Turbulence and Scalar Gradient Dynamics in Premixed Reacting Flows

Peter E. Hamlington, Alexei Y. Poludnenko, and Elaine S. Oran
Laboratory for Computational Physics and Fluid Dynamics
Naval Research Laboratory, Washington, DC, 20375, USA

The interaction between turbulence and premixed flames is examined for a range of turbulence intensities using results from direct numerical simulations of premixed stoichiometric hydrogen-air combustion. Particular focus is placed on the interaction of the turbulent vorticity and strain rate fields with the scalar gradient in the presence of very intense turbulence, where the scalar is the reactant mass fraction. Analysis of the scalar-gradient magnitude shows that, for all turbulence intensities, the flame is broadened in the preheat zone, but remains close to the laminar flame width in the reaction zone. In agreement with previous studies, broadening of the reaction zone is not observed for even the largest intensities. Consideration of the terms in the scalar gradient transport equation shows that the strain rate acts to reduce the scalar-gradient magnitude for small turbulence intensities, while it increases the magnitude for large intensities. The vorticity and strain rate magnitudes are suppressed in the reaction zone of the flame, but this suppression decreases in strength as the turbulence intensity increases. The interactions between the vorticity, strain rate, and scalar gradient are substantially influenced by heat release for small turbulence intensities. For intense turbulence, however, these interactions are similar to those observed in nonreacting turbulence.

I. Introduction

This paper uses data from a series of direct numerical simulations to examine the interactions of flames and turbulence in premixed, stoichiometric hydrogen and air combustion. Particular focus is placed on the properties of the gradient of the reactant mass fraction, $Y$, where this scalar gradient reflects properties of the flame. The present simulations are extensions of those described in Ref. [1], and are carried out for a range of turbulence intensities, from $I_T \equiv U_{rms}/S_L = 2.45$ to 30.6, where $U_{rms}$ is the rms turbulent velocity in the unburned mixture and $S_L$ is the laminar flame speed. Previous studies of the scalar gradient in premixed flames have typically considered lower turbulence intensities; for example, Chakraborty and Swaminathan examined premixed flames where $I_T = 1.4$ and 7.6, and Kim and Pitsch examined $I_T = 13.8$ and 19.5. For the range of turbulence intensities examined here, substantial differences in the interaction between the flame and turbulence are expected, resulting in changes to the properties of both the turbulence and the scalar gradient. These changes, and their connection to variations in the turbulence intensity, are the focus of the present study.

In order to examine the interaction between the flames and turbulence, here we consider the coupled dynamics of the turbulent vorticity and strain rate with the dynamics of the scalar gradient. The vorticity, $\omega(x,t)$, is defined in terms of the velocity, $u_i(x,t)$, as

$$\omega_i(x,t) \equiv \epsilon_{ijk} \frac{\partial u_k}{\partial x_j},$$

where $\epsilon_{ijk}$ is the cyclic permutation tensor, and the strain rate, $S_{ij}(x,t)$, is given by

$$S_{ij}(x,t) \equiv \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right).$$

Copyright © 2010 by the American Institute of Aeronautics and Astronautics, Inc. All rights reserved.
The scalar gradient is defined in terms of $Y$ as

$$
\chi_i(x,t) = \frac{\partial Y}{\partial x_i}.
$$

The properties of $\omega_i$, $S_{ij}$, and $\chi_i$ can be used to obtain an understanding of the interaction between turbulence and premixed flames. In particular, the properties of $\chi_i$ reflect the internal structure of the flame separating the burned ($Y = 0$) and unburned ($Y = 1$) mixtures. This internal structure consists of isosurfaces of $Y$, which are not necessarily parallel. The orientation of the normal to these surfaces is given by the direction of $\chi_i$, and the separation between these surfaces is related to the magnitude of $\chi_i$. Larger values of $\chi_i$ indicate less separation between the surfaces, while smaller values indicate greater separation. Variations in the orientation of $\chi_i$ thus indicate the degree of wrinkling of the flame surfaces, and the magnitude of $\chi_i$ reflects the local flame width. Compared to the internal structure of the flame reflected in the properties of $\chi_i$, the turbulent flame brush consists of the entire region separating the purely burned and unburned mixtures (where $Y = 0$ and $Y = 1$, respectively, at all locations). The width of the flame brush can be large even when the flame itself is thin.

In any turbulent flow, the quantities $\omega_i$, $S_{ij}$ have important effects on the evolution of $\chi_i$. In particular, both $\omega_i$ and $S_{ij}$ directly affect the orientation of $\chi_i$, while $S_{ij}$ has an additional effect on the magnitude of $\chi_i$. The coupled dynamics of $\omega_i$, $S_{ij}$, and $\chi_i$ are complicated in premixed reacting flows, however, by the presence of the flame, the effects of heat release, and the non-conservative nature of $Y$. Due to chemical reactions, the scalar, $Y$, is not conserved, and its dynamics are substantially different from the advection-dominated dynamics of conserved scalars. Heat release in reacting flows also affects the dynamics of $\omega_i$ and $S_{ij}$ through temporal and spatial variations in the density and strength of diffusive processes. These variations can affect the turbulence dynamics, resulting in changes to the coupled evolution of $\omega_i$ and $S_{ij}$.

Through consideration of the dynamics of $\omega_i$, $S_{ij}$, and $\chi_i$, this paper examines several issues in premixed flames as a function of the turbulence intensity. In particular, while premixed turbulent flames have been shown to be broader than laminar flames in the preheat zone, the reaction zone is not substantially broadened, even for large intensities, for the hydrogen-air mixtures studied here. This result is examined in the context of the effects of turbulence, and in particular $S_{ij}$, on the magnitude of $\chi_i$. Previous studies have also indicated that the interaction between $S_{ij}$ and $\chi_i$ varies with turbulence intensity and location within the flame, and the present study explores this interaction in the limit of intense turbulence.

Prior studies have largely neglected the effects of $\omega_i$ in orienting $\chi_i$, as well as changes in the coupling between $\omega_i$ and $S_{ij}$ in the presence of premixed flames. The effect of $\omega_i$ on the orientation of $\chi_i$ is important in determining the degree of flame wrinkling as the turbulence intensity varies. The present paper thus includes effects due to $\omega_i$ in the analysis of $\chi_i$, and also examines the interaction between $\omega_i$ and $S_{ij}$ as a function of location in the flame and turbulence intensity. Particular emphasis is placed on the magnitudes and relative alignments of $\omega_i$, $S_{ij}$, and $\chi_i$. Together, these magnitudes and alignments give insights into the interactions between $\omega_i$, $S_{ij}$, and $\chi_i$, and provide quantitative measures of how the basic interaction between turbulence and flames varies as the turbulence intensity changes.

