instantaneous value of \(Y\). Once again, Eq. (10) is valid only if every scalar gradient trajectory beginning from the \(Y_a\) isosurface intersects the \(Y_b\) surface, and vice versa.

Although Eq. (10) provides a measure of the average separation between two isosurfaces in a turbulent flame, the flame width found using this relation depends on the choice of \(Y_a\) and \(Y_b\). To avoid placing arbitrary restrictions on the definition of the flame width (e.g., \(Y_a \approx 0.1\) and \(Y_b \approx 0.9\)), a local width can be defined at each \(Y\) as the separation between isosurfaces at \(Y\) and \(Y + \Delta Y\). Further letting \(\Delta Y \to 0\), we can then define a local turbulent flame width, \(\langle \delta(Y | Y) \rangle\), as

\[
\langle \delta(Y | Y) \rangle \equiv \lim_{\Delta Y \to 0} \frac{\langle \delta(Y, Y + \Delta Y) \rangle}{\Delta Y} = \langle \tilde{Y}^{-1} | Y \rangle, \tag{11}
\]

where \(\delta(Y | Y)\) is the notation used to denote the local internal width of the turbulent flame, since \(\delta(Y | Y)\) is more commonly used for the width of the turbulent flame brush. From Eq. (11), large values of \(\tilde{Y}^{-1}\) indicate a broad flame, while small values indicate a thin flame.

Figure 7 shows that, for all \(I_f\), \(\langle \delta(Y | Y) \rangle\) has a minimum at \(Y \approx 0.4\), and that it becomes larger than the laminar values with both increasing \(Y\) and \(I_f\). Values of \(\langle \delta(Y | Y) \rangle\) greater than one occur since \(\delta_L \sim (dT / dx)^{-1} L_{max}\) corresponds to the minimum local width of the laminar flame, and both the turbulent and laminar widths are larger than this value at most locations in the flame. Comparison of the turbulent and laminar curves in Fig. 7 thus indicates that turbulent flame broadening is greater in the preheat zone than in the reaction zone and that the broadening increases at all \(Y\) with \(I_f\). As in prior studies, however, there is relatively little flame broadening for \(Y < 0.6\) within the reaction zone, even for high \(I_f\).
FIG. 7. (Color online) Conditional averages of the local flame width \(\langle \delta_0 Y \rangle = \langle \tilde{\chi}^{-1} Y \rangle\) in the flame brush for F1–F5. Conditional averages are normalized using \(\delta_t\). Inset shows \(\langle \tilde{\chi} Y \rangle\) normalized by \(\delta_t\). Legend is given in Fig. 8.

With respect to the \(\tilde{\chi}\) field itself, the inset of Fig. 7 shows that \(\langle \tilde{\chi} Y \rangle\) reaches a maximum near \(Y \approx 0.4\) and decreases towards the products and reactants. The qualitative dependence of \(\langle \tilde{\chi} Y \rangle\) on \(Y\) is similar for all \(I_T\), but Fig. 7 does show that \(\langle \tilde{\chi} Y \rangle\) decreases at all \(Y\) with increasing \(I_T\). Only for low \(I_T\) (i.e., F1 and F2) is there reasonable agreement between the laminar and turbulent curves. It should be noted that although curves of \(\langle \tilde{\chi}^{-1} Y \rangle\) and \(\langle \tilde{\chi} Y \rangle^{-1}\) are equal for a laminar flame, this is not generally true for a turbulent flame.

Using the distributions of \(\langle \delta_0 Y \rangle\) in Fig. 7, an average local internal structure of the turbulent flames can be reconstructed from Eq. (10). The average flame-normal coordinate, denoted \(\langle n Y \rangle\), corresponding to each \(Y\) can be calculated from \(\langle \tilde{\chi}^{-1} Y \rangle\) as

\[
\langle n Y \rangle = \langle n Y = 0 \rangle + \int_0^Y \langle \tilde{\chi}^{-1} \rangle d\eta, \quad (12)
\]

where \(\langle n Y = 0 \rangle\) denotes the (arbitrary) location corresponding to \(Y = 0\), and \(\eta\) is a dummy integration variable. Numerical integration of Eq. (12) is carried out after first interpolating \(\langle \tilde{\chi}^{-1} Y \rangle\) to a grid with smaller \(Y\) spacing. This approach gives profiles of \(Y\) as a function of \(\langle n Y \rangle\), which reflect the average local internal structure of the turbulent flame. The resulting profiles in Fig. 8 show that the preheat zone is broader than the reaction zone, and that the flame width increases with \(I_T\) for all \(Y\). The reconstructed profiles in Fig. 8 are consistent with the flame structure for F4 obtained using an alternative method outlined in a previous study.

Quantitative measures of the reaction and preheat zone widths can be obtained from the profiles in Fig. 8. Table III shows that while the reaction and preheat zones have similar widths for F1, the preheat zone is nearly twice as wide as the reaction zone for the highest \(I_T\) examined here (F5). Similarly, while the width of the preheat zone increases by nearly a factor of three from F1 to F5, there is a much less dramatic increase in the width of the reaction zone with \(I_T\) (the reaction zone broadens by \(\approx 50\%\) from F1 to F5). Table III also shows that the width of the overall flame brush increases weakly with \(I_T\), consistent with the 2D fields in Fig. 5.

C. Flame-structure dynamics

The dynamics of \(n_i\) and \(\delta_t = \tilde{\chi}^{-1}\) are given by the transport equations

\[
\frac{Dn_i}{Dt} = \frac{1}{\chi} (\delta_{ij} - n_i n_j) \frac{D\tilde{\chi}_j}{Dt}, \quad (13)
\]

\[
\frac{D\delta_t}{Dt} = -\delta_t^2 n_i \frac{D\tilde{\chi}_i}{Dt}, \quad (14)
\]

where \(D/Dt = \partial/\partial t + u_j \partial/\partial x_j\) and \(D\tilde{\chi}/Dt\) is obtained from Eq. (6) as

\[
\frac{D\tilde{\chi}_i}{Dt} = -n_j \tilde{\chi}_{ij} - \frac{\tilde{\chi}}{2} \epsilon_{ijk} n_k \omega_k + \frac{\partial}{\partial x_i} \left[ \mathbf{v} + \frac{1}{\rho} \partial (\rho D\tilde{\chi}_j) / \partial x_j \right]. \quad (15)
\]

Due to the prefactors involving \(n_i\) in Eqs. (13) and (14), only those terms of Eq. (15) that are perpendicular to \(n_i\) directly

<table>
<thead>
<tr>
<th>Simulation</th>
<th>Reaction zone ((\delta_t))</th>
<th>Preheat zone ((\delta_t))</th>
<th>Flame brush (\delta_t/\delta_L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1</td>
<td>0.60</td>
<td>0.61</td>
<td>12.1</td>
</tr>
<tr>
<td>F2</td>
<td>0.64</td>
<td>0.83</td>
<td>12.5</td>
</tr>
<tr>
<td>F3</td>
<td>0.71</td>
<td>1.2</td>
<td>13.6</td>
</tr>
<tr>
<td>F4</td>
<td>0.84</td>
<td>1.4</td>
<td>14.5</td>
</tr>
<tr>
<td>F5</td>
<td>0.91</td>
<td>1.7</td>
<td>15.7</td>
</tr>
</tbody>
</table>
affect the dynamics of \( n_i \), while only the terms parallel to \( n_i \) affect \( \delta_i \). Consequently, the first two terms on the right-hand side of Eq. (15) both affect the flame orientation and wrinkling, but the \( \omega_i \) term, which is always perpendicular to \( n_i \), plays no direct role in the evolution of the local flame width.