## II. Fundamental Equations

The governing equations for $\omega_i$, $S_{ij}$, and $\chi_i$ in premixed compressible reacting flows vary in several ways from those in noreacting flows, due primarily to the effects of heat release and chemical reactions. In such flows, the mass density, $\rho$, fluid viscosity, $\mu$, molecular diffusion, $D$, and thermal conduction, $K$, can vary spatially and temporally, and the presence of chemical reactions can have a significant effect on the dynamics of $\chi_i$. The fundamental equations governing the evolution of the flow are given by

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

$$
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_i u_j)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ 2\mu \left( S_{ij} - \frac{1}{3} S_{il} \delta_{lj} \right) \right],
$$

$$
\frac{\partial E}{\partial t} + \frac{\partial [(E + P)u_i]}{\partial x_j} = \rho \dot{\omega} + \frac{\partial}{\partial x_j} \left( K \frac{\partial T}{\partial x_j} \right),
$$

$$
\frac{\partial (\rho Y)}{\partial t} + \frac{\partial (\rho Y u_j)}{\partial x_j} = \rho \dot{\omega} + \frac{\partial}{\partial x_j} \left( \rho D \frac{\partial Y}{\partial x_j} \right),
$$

![Image](image.png)

American Institute of Aeronautics and Astronautics
where \( P \) is the pressure, \( E \) is the energy density, \( \dot{w} \) is the chemical reaction rate and \( q \) is the chemical energy release. From Eq. (5), an equation for \( u_i \) can be written in non-conservative form as\(^7\)

\[
\frac{Du_i}{Dt} = -\frac{1}{\rho} \frac{\partial P}{\partial x_i} + \frac{1}{\rho} \frac{\partial}{\partial x_j} \left( 2\mu \tilde{S}_{ij} \right) .
\]  

(8)

where \( D/Dt \equiv \partial/\partial t + u_j \partial/\partial x_j \) and \( \tilde{S}_{ij} \) is the deviatoric strain rate tensor defined as

\[
\tilde{S}_{ij} \equiv S_{ij} - \frac{1}{3} S_{kk} \delta_{ij} .
\]  

(9)

From Eq. (8), the governing equations for \( \omega_i, S_{ij} \) and \( \chi \) in premixed flames also include terms due to varying \( \rho, \mu, \) and \( D \).

II.A. Vorticity

The transport equation for \( \omega_i \), defined in Eq. (1), is obtained by taking the curl of Eq. (8), which yields

\[
\frac{D\omega_i}{Dt} = \omega_j \left( S_{ij} - S_{kk} \delta_{ij} \right) + \frac{\epsilon_{ijk}}{\rho^2} \frac{\partial P}{\partial x_j} \frac{\partial P}{\partial x_k} + \epsilon_{ijk} \frac{\partial}{\partial x_j} \left[ 2 \frac{\partial}{\partial x_l} \left( \mu \tilde{S}_{kl} \right) \right] .
\]  

(10)

The first term on the right hand side of Eq. (10) includes both the nonlinear vortex stretching term \( \omega_i S_{ij} \) and the dilatation term \( \omega_i S_{kk} \). The second term on the right in Eq. (10) is the baroclinic torque, which can be significant when the gradients of \( \rho \) and \( P \) are not aligned. The last term contains all viscous effects, including those due to gradients in \( \mu \).

Defining the vorticity magnitude \( \omega^2 \equiv \omega_i \omega_i \), the transport equation for \( \omega^2 \) is obtained from Eq. (10) as

\[
\frac{1}{2} \frac{D\omega^2}{Dt} = \omega_i \omega_j \left( S_{ij} - S_{kk} \delta_{ij} \right) + \frac{\omega_i \epsilon_{ijk}}{\rho^2} \frac{\partial P}{\partial x_j} \frac{\partial P}{\partial x_k} + \omega_i \epsilon_{ijk} \frac{\partial}{\partial x_j} \left[ 2 \frac{\partial}{\partial x_l} \left( \mu \tilde{S}_{kl} \right) \right] .
\]  

(11)

The quantity \( \frac{1}{2} \omega^2 \) is the local enstrophy, and the first term on the right side of Eq. (11) includes contributions due to both the enstrophy production rate \( \omega_i \omega_j S_{ij} \) and dilatation \( \omega^2 S_{kk} \). Equation (11) shows the effect of dilatation on \( \omega^2 \), since \( \omega^2 S_{kk} \) will either increase or decrease \( \omega^2 \) depending on the sign of \( S_{kk} \).

The evolution of the vorticity orientation\(^8,9\) is described by the transport equation for the normalized vorticity vector \( \tilde{\omega}_i \equiv \omega_i / \omega \), where \( \omega \equiv [\omega_i \omega_i]^{1/2} \). From this equation, effects that change the magnitude of \( \omega_i \) can be separated from those that change its direction. The transport equation for \( \tilde{\omega}_i \) is obtained from

\[
\frac{D\tilde{\omega}_i}{Dt} = \frac{1}{\omega} \frac{D\omega_i}{Dt} - \frac{\tilde{\omega}_i D\omega^2}{\omega^2} - \frac{1}{2} \frac{D\omega^2}{Dt} .
\]  

(12)

Substituting the transport equations for \( \omega_i \) and \( \omega^2 \) in Eqs. (10) and (11), we obtain

\[
\frac{D\tilde{\omega}_i}{Dt} = \eta^S_i + \eta^b_i + \eta^\mu_i ,
\]  

(13)

where

\[
\eta^S_i \equiv \omega_j S_{ij} - \tilde{\omega}_i \tilde{\omega}_j \tilde{\omega}_k S_{jk} ,
\]

(14)

is the contribution due to the vortex stretching term,

\[
\eta^b_i \equiv \frac{\epsilon_{ijk}}{\omega} \frac{\partial \rho}{\partial x_j} \frac{\partial P}{\partial x_k} - \frac{\tilde{\omega}_j \epsilon_{ijk}}{\omega^2} \frac{\partial \rho}{\partial x_k} \frac{\partial P}{\partial x_l} ,
\]

(15)

represents tilting by the baroclinic torque, and

\[
\eta^\mu_i \equiv \frac{\epsilon_{ijk}}{\omega} \frac{\partial}{\partial x_j} \left[ 2 \frac{\partial}{\partial x_l} \left( \mu \tilde{S}_{kl} \right) \right] - \frac{\tilde{\omega}_j \epsilon_{ijk}}{\omega} \frac{\partial}{\partial x_k} \left[ 2 \frac{\partial}{\partial x_m} \left( \mu \tilde{S}_{lm} \right) \right] ,
\]

(16)

is the effect of the viscous terms, including gradients in \( \mu \), on \( \tilde{\omega}_i \). Even though dilatation plays no direct role in orienting \( \omega_i \), it can still have an indirect effect on the orientation through its effect on the magnitudes of \( \omega_i \) and \( S_{ij} \). Thus, it affects all of the terms on the right side of Eq. (13), as well as the properties of the nonlinear coupling between \( \omega_i \) and \( S_{ij} \).
II.B. Strain Rate

The transport equation for \( S_{ij} \) is obtained by first deriving the equation for the velocity gradient, \( A_{ij} \equiv \partial u_i / \partial x_j \). This is obtained by taking the gradient of Eq. (8), which gives

\[
\frac{DA_{ij}}{Dt} = -A_{ik}A_{kj} - \frac{1}{\rho} \frac{\partial^2 P}{\partial x_i \partial x_j} + \frac{1}{\rho^2} \frac{\partial P}{\partial x_i} \frac{\partial \rho}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \frac{1}{\rho} \frac{\partial}{\partial x_k} (2\mu \hat{S}_{ik}) \right]. \tag{17}
\]

The transport equation for the strain rate \( S_{ij} \) in Eq. (2) is obtained by adding Eq. (17) and its transpose and multiplying by 1/2. This then gives

\[
\frac{DS_{ij}}{Dt} = -S_{ik}S_{kj} - \frac{1}{4} \left( \omega_i \omega_j - \omega^2 \delta_{ij} \right) - \frac{1}{2\rho} \frac{\partial^2 P}{\partial x_i \partial x_j} + \frac{1}{2\rho^2} \left( \frac{\partial P}{\partial x_i} \frac{\partial \rho}{\partial x_j} + \frac{\partial P}{\partial x_j} \frac{\partial \rho}{\partial x_i} \right) + \xi_{ij}, \tag{18}
\]

where

\[
-\frac{1}{2} (A_{ik} A_{kj} + A_{jk} A_{ki}) = -S_{ik} S_{kj} - \frac{1}{4} (\omega_i \omega_j - \omega^2 \delta_{ij}), \tag{19}
\]

and we have defined

\[
\xi_{ij} \equiv \frac{1}{2} \frac{\partial}{\partial x_j} \left[ \frac{1}{\rho} \frac{\partial}{\partial x_k} (2\mu \hat{S}_{ik}) \right] + \frac{1}{2} \frac{\partial}{\partial x_i} \left[ \frac{1}{\rho} \frac{\partial}{\partial x_k} (2\mu \hat{S}_{jk}) \right], \tag{20}
\]

to simplify the notation. By defining the strain rate magnitude \( S^2 \equiv S_{ij} S_{ij} \), and multiplying Eq. (18) by \( S_{ij} \), we obtain

\[
\frac{1}{2} \frac{DS^2}{Dt} = -S_{ik}S_{kj}S_{ij} - \frac{1}{4} \omega_i \omega_j \left( S_{ij} - S_{kk} \delta_{ij} \right) - \frac{S_{ij}}{\rho} \frac{\partial^2 P}{\partial x_i \partial x_j} + \frac{S_{ij}}{2\rho^2} \left( \frac{\partial P}{\partial x_i} \frac{\partial \rho}{\partial x_j} + \frac{\partial P}{\partial x_j} \frac{\partial \rho}{\partial x_i} \right) + S_{ij} \xi_{ij}. \tag{21}
\]

As in Eq. (11), there is a dilatation effect in Eq. (21) that increases \( S^2 \) during fluid expansion (when \( S_{kk} > 0 \)) and decreases \( S^2 \) during fluid compression (when \( S_{kk} < 0 \)). With the magnitude \( S = |S_{ij} S_{ji}|^{1/2} \), \( S_{ij} \) can be fully characterized by \( S \), its normalized eigenvalues, \( \lambda_i \), and the corresponding eigenvectors, \( \mathbf{e}_i \). The eigenvectors of \( S_{ij} \) in particular are important in understanding the interactions of \( \omega_i \) and \( \chi_i \) with \( S_{ij} \), as discussed in Section II.D.

II.C. Scalar Gradient

The evolution of the reactant mass fraction, \( Y \), which is the scalar of interest in the present study, can be written in non-conservative form from Eq. (7) as

\[
\frac{DY}{Dt} = \dot{w} + \frac{1}{\rho} \frac{\partial}{\partial x_k} (\rho D\chi_k). \tag{22}
\]

The transport equation for \( \chi_i \) can then be obtained by taking the gradient of Eq. (22), giving

\[
\frac{D\chi_i}{Dt} = -\chi_j S_{ij} - \frac{1}{2} \xi_{ijk} \chi_j \omega_k + \frac{\partial \dot{w}}{\partial x_i} + \frac{\partial}{\partial x_i} \left[ \frac{1}{\rho} \frac{\partial}{\partial x_k} (\rho D\chi_k) \right], \tag{23}
\]

which explicitly shows the effects of \( \omega_j \) and \( S_{ij} \) on \( \chi_i \). The effect of \( S_{ij} \) on \( \chi_i \) is similar to its effect on \( \omega_i \) through the vortex stretching term in Eq. (10). The primary difference between vortex stretching and the interaction between \( \chi_i \) and \( S_{ij} \) is the different sign in front of the two terms. Equation (23) also shows that the vorticity plays a role in the evolution of \( \chi_i \) through the outer product between \( \omega_i \) and \( \chi_i \). The reaction rate is shown in Eq. (23) to affect the dynamics of \( \chi_i \) through the gradient of \( \dot{w} \), and the effects of molecular diffusion enter through a similar gradient term.

A transport equation for the magnitude of the scalar gradient, \( \chi^2 \equiv \chi_i \chi_i \), can be obtained by multiplying Eq. (23) by \( \chi_i \), which gives

\[
\frac{1}{2} \frac{D\chi_i}{Dt} = -\chi_i \chi_j S_{ij} + \chi_i \frac{\partial \dot{w}}{\partial x_i} + \chi_i \frac{\partial}{\partial x_i} \left[ \frac{1}{\rho} \frac{\partial}{\partial x_k} (\rho D\chi_k) \right]. \tag{24}
\]

Equation (24) shows that \( \omega_i \) plays no direct role in the evolution of \( \chi^2 \), although it does have a direct effect on the orientation of \( \chi_i \), as in Eq. (23). The gradients of \( \dot{w} \) and the molecular diffusion term will either
There are specific interaction terms in the governing equations for II.D. Interactions Between Turbulence and Scalar Gradients describes the effects of molecular diffusivity.

For instance, the inner product \( \chi_i \partial \hat{w}_i / \partial x_i \) is positive when \( \chi_i \) and \( \partial \hat{w}_i / \partial x_i \) are aligned and negative when they are oppositely aligned.

We can also formulate a transport equation for the orientation of the scalar gradient, \( n_i \equiv \chi_i / \chi \), where \( \chi \equiv [\chi_i \chi_i]^{1/2} \), as

\[
\frac{D n_i}{D t} = \frac{1}{\chi} \frac{D \chi}{D t} - n_i \frac{1}{\chi} \frac{D \chi^2}{2 \frac{D t}{D t}}.
\]

(25)

Substituting Eqs. (23) and (24) into Eq. (25) gives

\[
\frac{D n_i}{D t} = \zeta_i^s + \zeta_i^\omega + \zeta_i^D,
\]

(26)

where

\[
\zeta_i^s = -\varepsilon_{ij} \varepsilon_{jk} \omega_j \chi_k,
\]

(27)

are effects of strain,

\[
\zeta_i^\omega = \frac{1}{2} \varepsilon_{ijk} n_j \omega_k,
\]

(28)

are effects due to the vorticity,

\[
\zeta_i^D = \frac{1}{\chi} \frac{\partial}{\partial x_i} \left[ \frac{1}{\rho} \frac{\partial}{\partial x_k} \left( \rho D \chi_k \right) \right] - \frac{n_i n_j}{\chi} \frac{\partial}{\partial x_j} \left[ \frac{1}{\rho} \frac{\partial}{\partial x_k} \left( \rho D \chi_k \right) \right],
\]

(30)

describes the effects of molecular diffusivity.

II.D. Interactions Between Turbulence and Scalar Gradients

There are specific interaction terms in the governing equations for \( \omega_i \), \( S_{ij} \), and \( \chi_i \) (Eqs. (10), (18), and (23), respectively) that can be used to examine the interaction between turbulence and flames in premixed reacting flows. In particular, the vortex stretching term \( \omega_i S_{ij} \) in Eq. (10) and the terms \( -\chi_j S_{ij} \) and \( \frac{1}{2} \varepsilon_{ijk} \omega_j \chi_k \) in Eq. (23), all involve turbulence and scalar gradient interactions. The vorticity production term, \( \omega_i \omega_j S_{ij} \), and \( -\chi_i \chi_j S_{ij} \) in Eqs. (11) and (24), respectively, also involve interactions between \( \omega_i \), \( S_{ij} \), and \( \chi_i \).

Since these terms involve products of vector or tensor quantities, they can be evaluated in terms of the magnitudes and alignments of the vectors and eigenvectors. The alignments, in particular, can be used to gain insights into the underlying physics and coupled dynamics of \( \omega_i \), \( S_{ij} \), and \( \chi_i \). The orientations of \( \hat{\omega} \), \( \hat{e}_i \) (the eigenvectors of \( S_{ij} \)), and \( \hat{n} \) are determined by the relative balance and individual properties of the terms on the right sides of Eqs. (10), (18), and (23). The resulting orientations then lead to alignments (or misalignments) between \( \hat{\omega} \), \( \hat{e}_i \), and \( \hat{n} \) that reflect the properties of the coupling between \( \omega_i \), \( S_{ij} \), and \( \chi_i \).