The effects of \( \omega_i \) and \( S_{ij} \) on \( n_i \) can be examined by considering the alignment of \( n_i \) with the unit vector \( \vec{\omega}_i = \omega_i / \omega_i \) (where \( \omega_i = [\omega_i, \omega_i]^{1/2} \)) and with the eigenvectors of \( S_{ij} \), denoted \( \vec{e}_i \), corresponding to eigenvalues, \( s_i, \) ordered as \( s_1 \geq s_2 \geq s_3 \). The alignments are given by \( |\vec{e}_i \cdot \vec{n}| \) and \( \vec{\omega}_i \cdot \vec{n} \), which are equal to 1 for perfectly aligned vectors, 0 for perfectly misaligned (i.e., perpendicular) vectors and -1 for anti-parallel vectors. These alignments give insights into the effects of \( \omega_i \) and \( S_{ij} \) on the flame orientation, as well as the nature of the coupling between the turbulence and the flame. For example, if \( \omega_i \) and \( S_{ij} \) are independent of \( n_i \), as occurs in passive scalar evolution in nonreacting turbulence, then \( n_i \) aligns perpendicular to \( \vec{\omega}_i \) and parallel to \( \vec{e}_i \). As the coupling between \( \omega_i \), \( S_{ij} \), and \( n_i \) changes in reacting flows, however, these alignments may vary or be lost altogether.

Figure 9 shows that throughout the flame for high \( I_T \) and within the preheat zone for low \( I_T \), alignments of \( n_i \) with \( \vec{e}_i \) and \( \vec{\omega}_i \) are similar to those found in passive scalar evolution in nonreacting flows \(^8, ^34\) (last column of Fig. 9). In particular, \( n_i \) is preferentially aligned with \( \vec{e}_3 \) and misaligned with \( \vec{\omega}_1 \). The similarity to passive scalar alignments suggests that, for high \( I_T \), the flame and its corresponding scalar gradient field have only weak effects on \( \omega_i \) and \( S_{ij} \). As \( I_T \) decreases, the alignments in Fig. 9 change substantially, and for low \( I_T \) (Fl in Fig. 9a), there is preferential alignment between \( n_i \) and \( \vec{e}_1 \) in the reaction zone. This result has been observed in prior studies of premixed flames, \(^2, ^15, ^16, ^18\) and is discussed in more detail in Sec. V. There is, additionally, no preferred alignment between \( \vec{\omega}_i \) and \( n_i \) for low \( I_T \) in the reaction zone (i.e., the two vectors are randomly oriented with respect to each other), indicating that the dynamics of \( n_i \) and the full \( \omega_i \) field are only weakly coupled (although, as will be shown in Sec. IV D, there are preferential alignments between \( n_i \) and intense vortical structures for low \( I_T \)).

The alignments in Fig. 9 indicate that the dynamics of \( n_i \), \( \omega_i \), and \( S_{ij} \) (and, hence, the flame and the turbulence) vary substantially as a function of \( I_T \) and location in the flame. These changes are ultimately responsible for the variations in flame wrinkling with \( I_T \) and \( Y \) observed qualitatively in Figs. 4 and 5, and quantitatively in Fig. 6. In particular, the increased wrinkling for high \( I_T \) and in the preheat zone for all \( I_T \) is due to the passive evolution of \( n_i \), where the flame orientation dynamics are dominated by \( \omega_i \) and \( S_{ij} \). Consequently, \( n_i \) becomes increasingly isotropic due to the isotropy of the \( \omega_i \) and \( S_{ij} \) fields, resulting in greater flame wrinkling. For lower \( I_T \) and within the reaction zone, \( n_i \) is no longer passive, the effects of \( \omega_i \) and \( S_{ij} \) on \( n_i \) and the flame are altered, and the flame is subsequently less wrinkled.

Changes in the alignments—and the underlying turbulence-flame dynamics—also affect the flame width through the interaction between \( S_{ij} \) and \( \delta_i \) in Eqs. (14) and (15). The alignments between \( n_i \) and \( \vec{e}_i \), in particular, determine the sign and magnitude of the production term \( n_i \delta_i \vec{S}_{ij} \) in the equation for \( n_i \delta_i \vec{S}_{ij} \) (which appears in Eq. (14) for the evolution of \( \delta_i \)). This term can be written explicitly as \(^2\)

\[
\frac{n_i \delta_i \vec{S}_{ij}}{Y} = \frac{\vec{\omega}_i}{2} \left( s_1 |\vec{e}_1 \cdot \vec{n}|^2 + s_2 |\vec{e}_2 \cdot \vec{n}|^2 + s_3 |\vec{e}_3 \cdot \vec{n}|^2 \right).
\]

where the alignments weigh the effects of the \( S_{ij} \) eigenvalues and play a critical role in determining whether strain acts to increase \( \delta_i \) and, thus, broaden the flame, or decrease it. Figure 10 shows that, for low \( I_T \), the conditional average of \( n_i \delta_i \vec{S}_{ij} \) is positive for nearly all \( Y \) and has a \( Y \)-dependence similar to that found in a laminar flame (with a peak near \( Y = 0.4 \)). As \( I_T \) increases, \( \langle n_i \delta_i \vec{S}_{ij} \rangle \) becomes increasingly negative, again with the largest magnitude occurring near \( Y = 0.4 \), resulting in thinning of the flame. The curves in Fig. 10 thus indicate that, on average, the effect of \( S_{ij} \) is to increase \( \delta_i \) for low \( I_T \) and to reduce it for high \( I_T \), consistent with results from prior studies of premixed flames. \(^15, ^16, ^18\)

The relatively thin flame in the reaction zone for high \( I_T \) (discussed in Sec. III B and shown in Figs. 7 and 8) is thus due, in part, to the thinning effect of \( S_{ij} \) on \( \delta_i \) shown in Fig. 10.