For instance, the alignment between \( \hat{\omega} \) and \( \hat{e}_i \) in nonreacting turbulent flows is affected by the nonlinear, two-way coupling between \( \omega_i \) and \( S_{ij} \), resulting in alignment of \( \hat{\omega} \) with \( \hat{e}_2 \). If \( S_{ij} \) did not depend on \( \omega_i \), then \( \hat{\omega} \) would evolve as a passive vector with respect to \( S_{ij} \) and become preferentially aligned with \( \hat{e}_1 \) instead. Alternatively, if \( \omega_i \) and \( S_{ij} \) were completely independent of each other, then \( \hat{\omega} \) would show no preferential alignment with any of the eigenvectors of \( S_{ij} \). The alignments of \( \hat{\omega} \), \( \hat{e}_1 \), and \( \hat{n} \) can thus provide insights into the interactions and coupling between \( \omega_i \), \( S_{ij} \), and \( \chi_i \).

The alignments are also important in determining the interaction terms in the equations for \( \omega^2 \), \( S^2 \), and \( \chi^2 \). For example, the production of \( \omega^2 \) by \( S_{ij} \), \( \omega_i \omega_j S_{ij} \), in Eq. (11) can be written as

\[
\omega_i \omega_j S_{ij} = \omega^2 \left[ \lambda_1 (\hat{e}_1 \cdot \hat{\omega})^2 + \lambda_2 (\hat{e}_2 \cdot \hat{\omega})^2 + \lambda_3 (\hat{e}_3 \cdot \hat{\omega})^2 \right],
\]

(31)

where \( \lambda_i \) are the eigenvalues of \( S_{ij} \) normalized by \( S \equiv [S_{ij} S_{ij}]^{1/2} \). The quantities \( \hat{e}_i \cdot \hat{\omega} \) represent the alignments of \( \hat{e}_i \) with the vorticity direction vector \( \hat{\omega} \). For complete alignment, \( \hat{e}_i \cdot \hat{\omega} = 1 \), for completely misaligned (or perpendicular) vectors, \( \hat{e}_i \cdot \hat{\omega} = 0 \), and for complete anti-alignment \( \hat{e}_i \cdot \hat{\omega} = -1 \). Similarly, the interaction between \( S_{ij} \) and \( \chi_i \) in Eq. (24), \( -\chi_i \chi_j S_{ij} \), can be written in terms of the magnitudes \( \chi^2 \) and \( S \) and the alignments \( \hat{e}_i \cdot \hat{n} \) as

\[
-\chi_i \chi_j S_{ij} = -\chi^2 S \left[ \lambda_1 (\hat{e}_1 \cdot \hat{n})^2 + \lambda_2 (\hat{e}_2 \cdot \hat{n})^2 + \lambda_3 (\hat{e}_3 \cdot \hat{n})^2 \right].
\]

(32)
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_0 )</td>
<td>293 K</td>
<td>Initial Temperature</td>
</tr>
<tr>
<td>( P_0 )</td>
<td>1.01 \times 10^6 \text{erg/cm}^3</td>
<td>Initial Pressure</td>
</tr>
<tr>
<td>( \rho_0 )</td>
<td>8.73 \times 10^{-4} \text{g/cm}^3</td>
<td>Initial Density</td>
</tr>
<tr>
<td>( \gamma )</td>
<td>1.17</td>
<td>Adiabatic Index</td>
</tr>
<tr>
<td>( M )</td>
<td>21 g/mol</td>
<td>Molecular weight</td>
</tr>
<tr>
<td>( A )</td>
<td>6.85 \times 10^{12} \text{cm}^3/\text{g-s}</td>
<td>Pre-exponential factor</td>
</tr>
<tr>
<td>( Q )</td>
<td>46.37 \text{RT}_0</td>
<td>Activation energy</td>
</tr>
<tr>
<td>( q )</td>
<td>43.28 \text{RT}_0/\text{M}</td>
<td>Chemical energy release</td>
</tr>
<tr>
<td>( \kappa )</td>
<td>2.9 \times 10^{-5} \text{g/s-cm-K}^n</td>
<td>Thermal conduction coefficient</td>
</tr>
<tr>
<td>( D_0 )</td>
<td>2.9 \times 10^{-5} \text{g/s-cm-K}^n</td>
<td>Molecular diffusion coefficient</td>
</tr>
<tr>
<td>( n )</td>
<td>0.7</td>
<td>Temperature exponent</td>
</tr>
<tr>
<td>( T_F )</td>
<td>2135 K</td>
<td>Post-flame temperature</td>
</tr>
<tr>
<td>( \rho_F )</td>
<td>1.2 \times 10^{-4} \text{g/cm}^3</td>
<td>Post-flame density</td>
</tr>
<tr>
<td>( \delta_L )</td>
<td>0.032 cm</td>
<td>Laminar flame thermal width</td>
</tr>
<tr>
<td>( S_L )</td>
<td>302 cm/s</td>
<td>Laminar flame speed</td>
</tr>
</tbody>
</table>

Table 1. Laminar flame properties and input model parameters common to all numerical simulations.

Even though the vorticity plays no direct role in the evolution of \( \chi^2 \), Eq. (32) shows that \( \omega_i \) does have an indirect role on \( \chi^2 \) through its effects on the evolution of \( S_{ij} \) (and hence \( e_i \)) and on the orientation of \( n \). In particular, the interaction between \( \omega_i \) and \( \chi_i \) in Eq. (23) can be written as

\[
- \frac{1}{2} \epsilon_{ijk} \chi_j \omega_k = - \frac{1}{2} \chi \hat{\omega}_{ijk} n_j \hat{\omega}_k = - \frac{1}{2} \chi \hat{\omega} (n \times \hat{\omega}).
\]

This thus shows that the vorticity tends to misalign the scalar gradient with itself.

Although \( \omega^2 \), \( S \), and \( \chi^2 \) are important in determining the magnitude of the interaction terms in Eqs. (31) and (32), the alignments of \( \hat{\omega} \) and \( n \) with \( e_i \), combined with the eigenvalues, \( \lambda_i \), determine the signs of these terms. This affects whether \( \chi^2 \), for example, is created or destroyed by \( S_{ij} \). In any turbulent flow, the \( \lambda_i \) can be ordered as \( \lambda_1 \geq \lambda_2 \geq \lambda_3 \). In incompressible flows, continuity requires \( \lambda_1 + \lambda_2 + \lambda_3 = 0 \), and thus \( \lambda_1 \geq 0 \) and \( \lambda_3 \leq 0 \). As a result, preferential alignment between \( n \) and \( e_3 \), for instance, and misalignment with \( e_1 \), would yield \( -\chi_i \chi_j S_{ij} > 0 \), and hence production of \( \chi^2 \) by \( S_{ij} \). This picture is complicated in compressible reacting flows, however, where compressibility effects result in \( \lambda_1 + \lambda_2 + \lambda_3 \neq 0 \). It thus may not always be the case that \( \lambda_1 \geq 0 \) and \( \lambda_3 \leq 0 \) in such flows. Nevertheless, the signs of both \( \omega_i \omega_j S_{ij} \) and \(-\chi_i \chi_j S_{ij} \) still completely depend on the alignments \( e_i \cdot \hat{\omega} \) and \( e_i \cdot n \), as well as the signs and magnitudes of the corresponding eigenvalues.

### III. Description of Numerical Simulations

The simulations used in the present study represent premixed hydrogen-air combustion in an infinite, unconfined domain, where the interaction between turbulence and the flame can be examined in isolation from additional effects due to the system geometry. The numerical simulations have been carried out using Athena-RFX,\(^1\) a reactive-flow version of the magnetohydrodynamic code Athena.\(^{13,14}\) The code solves the compressible, inviscid Navier-Stokes equations for a reactive flow based on Eqs. (4)-(7).