**IV. TURBULENCE PROPERTIES**

The evolution and properties of turbulent flames, which have been characterized in Sec. III C using \( n_i \) and \( \delta_i \), depend
directly on \( \omega \) and \( S_{ij} \), as shown in Eqs. (13)–(15). Because \( \omega \) and \( S_{ij} \) are functions of velocity gradients (see Eq. (2)), they reflect the small-scale structure of the turbulence, and their magnitudes, orientations, and relative alignments provide insights into the effects of the flame on the turbulence.

Instantaneous 2D fields of the magnitudes \( \omega_i = \frac{\partial u_i}{\partial x_i} \) and \( S_{ij} = \frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \) along the center of the y-axis are shown in Fig. 11 for F1, F3, and F5, where \( S \equiv [S_{ij}S_{ji}]^{1/2} \) and \( \langle \cdot \rangle \) denotes a time-dependent spatial average over the full domain. Both \( \omega \) and \( S \) are homogeneous in the reactants for all \( I_T \), and Fig. 11 shows that there are spatially localized, high-amplitude fluctuations in both fields. These fluctuations are larger for \( \omega \) than \( S \), consistent with results from prior studies of homogeneous isotropic turbulence.

For the lower values of \( I_T \) in Figs. 11(a) and 11(b), \( \omega \) and \( S \) are generally smaller on the product side of the flame, although relatively rare regions of intense \( \omega \) and \( S \) do still occur in the flame brush. The suppression of these fields occurs abruptly near the \( Y = 0.6 \) surface separating the preheat and reaction zones, and both \( \omega \) and \( S \) remain small downstream of the flame (i.e., into the products). For F1, the magnitudes are small even beyond the bounds of the flame brush, although the downstream extent of this suppressed region decreases as \( I_T \) increases (as shown in Fig. 11(b) for F3). For high \( I_T \) (F5 in Fig. 11(c)), there is little suppression of \( \omega \) and \( S \) across the flame.

The fields in Fig. 11 indicate that \( \omega \) and \( S \)—and hence small-scale turbulence—are suppressed by the flame for low \( I_T \), but this suppression becomes less pronounced as \( I_T \) increases. The characteristics of intense 3D vortical structures provide additional insights into the suppression of turbulence within the flame brush, as well as into the small-scale structure and anisotropy of the flow. Figure 12 shows vortical structures identified as regions of large second invariant of the traceless velocity gradient tensor, \( Q = -\frac{1}{4}A^*_{ij}A^*_{ji} \), where \( A^*_{ij} = \frac{\partial u_i}{\partial x_j} - \frac{1}{3}\delta_{ij}S_{kk} \), \( A_{ij}^* = (S_{ij}S_{ji})^{1/2} \), and \( S_{ij}^* = S_{ij} - \frac{1}{3}\delta_{ij}S_{kk} \). Physically, such regions are characterized by the dominance of vorticity over strain, as would be expected in the vicinity of a typical turbulent vortex (e.g., in the Burgers model of turbulent vortices). Following the approach used by Pirozzoli et al. in the study of supersonic boundary layers, the traceless tensors \( A^*_{ij} \) and \( S^*_{ij} \) are used here in the definition of \( Q \) in order to remove the influence of nonzero divergence within the flame brush; this divergence is not directly associated with the structure of turbulent vortices and thus is not included in the identification procedure. Alternative vortex identification methods are also possible, but, for homogeneous isotropic turbulence, it has been shown that most such approaches yield essentially identical vortical structure regions.
Vortical structures are identified in Fig. 12 by isosurfaces of $Q = 0.02 Q_{\text{max}}$, where $Q_{\text{max}}$ is the maximum value of $Q$ in the products for each $I_T$. The center of the flame brush is at $x/d_L = 0$, and the semi-transparent green isosurfaces correspond to the $Y = 0.6$ flame surface (see Fig. 4). Axes are in units of $d_L$.

Vortical structures are identified in Fig. 12 by isosurfaces of $Q = 0.02 Q_{\text{max}}$, where $Q_{\text{max}}$ is the maximum value of $Q$ in the domains shown in Fig. 12 for each $I_T$. The structures are tube-like, consistent with previous studies that cover a wide range of flows.\textsuperscript{38,40,41} The structures are suppressed across the flame for low $I_T$, but the suppression becomes less pronounced as $I_T$ increases, consistent with the behavior of $\omega$ and $S$ across the flame in Fig. 11. There are relatively few structures immediately downstream of the flame for F1 and F3, and the structures that are present tend to be oriented along the $x$-axis. This anisotropy in the flow is not present in the reactants and products far from the flame brush, where structures are randomly oriented. Similar anisotropy was also observed by Tanahashi \textit{et al.}\textsuperscript{23} for low $I_T$, and Fig. 12 further indicates that the anisotropy is increasingly lost as $I_T$ increases. In particular, there is no apparent change in the orientation of the structures across the flame brush for F5 in Fig. 12, suggesting that the turbulence remains isotropic throughout the flame for high $I_T$.

It should be noted that, despite the fact that the turbulence is homogeneous and isotropic in both the reactants and products far from the flame brush, $\omega$ and $S$ in Fig. 11 have slightly larger amplitudes in the products than in the reactants. This is due to the turbulence forcing described in Sec. II, which is maintained at a constant rate per unit volume throughout the simulation domain. Since the fluid density decreases from the reactants to products (due to heat release), this gives larger forcing per unit mass in the products, and, hence, more intense velocities.

A. Vorticity and strain rate magnitudes

While Figs. 11 and 12 provide qualitative insights into the properties of $\omega_i$ and $S_{ij}$ through the flame brush, quantitative changes in these fields through the flame itself can be examined using conditional statistics based on $Y$, as is also done in the turbulent flame analysis in Sec. III. Here, we examine the magnitudes $\omega$ and $S$, while the orientations of $\omega_i$ and $S_{ij}$ given by $\vec{e}_i$ and $e_i$, respectively, are examined in Sec. IV B.

For low $I_T$, the conditional averages of $\omega$ and $S$ in Figs. 13(a) and 13(b) are largest in the preheat zone and decrease towards the reaction zone, consistent with Figs. 11 and 12. As $I_T$ increases, the suppression of $\omega$ and $S$ becomes less pronounced, and for F5, there are only small changes in the conditional averages of $\omega$ and $S$ through the flame. As in Fig. 11, Figs. 13(a) and 13(b) indicate that small-scale
turbulence (the strength of which is reflected in the magnitudes $\omega$ and $S$) is suppressed in the flame for low $I_T$, but is only weakly affected by the flame for high $I_T$.

The basic shapes of the curves in Figs. 13(a) and 13(b) are similar for all $I_T$, with two exceptions. First, within the preheat zone for the highest $I_T$ (e.g., F5), the conditional average of $\omega$ is greater than the corresponding average near $Y = 1$. The exact mechanism by which this increase occurs is not immediately clear. Baroclinic torque provides a possible source of increased $\omega$ and is discussed in more detail in Sec. IV C.