The chemical-reaction source term \( \dot{w} \) in Eqs. (6) and (7) is modeled using first-order Arrhenius kinetics as

\[
\dot{w} \equiv \frac{\partial Y}{\partial t} = -A \rho Y \exp \left( -\frac{Q}{RT} \right),
\]

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

$$D = D_0 \rho^{n}, \quad K = C_p \kappa_0 \rho^{n},$$  \hspace{1cm} (35)$$

where $D_0$, $\kappa_0$, and $n$ are constants and $C_p = \gamma R/M(\gamma - 1)$. The values of all model parameters contained in Eqs. (4)-(7), (34), and (35) are summarized in Table 1. These values are based on the reaction model of Gamezo et al.\textsuperscript{15} and represent a stoichiometric hydrogen-air mixture. This model correctly reproduces the properties of laminar flames in the hydrogen-air mixture, including the dependence on $P$ and $T$, and has been tested and successfully used in a number of applications.\textsuperscript{15}

The system of equations given by Eqs. (4)-(7), (34), and (35) is solved in Athena-RFX using a high-order fully conservative Godunov-type method based on the unsplit corner transport upwind algorithm.\textsuperscript{14,16,17} Equation (5) is solved in inviscid form, and small-scale kinetic energy dissipation in the simulations is provided by numerical viscosity. This approach has been shown\textsuperscript{1} to extend the inertial range without placing prohibitive demands on computational resources. Resolution and accuracy tests show that a resolution of 16 cells per $\delta_L$, as used in the present simulations, is sufficient to provide a converged solution representative of a system with physical viscosity.\textsuperscript{1} A more detailed discussion of resolution considerations, as well as the numerical method, is outlined in Ref. [1].

Turbulence is sustained in the simulations by perturbing the velocity field at the largest scale of the flow, where the perturbations are isotropic, do not introduce any net momentum to the system, and are divergence-free.\textsuperscript{1} Such large-scale energy input is commonly used in numerical studies of homogeneous isotropic turbulence to generate fully-developed turbulence with a kinetic energy spectrum that follows a $k^{-5/3}$ wavenumber scaling in the inertial range. In the present simulations, the large-scale perturbations are continued even after ignition of the flame, resulting in a sustained turbulence-flame interaction, in contrast to prior studies of premixed flames in freely decaying turbulence.\textsuperscript{4} The turbulence intensity in the unburned gases is determined by the energy-injection rate, which is maintained at a constant rate per unit volume throughout the simulation domain.

<table>
<thead>
<tr>
<th>Simulation</th>
<th>$I_T$ ($U_{ rms}/S_L$)</th>
<th>$Da$</th>
<th>$\tau_{ ed}$ (s)</th>
<th>$t_a$ ($\tau_{ ed}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1</td>
<td>2.45</td>
<td>0.387</td>
<td>$2.14 \times 10^{-4}$</td>
<td>4.86</td>
</tr>
<tr>
<td>F2</td>
<td>4.90</td>
<td>0.195</td>
<td>$1.07 \times 10^{-4}$</td>
<td>4.49</td>
</tr>
<tr>
<td>F3</td>
<td>9.81</td>
<td>0.0965</td>
<td>$5.36 \times 10^{-5}$</td>
<td>13.7</td>
</tr>
<tr>
<td>F4</td>
<td>18.4</td>
<td>0.0515</td>
<td>$2.86 \times 10^{-5}$</td>
<td>13.8</td>
</tr>
<tr>
<td>F5</td>
<td>30.6</td>
<td>0.0310</td>
<td>$1.71 \times 10^{-5}$</td>
<td>18.7</td>
</tr>
</tbody>
</table>

Table 2. Initial turbulent-to-laminar flame speed ratio $I_T \equiv U_{ rms}/S_L$, Damkohler number, $Da = (l/U_{ rms})/(l_F/S_L)$, and eddy turnover time, $\tau_{ ed} = L/U_{ L,S}$ in the unburned mixture at ignition for the five premixed flame simulations, denoted F1–F5. The analysis time, $t_a$, is also shown for each simulation.

Five different simulations have been performed, with turbulence intensities in the unburned mixture from $I_T = U_{ rms}/S_L = 2.45$ to 30.6, corresponding to $Da$ from 0.387 to 0.0310. The simulations are denoted in Table 2 by F1–F5, where F4 corresponds to simulation S2 in Ref. [1]. The Damkohler number, $Da$, is defined as $Da \equiv l/(U_{ rms})/(l_F/S_L)$, where $l$ is the turbulence integral scale, $l_F = D/S_L \approx 2\delta_L$, and $\delta_L \equiv (T_k - T_o)/(\kappa T_{ L, max})$ is the thermal width of the laminar flame. For all simulations, the ratio of $l$ to $\delta_L$ is $l/\delta_L = 1.90$, and the simulation domain has a physical width of $L = 2.59 \times 10^{-3}$ m, with a length-to-width ratio of $L_x : (L_y, L_z) = 16 : 1$. The simulations are shown on the combustion regime diagram\textsuperscript{18} in Figure 1. Periodic boundary conditions are used in the spanwise directions, giving a statistically planar flame in the y-z plane, with a mean flow in the x-direction. The size of the computational grid for all simulations is $n_x \times n_y \times n_z = 2048 \times 128 \times 128$, giving 16 computational cells per $\delta_L$. Homogeneous isotropic turbulence is allowed to develop for 2–3 turbulent eddy turnover times, $\tau_{ ed} = L/U_L$, where $U_L$ is the turbulent velocity at the scale of the domain width $L$, prior to ignition of the flame near the center of the x-axis. The analysis of the numerical data is carried out for between $4\tau_{ ed}$ and $19\tau_{ ed}$ for each simulation, beginning approximately $2\tau_{ ed}$ after ignition. Instantaneous turbulence kinetic energy spectra immediately prior to ignition are shown in Figure 2 for F1–F5. In all cases the kinetic energy spectra follow an approximate $E(k) \sim k^{-5/3}$ scaling, which is indicative of fully-developed homogeneous isotropic turbulence.
Figure 1. Combustion regime diagram\textsuperscript{18} similar to that used in Ref. [1], showing the location of simulations F1–F5 (red squares). Here $Re = (\langle U_{rms} \rangle / (\langle I_p \rangle S_L)$ is the Reynolds number, $K_a$ and $K_{a_f}$ are Karlovitz numbers, and $Ma_F$ is the fuel Mach number.

IV. Results

IV.A. Scalars and Scalar Gradients

Figure 3 shows instantaneous isosurfaces of $Y$ for F1–F5. In all cases, there is less small-scale wrinkling of the $Y = 0.05$ flame surface on the burned side of the flame than the $Y = 0.95$ surface on the unburned side. This is consistent with previous observations reported\textsuperscript{1} for just the case F4. As $I_T$ increases, the degree of flame wrinkling on both sides of the flame brush increases, as does the width of the flame brush itself. There also appears to be some broadening in the preheat zone for high $I_T$. Figure 3 does not, however, indicate how the internal flame structure is different from that of a laminar flame, or allow statements to be made about the variation of the large-scale wrinkling with $I_T$.

The third column in Figure 3 shows isosurfaces of $\chi^2$. Regions of intense $\chi^2$ occur in relatively thin wrinkled sheets for small $I_T$ (Figures 3a and b), while for large $I_T$ (Figures 3c–e) there are more prominent regions of large $\chi^2$ within the flame brush and the spatial variation of the $\chi^2$ field increases. Comparing $\chi^2$ with the $Y$ isosurfaces reveals that the largest values of $\chi^2$ occur near the reaction zone on the burned side of the flame. The variation of the $\chi^2$ field with $I_T$ is thus associated with the variation of the reaction zone isosurfaces shown in the left two columns of Figure 3, where this surface becomes increasingly wrinkled as $I_T$ increases.