Furthermore, Fig. 13(b) shows that for the lowest $I_T$ (F1), $\langle S \rangle[Y]$ has a local maximum near $Y = 0.4$. This increase is due to nonzero (positive) divergence, $S_{kk}$, resulting from heat release and fluid expansion by the flame. Figure 13(c) shows that the conditional average of $S_{kk}$ is largest in the reaction zone and increases relative to $\langle S \rangle[Y = 1]$ as $I_T$ decreases. For low $I_T$, $S_{kk}$ dominates the divergence-free part of $S_{ij}$ associated with the turbulence entering the flame from the reactants, resulting in increased $\langle S \rangle[Y]$ at $Y \approx 0.4$. As $I_T$ increases, the intensity of the incoming turbulence is larger with respect to $S_{kk}$, and the local increase in $\langle S \rangle[Y]$ is lost. Inherent in this explanation is a distinction between the straining associated with the turbulence and that produced by the flame. These two constituents of the strain rate are used in Sec. V to understand many of the variations in turbulence and flame properties with $I_T$ and $Y$ outlined here and in Sec. III.

B. Vorticity and strain rate orientations

The orientations of $\omega_i$ and $S_{ij}$ provide insights into the anisotropy associated with the turbulence, and are characterized, respectively, by $\hat{\omega}_i$ and $e_i$. Similar to the analysis of $n_i$ in Fig. 6, Fig. 14 shows conditional pdfs, $P(|\hat{\omega}_i|)[Y]$, of the component of $\hat{\omega}_i$ along the $x$-axis. With the exception of the lowest value of $I_T$ (F1), $P(|\hat{\omega}_i|)[Y]$ becomes increasingly different from the isotropic pdfs with decreasing $I_T$ throughout the flame, particularly near the products, with $\hat{\omega}_i$ being preferentially oriented parallel to the $x$-axis. For high $I_T$ (F4 and F5), the pdfs are close to the isotropic profiles at all $Y$, although there is a slight preference for alignment parallel to the $x$-axis.

For F1, the variations in the $|\hat{\omega}_i|$, pdfs with $Y$ are qualitatively different from those at higher values of $I_T$. Within the preheat zone, the orientation of $\hat{\omega}_i$ along the $x$-axis is stronger for F1 than for the higher values of $I_T$, but this orientation actually becomes less pronounced in the reaction zone. In particular, Fig. 14 shows that, for F1, the deviations from isotropy are, in fact, largest near the reactants, whereas the pdfs near the products are closer to isotropy. This trend may be connected to the large suppression of $\omega$ by the flame for low $I_T$ (see Fig. 13(a)), since it will be shown in Sec. IV D that the variation of intense vortical structure orientations with $Y$ is similar for all $I_T$.

Conditional pdfs of the components of $e_1$ and $e_3$ along the $x$-axis, denoted $e_{1x}$ and $e_{3x}$, respectively, are shown in Figs. 15 and 16. The pdfs of $e_{3x}$ are relatively close to the isotropic profiles for all $I_T$ and $Y$, and thus are not shown here. Figure 15 shows that the pdfs of $e_{1x}$, are essentially isotropic for all but the lowest values of $I_T$ (F1 and F2). At these lower intensities, $e_1$ is preferentially oriented parallel to the $x$-axis, a tendency that is more pronounced near the products. More substantial variations with $I_T$ are observed in Fig. 16 for $e_{3x}$. For F1–F3, $e_3$ is preferentially oriented in the $y$–$z$ plane (corresponding to $e_{3y} \approx 0$), but this preferred orientation becomes weaker with both increasing $Y$ (from products to reactants) and $I_T$. Relatively close agreement with the isotropic pdfs is found near the reactants for all $I_T$, and for the
highest \( I_T \) (F4 and F5), \( \mathbf{e}_3 \) is approximately isotropically distributed at all \( Y \).

Figures 14–16 thus indicate that, for all but the lowest \( I_T \) (F1), the turbulence is close to isotropy in the preheat zone (\( Y > 0.6 \)) for low \( I_T \) and at all \( Y \) for high \( I_T \). Substantial anisotropy does occur for low \( I_T \) within the reaction zone (\( Y < 0.6 \)). For F1, however, \( \tilde{\omega}_1 \) is actually more anisotropic near the reactants than the products, while \( \mathbf{e}_3 \) is more anisotropic near the products.

C. Dynamics and alignments of vorticity and strain rate

The evolution of \( \omega_i \) is given by the transport equation

\[
\frac{D\omega_i}{Dt} = \omega_j S_{ij} - \omega_i S_{ik} + \frac{\epsilon_{ijk}}{\rho^2} \frac{\partial \rho}{\partial x_j} \frac{\partial P}{\partial x_k},
\]

(17)

where viscous effects have been neglected, consistent with Eq. (4). The first term on the right in Eq. (17) is a vorticity production term involving interactions between \( \omega_i \) and \( S_{ij} \). The second and third terms arise due to variable density effects and represent dilatation and baroclinic torque, respectively. These last two terms are of particular importance in reacting flows since fluid expansion across the flame results in values of \( |\varepsilon_{3s}| \) equal to 0 are perpendicular to the \( x \)-axis and values equal to 1 are parallel to the \( x \)-axis.

The evolution of \( S_{ij} \) is given by the transport equation

\[
\frac{DS_{ij}}{Dt} = -S_{ik} S_{kj} - \frac{1}{\rho^2} \left( \frac{\partial \rho}{\partial x_i} \frac{\partial P}{\partial x_j} + \frac{\partial P}{\partial x_i} \frac{\partial \rho}{\partial x_j} \right) + \frac{1}{\rho^2} \left( \frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_j} + \frac{\partial \rho}{\partial x_j} \frac{\partial \rho}{\partial x_i} \right)
\]

(19)

dilatation and baroclinic torque are significant with respect to production, but for high \( I_T \), they have only weak effects on the evolution of \( \omega \). The growing influence of dilatation on \( \omega \) at lower \( I_T \) is responsible for the suppression of \( \omega \) shown in Fig. 13(a). As \( I_T \) increases, this term becomes overwhelmed by the (positive) production term, and the resulting dynamics are similar to those found in nonreacting turbulence. While the baroclinic torque becomes less important relative to the production term as \( I_T \) increases, the absolute magnitude of this term (not shown here) actually grows with \( I_T \). This suggests, in part, that the gradients of \( \rho \) and \( P \) become increasingly misaligned for high \( I_T \), consistent with the increasingly wrinkled flame surfaces shown in Figs. 4 and 5.