IV.B. Statistics of the Scalar Gradient

The magnitude of $\chi^2$ provides an indication of the flame width; broader local flame structures occur for small $\chi^2$, and thinner structures occur for large $\chi^2$. Figure 4 shows conditional averages of $\chi^2$ as a function of $Y$ within the flame brush. For all simulations, $\chi^2$ reaches a maximum near $Y \approx 0.4$ and decreases as $Y \rightarrow 0$ and $Y \rightarrow 1$, towards the burned and unburned sides of the flame, respectively. Even though the qualitative dependence of $\chi^2$ on $Y$ is similar for all $I_T$, Figure 4 does indicate that there are trends in the behavior of $\chi^2$. In particular, for $Y \gtrsim 0.6$, $\chi^2$ decreases with increasing $I_T$, while for $Y \lesssim 0.6$, $\chi^2$ increases with increasing $I_T$.

These results are consistent with prior studies of the flame width in premixed combustion,\textsuperscript{1,3,4} and indicate that both flame thinning and flame broadening can occur for the values of $I_T$ examined here, depending on the location within the flame. In particular, Ref. [1] outlined a method by which the internal structure of flamelets folded inside the turbulent flame brush can be reconstructed. This method has been applied here to F1–F5, and the resulting profiles of $Y$ are shown in Figure 5. These profiles are a direct measure of the internal structure of the flame, and are particularly useful when the flame is highly convolved in the flame brush. The coordinate $x/\delta_L$ in Figure 5 is at $Y = 0.5$ by definition, with $x/\delta_L > 0$ corresponding
Figure 3. Isosurfaces of the reactant mass fraction \( Y \) and the scalar gradient magnitude \( \chi^2 \) for (a) F1 – (e) F5. Left column shows the \( Y = 0.05 \) isosurface on the burned side of the flame, middle column shows the \( Y = 0.95 \) isosurface on the unburned side, and the right column shows the isosurface \( \chi^2 = 1/\delta^2_L \) with the same perspective as that used in the left column.
to $Y > 0.5$ and $x/\delta_L < 0$ corresponding to $Y < 0.5$. Figure 5 shows that flame broadening occurs in the preheat zone for all $I_T$, and that the broadening increases with increasing $I_T$. This direct picture of the internal flame structure is consistent with the structure inferred from the magnitude of $\chi^2$ in Figure 4.

The statistical spread of $\chi^2$ at each $Y$ provides information about the prevalence of instantaneously thin or broad regions in the flame brush that the conditionally averaged profiles in Figure 4 cannot capture. Figure 6 shows conditional probability density functions (pdfs) of $\chi^2$ normalized by the corresponding laminar value $\chi^2_L$ at each value of $Y$. Values of $\chi^2/\chi^2_L > 1$ (the region above the dashed white line in Figure 6) indicate flame thinning relative to the laminar profile, and $\chi^2/\chi^2_L < 1$ indicates flame broadening. Similar conditional pdfs were examined by Kim and Pitsch at several values of $Y$ for $I_T = 13.8$ and 19.5. Figure 6 shows that the range of $\chi^2$ is greatest in the preheat zone for all $I_T$, with a substantially higher probability of obtaining small values of $\chi^2$ than large values. As $I_T$ increases, however, the range of $\chi^2$ for all $Y$ also increases. For F1, where $I_T$ is small, the most probable value of $\chi^2/\chi^2_L$ is near 1 for all $Y$, while for higher $I_T$ (F3–F5), the most probable value is less than 1 in the preheat zone. Thus, as $I_T$ increases, there is an increasingly high probability of obtaining locally broadened flame regions, particularly in the preheat zone. The probability of obtaining locally broad regions in the reaction zone also increases with $I_T$, although the most probable value of $\chi^2/\chi^2_L$ in this region remains near 1. The smaller variability of $\chi^2/\chi^2_L$ in the reaction zone is consistent with results obtained by Kim and Pitsch and also from the direct reconstruction of the flame profiles in Ref. [1].

In order to understand the variation of $\chi^2$ in Figures 4–6 as a function of $Y$ and $I_T$, it helps to look at the balance of terms for $D\chi^2/Dt$ in Eq. (24). Figure 7 shows the conditionally averaged values of the terms on the right side of Eq. (24). For all values of $I_T$, the chemical reaction term, $\chi_i \partial \delta/\partial x_i$ in Eq. (24), is small in the preheat zone, reaches a maximum near $Y \approx 0.3 – 0.4$, and becomes negative for $Y < 0.1$. As a result, the gradient of the chemical reaction acts to increase $\chi^2$ at nearly all locations in the flame, particularly in the reaction zone. The third term on the right side of Eq. (24), representing the effects of diffusion, is negative almost everywhere and almost exactly balances the reaction gradient term for small $I_T$. The greatest change as $I_T$ varies is in $-\chi_i \chi_j S_{ij}$, which represents the interaction between $\chi_i$ and $S_{ij}$. For small $I_T$, the effect of $S_{ij}$ on $\chi^2$ is small and negative. As $I_T$ increases, however, this term becomes increasingly large and positive, with a maximum near $Y \approx 0.4$. As this term becomes large, the contribution from diffusion also becomes increasingly negative and approximately balances the combined effects of $S_{ij}$ and the reaction gradient.

The decomposition of $D\chi^2/Dt$ (Figure 7) thus confirms the importance of $S_{ij}$ in the balance and evolution of $\chi^2$, and shows how this contribution varies as $I_T$ increases. For small $I_T$, $S_{ij}$ decreases $\chi^2$ and hence contributes to flame broadening, while for large $I_T$, $S_{ij}$ increases $\chi^2$, contributing to flame thinning. It should be noted that the sign of the balance in Figure 7, corresponding at each $Y$ to the conditional average $\frac{1}{T}(D\chi^2/Dt|Y)$, does not necessarily indicate whether the flame is thinned or broadened with respect to the laminar flame. The positive and negative balances shown in Figure 7 would also be present in a laminar

![Figure 4](image-url)  
**Figure 4.** Conditional average of $\chi^2$ in the flame brush based on the local value of $Y$ for F1–F5. The conditional averages are normalized using $\delta_L$.  

![Figure 5](image-url)  
**Figure 5.** Time-averaged flamelet profiles of $Y$ in the turbulent flame brush for simulations F1–F5. The profiles are reconstructed by the method outlined in Ref. [1].
flame, since the laminar profile of $\chi^2$ (Figure 4) follows similar trends as the profiles for the turbulent flames. Figure 7 does give an indication of the role of $S_{ij}$, chemical reactions, and diffusion in flame thinning and broadening. Comparing the turbulent flame width with the laminar profile, however, requires consideration of, for example, Figure 4, which explicitly shows the relative magnitudes of $\chi^2$ at each value of $Y$ for the turbulent and laminar flames.

Finally, the orientation of the scalar gradient, $n$, indicates the degree of flame wrinkling. Figure 8 shows distributions of the angle made by $n$ with the mean direction of the flow, $\theta_e = \cos^{-1}(n_x)$ for $Y = 0.05, 0.5$, and $0.95$, where the distributions at $Y = 0.05$ and $Y = 0.95$ correspond to the left and middle columns of Figure 3. In a one-dimensional laminar flame, this angle is identically zero, which would give a $\delta$-function distribution at $\theta_e = 0$. Figure 8 shows that for all values of $Y$, the most probable orientation of $n$ is near $\theta_e \approx \pi/4$. As $I_T$ increases, however, the probability of obtaining values of $\theta_e$ far from 0 also increases. This indicates that the range of orientations is increased and that there is more flame wrinkling. There is relatively little variation with $Y$ in the qualitative shape of the orientation distributions, although somewhat broader distributions are obtained for $Y = 0.95$ within the preheat zone than for $Y = 0.05$ near the burned gases. This is consistent with reduced flame wrinkling in the reaction zone compared to the preheat zone, as shown in Figure 3.