The production term in the transport equation for \( \omega \), which is given using Eq. (17) as \( \tilde{\omega}_i \omega_j S_{ij} \), is responsible for the creation of small-scale structure and the transfer of energy from large to small scales in turbulent flows.\(^{35}\) The relative alignments between \( \tilde{\omega}_i \) and \( \mathbf{e}_j \) play a key role in determining the magnitude of this term (similar to the \( \delta \) production term in Eq. (16)), as shown by

\[
\tilde{\omega}_i \omega_j S_{ij} = \omega \left( s_1 |\mathbf{e}_1 \cdot \tilde{\omega}|^2 + s_2 |\mathbf{e}_2 \cdot \tilde{\omega}|^2 + s_3 |\mathbf{e}_3 \cdot \tilde{\omega}|^2 \right).
\]

(18)

As in the analysis of the \( n_i \) dynamics in Sec. III C, the alignments between \( \tilde{\omega}_i \) and \( \mathbf{e}_j \) also reflect the nature of the coupling between \( \omega_i \) and \( S_{ij} \) in turbulent flows. This coupling is nonlinear, as indicated by the transport equation for \( S_{ij} \) given by

\[
\frac{DS_{ij}}{Dt} = -S_{ik} S_{kj} - \frac{1}{\rho^2} \left( \frac{\partial \rho}{\partial x_i} \frac{\partial P}{\partial x_j} + \frac{\partial P}{\partial x_i} \frac{\partial \rho}{\partial x_j} \right) + \frac{1}{\rho^2} \left( \frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_j} + \frac{\partial \rho}{\partial x_j} \frac{\partial \rho}{\partial x_i} \right)
\]

(19)
where viscous effects have again been neglected. In non-reacting turbulence, the nonlinear coupled dynamics of $\omega_i$ and $S_{ij}$ given by Eqs. (17) and (19) result in $\omega_i$ being preferentially aligned with $e_2$, preferentially misaligned with $e_3$, and randomly aligned with $e_1$.

The conditional pdfs in Fig. 18 show that the alignments between $\omega_i$ and $e_i$ in premixed flames are generally similar to those found in nonreacting turbulence for all $Y$ and $I_T$. In particular, there is preferential alignment between $\omega_i$ and $e_2$, misalignment with $e_3$, and no preferred alignment with $e_1$. Within the reaction zone for low $I_T$, however, there is weak alignment between $\omega_i$ and $e_1$. A similar increase in this alignment has also been observed in non-premixed reacting flows and suggests that the two-way nonlinear coupling between $\omega_i$ and $S_{ij}$ is affected in the reaction zone for low $I_T$. In particular, these alignments for low $I_T$ are consistent with a decoupling of the two-way nonlinear interactions between $\omega_i$ and $S_{ij}$, which are responsible for the alignment between $e_2$ and $\omega_i$ observed in nonreacting turbulence and in reacting turbulence at high $I_T$.

D. Vortical structure orientations

The $Q$ isosurfaces in Fig. 12 indicate that, for low $I_T$, intense vortical structures are preferentially aligned in the $x$-direction on the product side of the flame. The orientation of these structures through the flame itself can be examined quantitatively by calculating conditional pdfs of $\omega_i$ within regions of intense $Q$. Figure 19 shows that, for low $I_T$, the vorticity within these regions is preferentially oriented parallel to the $x$-axis, particularly in the reaction zone. For $F1$, this preferential orientation is actually more pronounced near the products than the reactants, contrary to the orientations between $\omega_i$ and $e_1$ observed in nonreacting turbulence and in reacting turbulence at high $I_T$.

While the pdfs in Fig. 19 suggest that substantial vortical structure anisotropy is generated in the flame for low $I_T$, the instantaneous fields in Fig. 12 further indicate that this anisotropy persists within the flame brush downstream of the flame. This persistence can be quantified by calculating vortical structure pdfs $P(\{|\omega_i|\} | Q > 0.01Q_{\text{max}})$ in $y$–$z$ planes downstream of the center of the flame brush ($x/\delta L = 0$). Figure 20 shows these pdfs up to $x/\delta L = 10$, where the statistics have been calculated over nine consecutive $y$–$z$ planes centered on each downstream value of $x/\delta L$. As in Figs. 14 and 19, vortical structures are preferentially oriented parallel to the $x$-axis, particularly for low $I_T$ and at locations near the flame brush center. For $F1$, departures from the isotropic pdfs are observed up to $x/\delta L \approx 10$, consistent with the 3D structure orientations shown in Fig. 12(a). The departures from isotropy downstream of the flame become weaker as $I_T$ increases, and are lost after $x/\delta L \approx 6$ for $F2$ and $x/\delta L \approx 4$ for $F3$. The pdfs for $F4$ and $F5$ are nearly identical to the isotropic profiles at all $x/\delta L$. Figures 19 and 20 thus indicate that the anisotropy generated in the flame brush is strongest—and persists the greatest downstream distance—when $I_T$ is low. For high $I_T$, there is essentially no vortical structure anisotropy generated near the flame.
Finally, conditional pdfs of vortical structure alignment with \( n_i \) are shown in Fig. 21. These pdfs directly probe the interactions between intense vortices and the flame. For low \( I_T \), Fig. 21 shows that the alignments between the structures and \( n_i \) are different than those observed for the full \( \omega_i \) field (Fig. 9) or for nonreacting, passive scalar evolution (last column in Fig. 21). In particular, \( \tilde{\omega}_i \) and \( n_i \) are preferentially aligned in the reaction zone for F1 in Fig. 21(a). This alignment between vortical structures and \( n_i \) is even stronger than that observed for the full \( \omega_i \) field in nonreacting, passive scalar evolution. This suggests that the flame responds in a nearly completely passive manner to intense vortices for sufficiently high \( I_T \), and that the effect of the vortices is to orient the local flame normal \( (n_i) \) in a direction that is perpendicular to their axes.

V. DISCUSSION

The results in Secs. III and IV show that properties of both the flame and the turbulence vary smoothly with \( I_T \) and \( Y \) (i.e., location in the flame). The internal structure of the flame is similar to that of a laminar flame for low \( I_p \), but becomes increasingly wrinkled and broadened as \( I_T \) increases (although broadening remains relatively weak in the reaction zone even for high \( I_T \)). Conversely, the \( \omega_i \) and \( S_{ij} \) fields are anisotropic with suppressed magnitudes in the flame brush for low \( I_T \), but are only weakly affected by the flame for high \( I_T \). Analyses of the alignments between \( n_i \), \( \tilde{\omega}_i \), and \( e_i \) indicate that the flame responds passively to \( \omega_i \) and \( S_{ij} \) at all \( Y \) for high \( I_T \), and in the preheat zone for lower \( I_T \). For low \( I_T \), heat release effects play a substantial role in the dynamics of \( \omega_i \) and \( S_{ij} \), particularly in the reaction zone, resulting in qualitatively different alignments and interactions between the turbulence and the flame.