IV.C. Instantaneous Vorticity and Strain Rate

Figure 9 shows instantaneous isosurfaces of $\omega^2$ and $S^2$ for F1–F5. Both $\omega^2$ and $S^2$ are suppressed within the flame brush for all values of $I_T$, although this suppression becomes weaker as $I_T$ increases. In the unburned and burned gases, the $\omega^2$ field is organized primarily into coherent tube-like vortical structures, and the $S^2$ field is organized into sheet-like structures, both of which are consistent with prior studies of nonreacting turbulence. For the smallest value of $I_T$ shown in Figure 9a, vortical structures in the flame brush appear to have a larger characteristic size than the structures in the unburned or burned regions. The structures also appear to be oriented primarily in the downstream direction.

Figure 6. Conditional distributions of $\chi^2$ normalized by the corresponding laminar value at each $Y$ within the flame brush for (a) F1 – (e) F5.
Figure 7. Balance of the $\chi^2$ transport equation in Eq. (24) within the flame brush based on $Y$ for (a) F1 – (e) F5. Normalization of all quantities is carried out using $\delta_L$.

Figure 8. Orientation of $n$ with respect to $\hat{x}$ for F1–F5, where $\theta_e = \cos^{-1}(n_z)$, for (a) $Y = 0.95$, (b) $Y = 0.5$, and (c) $Y = 0.05$.

IV.D. Statistics of the Vorticity and Strain Rate

Figure 10 shows the variation of $\omega^2$ and $S^2$ as a function of $Y$ for F1–F5. For F2–F5, the magnitudes of both $\omega^2$ and $S^2$ decrease with decreasing $Y$ inside the flame, reaching a minimum near $Y \approx 0.2$. The suppression of these magnitudes relative to the mean value in the unburned mixture is somewhat stronger for $\omega^2$ than $S^2$, and the variation of the magnitudes with $Y$ becomes less pronounced as $I_T$ increases. The magnitudes of $\omega^2$ and $S^2$ are largest for nearly all values of $I_T$ in the preheat zone, with an essentially monotonic decrease as $Y$ decreases. This monotonic decrease is lost for F1, however, where Figure 10b shows that there is a local increase in $S^2$ at $Y \approx 0.4$. There is also a small decrease in $\omega^2$ and $S^2$ for F5 as $Y \rightarrow 1$, although in general the dependence of $\omega^2$ and $S^2$ on $Y$ for this case remains relatively weak. Many of the features in Figure 10 can be explained by considering the effects of heat release on $\omega^2$ and $S^2$. In particular, Eq. (11) indicates that dilatation destroys $\omega^2$, resulting in the decrease in $\omega^2$ within the flame brush. As heat release effects increase in the reaction zone, $S^2$ becomes increasingly dominated by $S_{kk}$, resulting in increased $S^2$ near $Y \approx 0.4$ for F1 in Figure 10.
Figure 9. Isosurfaces of $\omega^2$ (left column) and $S^2$ (right column) for (a) F1 – (e) F5. The isosurfaces are calculated at $0.05\omega_{max}^2$ and $0.05S_{max}^2$, where $\omega_{max}$ and $S_{max}$ are the maximum values of $\omega^2$ and $S^2$ in the instantaneous fields.
Figure 10. Conditional averages of (a) $\omega^2$ and (b) $S^2$ within the flame brush based on the local value of $Y$ for F1–F5. The conditional averages are normalized by the averages of $\omega^2$ and $S^2$ in the unburned mixture (where $Y = 1$), denoted $\langle \cdot \rangle_u$.

Figure 11. Conditional average based on $Y$ of $S_{kk}/S$ within the flame brush, for F1–F5.

This last point can be examined in more detail by considering the ratio of $S_{kk}$ to the strain rate tensor norm $S \equiv [S_{ij}S_{ji}]^{1/2}$ throughout the flame. This ratio reflects the competition between the effects of heat release and the turbulent strain. When $S_{kk}/S$ is large, the effects of heat release will dominate those of the strain; when $S_{kk}/S$ is small the turbulent strain will dominate the effects of heat release. Figure 11 shows that $S_{kk}/S$ decreases as $I_T$ increases, and that the ratio is largest within the reaction zone, where the chemical reaction rate, and hence the effects of heat release, are greatest. As noted in previous studies, the ratio of dilatation effects to turbulent straining increases with $Da$, and the ratio of $S_{kk}/S$ in Figure 11 supports this dependence.

IV.E. Interactions Between the Vorticity, Strain Rate, and Scalar Gradient

The interactions between the vorticity, strain rate, and scalar gradient can be understood by looking at the relative alignments of $\hat{\omega}$, $e_i$ (the eigenvectors of $S_{ij}$), and $n$. Figure 12 shows the conditionally averaged alignment of $\hat{\omega}$ with $e_i$. For F1, where $I_T$ is small, there is increased alignment between $\hat{\omega}$ and $e_1$, and preferential misalignment with $e_3$. The misalignment with $e_3$ is consistent with results in nonreacting flows, but the increased alignment with $e_1$ is in contrast to the weak alignment with this eigenvector observed in nonreacting flows. The increased alignment between $\hat{\omega}$ and $e_1$ has been observed previously in
nonpremixed flames, and the present results indicate that this increase also occurs in premixed flames, particularly for small $I_T$. For all $I_T$, the alignment of $\hat{\omega}$ with $e_1$ is greatest in the reaction zone for $Y \approx 0.4$, although as $I_T$ increases, the dependence on $Y$ becomes increasingly weak. The alignment between $\hat{\omega}$ and $e_i$ for $F4$ and $F5$ is similar to that found in nonreacting turbulence, with the strongest alignment occurring with the intermediate eigenvector $e_2$.

Figure 13 shows that there are substantial variations in the alignment of the scalar-gradient orientation, $n$, with $e_i$ as $I_T$ increases. For the smallest value of $I_T$, $n$ is preferentially aligned with $e_1$ and strongly misaligned with $e_3$, consistent with prior studies, and in contrast to results in nonreacting flows. As with the alignment between $\hat{\omega}$ and $e_i$, the alignment between $n$ and $e_i$ depends strongly on $Y$ for smaller values of $I_T$, with, for instance, the strongest alignment between $n$ and $e_1$ occurring in the reaction zone where $Y \approx 0.4$. As $I_T$ increases, however, the dependence on $Y$ is again weakened, and for $F4$ and $F5$ the alignment between $n$ and $e_1$ is similar to that found in nonreacting flows with passive scalars. That is, for large $I_T$, $n$ is preferentially aligned with $e_3$ and essentially equally misaligned with $e_1$ and $e_2$.

Figure 14 shows joint pdfs of the alignments between $\hat{\omega}$, $n$, and $e_i$ as a function of $Y$ and $I_T$. Such joint pdfs are useful for understanding the distribution of the alignments at each $Y$, as well as the alignment of $\hat{\omega}$ with $n$, which is expected to have a mean value near 0 for all $Y$ and $I_T$. For values of $Y$ near 1, within the preheat zone, Figure 14 shows that $\hat{\omega}$ and $n$ are misaligned for all $I_T$. For $F1$ and $F2$ there is essentially no preferred alignment, or misalignment, between $\hat{\omega}$ and $n$ outside of the preheat zone, and it is only for the two largest values of $I_T$ in $F4$ and $F5$ that $\hat{\omega}$ and $n$ show substantial misalignment in the reaction zone.

---

Figure 12. Conditional averages of alignment between $\hat{\omega}$ and the eigenvectors of $S_{ij}$, denoted $e_i$, within the flame brush for $F1$–$F5$. Conditioning is based on the local value of $Y$, and alignment is shown with (a) $e_1$, (b) $e_2$ and (c) $e_3$, where the corresponding eigenvalues of $S_{ij}$ are ordered $\lambda_1 \geq \lambda_2 \geq \lambda_3$.