These changes to the turbulence and the flame are fundamentally due to a shift in the relative balance between heat release and turbulent motions as \( I_T \) and \( Y \) vary. Here, we examine this balance by splitting \( S_{ij} \) into parts due to fluid expansion by the flame, denoted \( S_{ij}^{SF} \), and due to turbulence, denoted \( S_{ij}^{ST} \). A similar decomposition has been proposed from a qualitative standpoint in several prior studies,\(^{2,15,16,46,47}\) and has been used, for example, in explanations of the alignment between \( e_i \) and \( n_i \) for low \( I_T \) shown in Fig. 9(a). Here, we propose more explicit, quantitative forms for the constituent strain rates in order to understand variations in the dynamics of \( n_i \), \( \delta_i \), and, in particular, \( \omega_i \) with \( I_T \) and \( Y \).

Assuming that fluid expansion by the flame acts along the flame surface normal at all points and times, the flame strain rate can be written as \( S_{ij}^{SF} = n_i n_j S_{ij} \), where \( S_{ij} = [S_{ij}^{SF}]^{1/2} \). The extensional eigenvector of \( S_{ij}^{SF} \), denoted \( e_i^{SF} \), is coincident with \( n_i \) and corresponds to the eigenvalue \( s_{ij}^{SF} = 1 \). The remaining eigenvectors, \( e_i^{ST} \) and \( e_i^{ST'} \), lie in the plane tangential to the local surface of the flame, with \( s_{ij}^{ST} = s_{ij}^{ST'} = 0 \). Using this form for \( S_{ij}^{SF} \), we propose that \( S_{ij} \) can then be decomposed as

\[
S_{ij} = S_{ij}^{SF} + n_i n_j S_{ij}^{ST}. \tag{20}
\]
It is emphasized that this decomposition is not the same as considering $S_{ij}$ in terms of flame normal, $n_i n_j S_{ij}$, and tangential, $(\delta_{ij} - n_i n_j)S_{ij}$, components. In particular, $S_{ij}^T$ has components both normal and tangential to the local flame surface. Here, we assume that the flame strain is approximately equal to the corresponding laminar strain, denoted $S_{ij}^{lam}$, which is a function of $Y$ only. This then gives $S^F(Y, x, t) \approx S_{ij}^{lam}(Y(x, t))$.

The changing balance of terms in Eq. (20) as a function of $I_T$ and $Y$ can be used to explain many of the changes in the flame and turbulence properties outlined in Sects. III and IV. Since $S_{ij}$ and $S_{ij}^T$ are known, $S_{ij}^T$ can be found from Eq. (20), and conditional averages of $S^F/S^T$ (where $S^T \equiv [S_{ij}^T]^{1/2}$) are shown as a function of $I_T$ and $Y$ in Fig. 22. $S^F/S^T$ is largest within the reaction zone for all $I_T$, but becomes progressively smaller as $I_T$ increases. Consequently, for low $I_T$, and particularly within the reaction zone, we assume that $S_{ij} \approx n_i n_j S_{ij}^F$, while for high $I_T$ and within the preheat zone, we assume that $S_{ij} \approx S_{ij}^T$. When the turbulent Mach number is low, we can also assume $S^F \approx S_{ij}^T$, which requires that $S_{ij}^T$ be close to zero. This condition only holds, however, for the smaller values of $I_T$ examined here (i.e., F1-F3, see Fig. 1). As a result, we use the more general form $S^F \approx S_{ij}^{lam}$ in the following analysis.

The decomposition in Eq. (20) allows the origin of the alignments in Fig. 9 to be understood, since substitution of Eq. (20) into Eqs. (13) and (15) shows that the evolution of $n_i$ has no direct dependence on the flame strain. This is true because $-n_i \bar{S}_{ij}^F = -n_i \bar{S}^F$ in Eq. (15) is always parallel to $n_i$, and only perpendicular terms directly affect the evolution of $n_i$ in Eq. (13). As a result, only $S_{ij}^T$ has a direct effect on the dynamics of $n_i$. The alignment between $n_i$ and $e_1$ arises because, regardless of the specific alignments between $e_1^F$ (the eigenvectors of $S_{ij}^F$) and $n_i$, $S_{ij}$ in Eq. (20) is dominated by $S_{ij}^T$ when $I_T$ is low (as shown in Fig. 22). As a result, we obtain $e_1 \approx e_1^F$, and since $e_1^F$ is, by definition, coincident with $n_i$, this then gives preferential alignment between $e_1$ and $n_i$. This purely kinematic alignment mechanism is particularly pronounced in the reaction zone, because this is where $e_1$ is most nearly equal to $e_1^F$. As $I_T$ increases and $S_{ij}$ is no longer dominated by $S_{ij}^T$, the kinematic alignment between $n_i$ and $e_1$ is lost, and the dynamic alignment between $n_i$ and $e_1 \approx e_1^F$ characteristic of nonreacting, passive scalar evolution is recovered (as shown in Fig. 9).

The decomposition of $S_{ij}$ in Eq. (20) also allows us to understand the effects of $S_{ij}$ on $\delta_T$ shown in Fig. 10. Using Eq. (20), the production term in Eq. (16) can be rewritten as

$$n_i n_j \tilde{\tau}_{ij} = n_i n_j \tilde{\tau}_{ij}^T + \tilde{\tau}^F.$$  

Figure 23 shows that the conditional average of $\tilde{\tau}^F$ is positive (again using $S^F \approx S_{ij}^{lam}$), with a maximum near $Y = 0.4$, and is essentially identical to the production term in laminar flames for all $I_T$. The conditional average of the term due to $S_{ij}^T$ in Eq. (21), by contrast, is negative, peaks near $Y = 0.4$ for all $I_T$, and increases in magnitude substantially as $I_T$ increases. As a result, while $S_{ij}^T$ has essentially no additional contribution to flame broadening (compared to the laminar flame) for all $I_T$, $S_{ij}^T$ acts to thin the flame with increasing strength as $I_T$ increases. In the past, these two effects have often been combined (as in Fig. 10), leading to ambiguity about the effects of $S_{ij}$ on the flame width. Figure 23 shows that, for low $I_T$ where $S_{ij}^T$ is small, $S_{ij}^T$ is dominant and the combined effect of $S_{ij}$ is to leave the flame essentially unchanged from its laminar structure. For high $I_T$, $S_{ij}^T$ dominates $S_{ij}$, and the overall effect of $S_{ij}$ is to thin the flame (i.e., decrease $\delta_T$).

This analysis considers only the effects of $S_{ij}$ on the flame width. Turbulent diffusion plays an important additional role in determining the width of the flame and is expected to increase in strength as $I_T$ increases. As a result, the flame width at high $I_T$ is set by a competition of flame
broadening due to turbulent diffusion and flame thinning due to $S_{ij}$. Turbulent diffusion is also responsible for broadening of the preheat region, even though the average of $n_i n_j \delta S_{ij}$ is negative in this region for all but the lowest $I_T$ (see Fig. 10).

In addition to clarifying the effects of $S_{ij}$ on $n_i$ and $\delta n_i$, the decomposition in Eq. (20) sheds light on the dependence of $\omega_i$ on $I_T$ and $y$ outlined in Sec. IV. The direct effect of $S_{ij}$ on $\omega$ is given by the first two terms in Eq. (17), namely $(\langle \omega_i \omega_j S_{ij} \rangle - \omega_i \omega_j S_{kk})$. Again using Eq. (20), we can write

$$\omega_i \omega_j S_{ij} - \omega_i S_{kk} = \omega_i \omega_j S_{ij} - \omega_S S_{kk} \left[ 1 - \frac{(\langle \omega \cdot n \rangle)^2 S_F}{S_{kk}} \right]. \quad (22)$$

This expression shows that the suppression of $\omega$ by fluid expansion due to heat release (which gives $S_{kk} > 0$) is orientation dependent. For low turbulent Mach numbers, such as in F1-F3, we obtain $S_F/S_{kk} \approx 1$, and the magnitude of the $S_{kk}$ suppression term in Eq. (22) is reduced by a factor of approximately $[1 - (\langle \omega \cdot n \rangle)^2]$. As a result, if $\omega_i$ is perfectly aligned with $n_i$ (i.e., $|\langle \omega \cdot n \rangle| = 1$), then the suppression of $\omega$ is close to zero.

The orientation-dependent suppression of $\omega$ given by Eq. (22) can be used to explain the anisotropic orientation of intense vortical structures shown qualitatively in Fig. 12, and quantitatively in Figs. 19 and 20. It can also be used to explain the preferential alignment between these structures and $n_i$ for low $I_T$ in Fig. 21. Since the dynamics of $\omega_i$ are strongly influenced by $S_{ij}^F$ for low $I_T$ (as indicated by Fig. 22), and since the suppression of $\omega$ by $S_{ij}^F$ is orientation dependent (via Eq. (22)), vortical structures pass relatively unattenuated through the flame if they are well aligned with the flame surface normal ($n_i$). As a result, the most intense vortical structures within the flame will tend to occur, for low $I_T$, when $\omega_i$ and $n_i$ are aligned. In a sense, the flame acts as a filter that selectively suppresses all vorticity that is not aligned with $n_i$, which gives the preferential alignment between $\omega_i$ and $n_i$ within intense vortices for low $I_T$ in the reaction zone, as shown in Fig. 21(a).

Intense vortices are anisotropically oriented along the $x$-axis because $n_i$ is preferentially oriented along this direction for low $I_T$ (as shown in Fig. 6). This preferential orientation persists downstream of the flame (i.e., into the products) until the self-induced interactions of the vorticity field and the perturbations introduced by the turbulence driving scramble the vortices. The persistence of the anisotropy downstream, shown in Fig. 20, is greatest for F1 and F2 since the anisotropy and suppression generated by the flame is strongest for low $I_T$, and the post-flame vorticity field responsible for scrambling is at its weakest. As $I_T$ increases, the orientation-dependent suppression term in Eq. (22) becomes weaker with respect to the term involving $S_{ij}^F$, and intense vortices remain essentially isotropic throughout the flame. Moreover, as $S_{ij}^F$ and dilatation play a weaker role in the dynamics of $\omega_i$, the flame begins to respond in a passive manner to all vorticity. This results in misalignment between $\omega_i$ and $n_i$ for high $I_T$, as shown in Figs. 9 and 21, which is characteristic of non-reacting, passive scalar evolution.

In addition to the anisotropy resulting from the orientation-dependent suppression of $\omega$ at low $I_T$, there is also a closely related tilting effect exerted by $S_{ij}^F$ on $\omega_i$. This can be seen from the $S_{ij}$ interaction terms in Eq. (17), which are given after substitution of Eq. (20) by

$$\omega_j S_{ij} - \omega_i S_{kk} = \omega_j S_{ij}^F - \omega_S S_{kk} \left[ \omega_i - (\langle \omega \cdot n \rangle) \frac{S_F}{S_{kk}} \right]. \quad (23)$$

Similar to the transport equation for $n_i$ in Eq. (13), the dynamics of $\omega_i$ are given by

$$\frac{D\omega_i}{Dt} = \frac{1}{\omega} (\delta \omega_j - \omega_j \delta \omega_i) \frac{D\omega_j}{Dt}. \quad (24)$$

For low $I_T$, where the effects of $S_{ij}^F$ play a role in establishing the alignment between $\omega_i$ and $n_i$, shown in Fig. 21 for low $I_T$, although future work is required to understand the relative importance of this tilting mechanism and the anisotropic suppression of $\omega_i$. The nature of the large-scale turbulence driving process plays an additional role in the turbulence dynamics that has not been explicitly examined in the preceding analysis. For instance, $\omega$ and $S$ in Fig. 11 have slightly larger amplitudes in the products than in the reactants for all $I_T$. These differences are due to the fact that the forcing is maintained at a constant rate per unit volume throughout the simulation domain. The decrease in fluid density across the flame results in larger forcing per unit mass in the products and hence in more intense velocities. The forcing, which is isotropic, may also play a role in the orientation of the structures. The increasing isotropy of the $\omega_i$ pdfs for F1 in the reaction zone (Fig. 14(c)), for example, may be due to the increased influence of isotropic large scale forcing.

Finally, turbulent diffusion will have an additional effect on the orientation of premixed flames and is expected, in particular, to broaden the flames. Substantial broadening of the reaction zone has not been observed here or in prior studies, however, even when $I_T$ is high. Although turbulent diffusion has not been explicitly examined here, a number of qualitative insights into the robustness of thin reaction zones can, nevertheless, be obtained from the present study. In order for flame broadening to occur, the turbulent velocity field must be sufficiently strong at the scale of the local flame width, $\delta_i$. As shown in Fig. 7, however, $\delta_i$ is smallest within the reaction zone for all $I_T$, thus requiring large turbulent velocities at scales where the energy content is naturally small due to the $k^{-5/3}$ Kolmogorov energy cascade (see, e.g., Fig. 2). Moreover, Fig. 13 shows that $\omega$ and $S$ are suppressed most strongly within the reaction zone, indicative of weaker small-scale turbulence. Consequently, small-scale turbulence...
is weakest in the region (the reaction zone) where it is most important in order for flame broadening to occur. Figure 23 further shows that flame thinning by $S_{ij}^T$ is largest within the reaction zone for all $I_T$, thus providing an additional mechanism by which thin reaction zones are maintained. Finally, the anisotropic suppression of $\omega$ given in Eq. (22) may play a further role in reducing the strength of turbulent diffusion within the reaction zone and deserves further study in the future. Ultimately, the width of the flame for all $Y$ and $I_T$ is determined by the combined action of several effects, including turbulent diffusion, thinning by $S_{ij}^F$, and anisotropic suppression of small-scale turbulence.