Figure 13. Conditional averages of alignment between $n$ and $e_i$ within the flame brush for $F1$–$F5$. Conditioning is based on the local value of $Y$, and alignment is shown with (a) $e_1$, (b) $e_2$ and (c) $e_3$, where the corresponding eigenvalues of $S_{ij}$ are ordered $\lambda_1 \geq \lambda_2 \geq \lambda_3$. 

Figure 14 shows joint pdfs of the alignments between $\hat{\omega}$, $n$, and $e_i$ as a function of $Y$ and $I_T$. Such joint pdfs are useful for understanding the distribution of the alignments at each $Y$, as well as the alignment of $\hat{\omega}$ with $n$, which is expected to have a mean value near 0 for all $Y$ and $I_T$. For values of $Y$ near 1, within the preheat zone, Figure 14 shows that $\hat{\omega}$ and $n$ are misaligned for all $I_T$. For $F1$ and $F2$ there is essentially no preferred alignment, or misalignment, between $\hat{\omega}$ and $n$ outside of the preheat zone, and it is only for the two largest values of $I_T$ in $F4$ and $F5$ that $\hat{\omega}$ and $n$ show substantial misalignment in the reaction zone.
Figure 14. Joint pdfs of the alignment between the vorticity and scalar gradient, $\vec{\omega} \cdot \mathbf{n}$, (left column) and the strain rate eigenvectors and scalar gradient, $|e_i \cdot \mathbf{n}|$, (right three columns). Statistics are calculated only within the flame brush and results are shown for (a) F1 – (e) F5.
Figure 14 thus indicates that the effects of $\omega_i$ on $\chi_i$ are strongest within the preheat zone and for large $I_T$. The joint pdfs of $e_1$ with $n$ in Figure 14 essentially confirm the results in Figure 13. That is, preferential alignment of $n$ with $e_1$ occurs primarily in the reaction zone for small values of $I_T$, while for large $I_T$, $n$ is aligned with $e_3$ for essentially all $Y$, consistent with results for nonreacting, passive scalars.

Figures 12-14 thus indicate that for large $I_T$, the alignments between $\hat{\omega}$, $e_1$, and $n$ are essentially unchanged from the alignments observed in nonreacting flows. Thus, for large $I_T$, the turbulence dynamics are largely independent of the effects of heat release due to the flame. In particular, $\omega_i$ and $S_{ij}$ retain their strong nonlinear, two-way coupling observed in nonreacting turbulence, while $\chi_i$ responds as an essentially passive vector with respect to $\omega_i$ and $S_{ij}$. This results in the observed preferential alignment of $\hat{\omega}$ with $e_2$, the preferential alignment of $n$ with $e_3$, and the misalignment of $n$ and $\hat{\omega}$ for large $I_T$. For small $I_T$, however, Figures 12-14 indicate that there are substantial differences from the nonreacting case. This is, in turn, indicative of modified interactions and coupling between the dynamics of $\omega_i$, $S_{ij}$, and $\chi_i$. Similar modifications for low $I_T$ have been observed previously,$^{2,6}$ and reflect the increasing influence of heat release effects on the dynamics of $\omega_i$, $S_{ij}$, and $\chi_i$.

V. Summary and Conclusions

Stoichiometric hydrogen-air premixed flames subjected to a range of turbulence intensities ($I_T$) have been studied using direct numerical simulations. Particular emphasis has been placed on the effects of $\omega_i$ and $S_{ij}$ on the evolution of $\chi_i$, which is used to describe the local flame structure in the flame brush. The interactions between $\omega_i$, $S_{ij}$, and $\chi_i$ are evaluated by considering the magnitudes $\omega^2$, $S^2$, and $\chi^2$, as well as the relative alignments of $\omega_i$, the eigenvectors of $S_{ij}$, and $\chi_i$. These magnitudes and alignments reflect the underlying physics of the interaction terms in Eqs. (11), (23), and (24), and provide insights into the relative balance of turbulence and heat release effects in premixed flames.

Analysis of $\chi^2$ and the reconstructed flamelet profiles of $Y$ in Figures 4-6 shows that the preheat zone is broadened for all $I_T$, and that this broadening increases with $I_T$. The reaction zone is not broadened for any of the values of $I_T$ considered in the present study, which is consistent with results for the one value of $I_T$ analyzed in Ref. [1]. Figure 6 also shows that the range of $\chi^2$ at each $Y$ relative to the corresponding laminar value, $\chi_{Lj}^2$, is largest in the preheat zone, with a substantially higher probability for $\chi^2/\chi_{Lj}^2 < 1$ than $\chi^2/\chi_{Lj}^2 > 1$. This is consistent with prior studies$^4$ for smaller values of $I_T$. As $I_T$ increases, Figure 7 shows that the effect of $S_{ij}$ on $\chi^2$ becomes increasingly positive, particularly in the reaction zone, which may play a role in maintaining thin reaction zones for the values of $I_T$ considered here. Figures 3 and 8 indicate that wrinkling in both the preheat and reaction zones increases as $I_T$ increases.

Figures 9 and 10 show that $\omega^2$ and $S^2$ are both suppressed near the reaction zone, but that this suppression becomes less pronounced as $I_T$ increases. This suppression can be understood from the effects of heat release, and, in particular, of dilatation on $\omega^2$ and $S^2$. Figure 11 shows that $S_{kl}/S$, which provides an indication of the magnitude of heat release effects relative to the total $S_{ij}$, is largest for small $I_T$, particularly within the reaction zone.

The alignments shown in Figures 12-14 indicate that when $I_T$ is large, the interactions between $\omega_i$, $S_{ij}$, and $\chi_i$ are similar to those found in nonreacting turbulence. In particular, $\omega_i$ and $S_{ij}$ remain nonlinearly coupled, while $\chi_i$ responds as a passive vector with respect to $\omega_i$ and $S_{ij}$. These alignments suggest that the turbulence dynamics are largely unaffected by heat release effects due to the flame when $I_T$ is large. When $I_T$ is small, however, the alignments show substantial differences from those observed in nonreacting turbulence, particularly in the reaction zone. This indicates that when $I_T$ is small, heat release effects play an important role in the dynamics of $\omega_i$ and $S_{ij}$. In such situations, the nonlinear coupling between $\omega_i$ and $S_{ij}$ observed in nonreacting turbulence is altered, and the dynamics of $\chi_i$ become increasingly independent of effects due to $\omega_i$ and $S_{ij}$.

A number of important directions for future research are suggested by the present study. A more detailed comparison of turbulent premixed flame widths with laminar flames requires analysis of a dynamical equation for the difference between the turbulent and laminar flame profiles. Several prior studies have attempted such an analysis$^4,5$ and the present simulations over a broad range of turbulence intensities may provide more detailed indications of the physics responsible for flame thinning and broadening, particularly in the reaction zone. Effects of flame curvature, and in particular cusps, also deserve future investigation, since these effects can play an important role in the flame structure and evolution.$^1,4$ The variations in the kinetic energy spectra throughout the flame are also important in understanding flame broadening, and an approach
that can examine spectra within the highly inhomogeneous flame brush would yield insights into the roles of both large and small scale turbulence on the flame evolution. Finally, the simulations outlined here model premixed flames for stoichiometric hydrogen-air mixtures. Analysis of different types of flames, such as 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 scalar gradient to be studied in situations where the reaction zone may be broadened.

Acknowledgments

This work was supported by the National Research Council Research Associateship Program, the Naval Research Laboratory through the Office of Naval Research, the Air Force Office of Scientific Research, and by the National Science Foundation through TeraGrid resources provided by NCSA and TACC. Additional computing facilities were provided by the Department of Defense High Performance Computing Modernization Program.

References