VI. SUMMARY AND CONCLUSIONS

The interactions between turbulence and flames in stoichiometric H₂-air premixed combustion have been studied for a range of turbulence intensities ($I_T$) using numerical simulations. Particular emphasis has been placed on the internal structure of the flame, which is characterized by the local flame orientation, $n_i = \chi_i/\chi$, and the local thickness, $\delta_i = \chi^{-1}$, and on the properties of the turbulence represented by the vorticity, $\omega_i$, and strain rate, $S_{ij}$.

A reconstruction method for the internal structure of the flame has been formulated using conditional averages of $\delta_i$ based on local, instantaneous values of $Y$. For low $I_T$, the flame structure is similar to that of a laminar flame, and there is relatively little flame wrinkling (as determined using pdfs of $n_i$). As $I_T$ increases, however, the flames become broader than laminar flames, particularly in the preheat zone, and the orientation of $n_i$ becomes increasingly isotropic. There is, however, relatively little broadening of the flame in the reaction zone, even for the highest value of $I_T$ studied here. This is consistent with prior results $^5$ for F4.

Examination of the turbulence has focused on the properties of $\omega_i$ and $S_{ij}$. The magnitudes of $\omega_i$ and $S_{ij}$ are suppressed by heat release effects in the flame for low $I_T$, but are only weakly affected by the flame for high $I_T$. The orientations of $\hat{\omega}_i = \omega_i/\omega$ and the eigenvectors of $S_{ij}$, denoted $e_i$, are essentially isotropic throughout the flame for high $I_T$, but for low $I_T$, substantial anisotropy is generated in the direction parallel to the $x$-axis. Intense vortical structures show similar behavior; there are fewer intense structures on the product side of the flame for low $I_T$ and the structures that are present are anisotropically oriented. For high $I_T$, however, the prevalence and orientation of these structures is relatively unchanged through the flame.

The interactions between the turbulence and the flame have been examined by considering the transport equations for $n_i$, $\delta_i$, $\chi_i$, $\omega_i$, and $S_{ij}$. Analysis of the alignments of $n_i$ with $e_i$ and $\hat{\omega}_i$ shows that, for high $I_T$, the interactions between $\omega_i$, $S_{ij}$, and $\chi_i$ are statistically similar to those found in nonreacting, passive scalar evolution. In particular, $\omega_i$ and $S_{ij}$ are nonlinearly coupled, while $n_i$ responds as a passive vector with respect to $\omega_i$ and $S_{ij}$. These alignments suggest that the dynamics of $\omega_i$ and $S_{ij}$ are largely unaffected by heat release effects due to the flame when $I_T$ is large and that the flame responds in a passive manner with respect to the turbulence. This passivity results, in particular, in greater flame wrinkling in the preheat zone for all $I_T$ and at all $Y$ for high $I_T$. It also results in a net thinning effect on the flame by $S_{ij}$.

When $I_T$ is low, the interactions and alignments between $n_i$, $\hat{\omega}_i$, and $e_i$ are substantially different from those found in nonreacting turbulence, particularly in the reaction zone. In particular, the nature of the coupling between $\omega_i$ and $S_{ij}$ is altered, and the flame structure is only weakly affected by the turbulence (resulting in reduced flame wrinkling and an overall similarity to laminar flames). The effect of $S_{ij}$ on the flame width for low $I_T$ is similar to that found in laminar flames.

An explanation for the variation of turbulence-flame properties and interactions with $I_T$ and $Y$ has been proposed using a decomposition of $S_{ij}$ into the components associated with the fluid expansion in the flame, $S_{ij}^E$, and with the turbulent flow field, $S_{ij}^F$. This allows changes in the alignments of $n_i$, $e_i$, and $\hat{\omega}_i$ to be understood and also provides an explanation for the anisotropic orientation of intense vortical structures when $I_T$ is low. In particular, the suppression of $\omega$ is anisotropic and depends on the relative alignment between $\hat{\omega}_i$ and $n_i$. Moreover, the effect of $S_{ij}$ on $\delta_i$ is shown to be composed of two parts; flame straining results in essentially no net broadening of the flame, compared to the laminar case, for all $I_T$, while turbulent straining acts to thin the flame with increasing strength as $I_T$ increases.

The present study suggests a number of directions for future research. Recent studies of premixed flames $^{19,20}$ have shown that the alignment between $e_i$ and $n_i$, as well as the strength of the dilatational strain rate (as compared to the tangential strain rate), increases as the Lewis number, $Le$, decreases below unity. Future work is required to examine how the present trends with $I_T$ and $Y$ depend on $Le$. In particular, changes to the balance between $S_{ij}^E$ and $S_{ij}^F$ and the anisotropic suppression of vorticity should be examined. The effects of turbulent diffusion on the flame structure also require more detailed future investigation. Turbulent diffusion balances the thinning effects of $S_{ij}^T$ and its strength should be quantified as a function of both $I_T$ and location in the flame. This requires an appropriate quantitative measure of turbulent diffusion, as well as consideration of counter-gradient transport. $^{48-50}$ Since turbulent diffusion depends on sufficiently strong turbulent motions at the scale of the flame, determining the variation of turbulent spectra with $Y$ and $I_T$ is an important aspect of this analysis. In particular, an approach that can examine turbulence kinetic energy spectra within the highly inhomogeneous flame brush would provide insights into the mutual interactions between the flame and small-scale turbulent transport. Similar spectral analyses are also required to understand the scales associated with flame wrinkling. The anisotropic suppression of vorticity by the flame may play an additional role in determining small-scale turbulent transport, and several prior studies $^{2,5}$ have indicated the importance of flame curvature and, in particular, cusps in the flame evolution. Future work is required to understand all of these effects. Finally, analyses of different reactive mixtures, for example, those that are off-stoichiometric or have different activation energies, and at substantially higher values of $I_T$, would allow the coupled
dynamics of turbulence and the flame to be studied over a broader range of conditions.

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31Since kinetic energy dissipation is provided by numerical, rather than physical, viscosity, it is more difficult to estimate the Reynolds numbers and the Kolmogorov length scales. If the physical fluid is characterized by Schmidt, $Sc = \nu / D$, and Prandtl, $Pr = \nu / K$, numbers of unity, then the kinematic viscosity is given in analogy with Eq. (8) as $\nu = \nu_0 T / \rho_0$, where $\nu_0 = D_0 = \kappa_0 = 2.9 \times 10^{-3} \text{g} / (\text{s} \cdot \text{cm} \cdot \text{K})$. This gives outer scale Reynolds numbers, $Re = UL/v$, between 180 and 2200 in the reactants for $F_1 < F_5$. This corresponding Kolmogorov length scales, $\eta_0 = U_{1/3} H^{1/3}$, are between 0.165 and 0.0255.
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