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Flame thickness and conditional scalar dissipation rate in a premixed temporal turbulent reacting jet

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ABSTRACT

The flame structure corresponding to lean hydrogen–air premixed flames in intense sheared turbulence in the thin reaction zone regime is quantified from flame thickness and conditional scalar dissipation rate statistics, obtained from recent direct numerical simulation data of premixed temporally-evolving turbulent slot jet flames [1]. It is found that, on average, these sheared turbulent flames are thinner than their corresponding planar laminar flames. Extensive analysis is performed to identify the reason for this counter-intuitive thinning effect. The factors controlling the flame thickness are analyzed through two different routes i.e., the kinematic route, and the transport and chemical kinetics route. The kinematic route is examined by comparing the statistics of the normal strain rate due to fluid motion with the statistics of the normal strain rate due to varying flame displacement speed or self-propagation. It is found that while the fluid normal straining is positive and tends to separate iso-scalar surfaces, the dominating normal strain rate due to self-propagation is negative and tends to bring the iso-scalar surfaces closer resulting in overall thinning of the flame. The transport and chemical kinetics route is examined by studying the non-unity Lewis number effect on the premixed flames. The effects from the kinematic route are found to couple with the transport and chemical kinetics route. In addition, the intermittency of the conditional scalar dissipation rate is also examined. It is found to exhibit a unique non-monotonicity of the exponent of the stretched exponential function, conventionally used to describe probability density function tails of such variables. The non-monotonicity is attributed to the detailed chemical structure of hydrogen-air flames in which heat release occurs close to the unburnt reactants at near free-stream temperatures.

1. Introduction

Scalar dissipation rate (SDR) is a central quantity in both non-reacting and reacting turbulent flows involving scalar transport. It denotes the rate at which large scale inhomogeneity of the scalar field is broken down into smaller scales under the straining action of turbulence, and is eventually dissipated by molecular diffusion. Hence, scalar mixing in a turbulent flow is characterized by SDR. In reacting flows, the interpretation of SDR becomes richer. For non-premixed turbulent flames where the fuel and oxidizer must be mixed at the molecular level to sustain reactions, Peters [2] identified SDR as the inverse of the characteristic diffusion time scale. The connections between the mean reaction rate and the scalar dissipation rate have been utilized and derived in [3,4] and [5–7], respectively. Thereafter, the mean scalar dissipation rate of the progress variable [8], the mean dissipation rate of a level set variable [9], or a functional of the scalar dissipation rate spectrum of a level set variable [10] have been shown to be related to the turbulent flame speed. For premixed combustion, one can connect the conditional scalar dissipation rate (CSDR) to the local flame thickness. CSDR is defined as the square of the magnitude of the gradient of a scalar; the flame thickness can be defined proportional to the inverse of the magnitude of the scalar gradient. The flame thickness is the width over which the entirety of the chemical to thermal energy conversion occurs, and thus the distribution of this quantity is of fundamental importance. Flame thickness is

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also an important parameter in the definition of regime diagrams of premixed turbulent combustion.

In a premixed flame, a strong scalar gradient spanning over the flame thickness separates the unburnt cold reactants from the hot burnt products. On interaction with turbulence, the flame shape and local structure may be modified and turbulence may either lead to production of the scalar gradient or its dissipation depending upon the Damköhler number (Da) and the Karlovitz number (Ka) among other parameters. If the scalar is passive without any source to support the gradient, the ultimate state would be a homogeneous mixture at the end of the collective stretching and diffusion processes. But for premixed flames the heat release sustains the gradient and also tends to destroy the local turbulent strain due to dilatation. The dilatation of fluid volume in regions of substantial heat release within the flame can strongly alter the eigenvalues (i.e. principal strains) and the alignment of the eigenvectors of the fluid deformation rate tensor (S_{ij}) with respect to the scalar gradient (or local normal) [11]. This has a profound effect on the scalar gradient production or dissipation. Hence, it is of interest to understand how turbulence and heat release compete to define the scalar gradient, and consequently the flame thickness and SDR. Fundamental understanding of the turbulence–scalar interaction gleaned from the statistics of SDR or CSDR and flame thickness can also aid in turbulent flame modeling [11–13].

It must be recognized that while fluid strain rates are ubiquitous and well understood, additional strain rates exist in the premixed flames due to the change in the flame displacement speed (S_d). For example, in a standard, steady one-dimensional laminar premixed flame S_d monotonically increases from unburnt to burnt region, just like the fluid velocity, due to the density decrease. While the increase in the fluid velocity induces a positive fluid normal strain rate (a_N) trying to separate two iso-scalar surfaces, the increase in the flame displacement speed induces a negative strain rate along the local normal direction and tends to bring the two iso-scalar surfaces closer. These two strain rates balance each other in this planar, laminar, unstretched, premixed flame, resulting in a constant flame thickness. The behavior of these strain rates in a turbulent premixed flame, however, may vary in a more complicated manner. The statistics of these two strain rates in a shear driven turbulent reacting flow with non-unity Lewis number effects and their consequent role in controlling the flame thickness and SDR are extensively studied and discussed in the present study.

One of the hallmarks of passive scalar turbulence is that, similar to the energy dissipation rate, the scalar dissipation rate is also a highly intermittent quantity. Intermittency in the fields is characterized by instantaneous values which may deviate significantly from the corresponding mean values. In the probability density function (pdf) description, the probability of occurrence of such extreme events is higher compared to the measures from the Gaussian distribution. In addition, these extreme values are randomly distributed in time or space. Intermittency of the scalar dissipation rate of passive scalars is a major topic in turbulence research which has received extensive attention over the decades. For reactive scalars, though the importance of intermittency has been recognized [14], it has seldom been addressed in the context of turbulent premixed flames except for its introduction in models [15,16] and recently in [17].

The paper is organized as follows. The next section briefly introduces the datasets obtained from the direct numerical simulation (DNS) of temporally evolving jet. Section-3 defines the slightly modified definition of flame thickness and SDR used in this paper. Section-4 presents the results and discussions on the pdfs of normalized flame thickness and CSDR; the statistics of the strain rates discussed above; the effect of mean shear; the intermittency of the CSDR and its implications along with some few additional important points. The final section concludes with the findings of this study.

Table 1
Simulation parameters reproduced from [1].

Parameter	Case $Da-$	Case $Da+$
$\boldsymbol{Da_{jet}}$	0.13	0.54
$\boldsymbol{H}$ (mm)	2.7	5.4
$\boldsymbol{U}$ (m/s)	312.6	156.3
$\boldsymbol{dx}$ (mm)	18	36
$\boldsymbol{dt}$ (ns)	2.5	5

2. DNS of lean hydrogen–air premixed temporally-evolving slot jet flame

Statistics related to the pdfs of flame thickness and CSDR were obtained from a recent petascale DNS of lean hydrogen-air combustion with detailed chemistry in a temporally evolving slot-jet configuration [1]. In this configuration, two initially planar lean hydrogen-air premixed flames at an equivalence ratio of $\phi = 0.7$ and unburnt temperature of 700 K propagate towards each other, crossing through a plane turbulent jet of unburnt premixed reactants. Spatio-temporal scales down to the mean Kolmogorov length scales and time scales were resolved in the simulation. The H_2–air chemistry was modeled by the detailed chemical reaction mechanism of [18]. DNS of turbulent premixed flames has been performed predominantly in the absence of mean shear with the exception of a few studies [19,20]. Mean shear contributes to turbulence production, which enhances its interaction with the flame. In the absence of mean shear, heat release can dissipate turbulence within the flame, targeting particularly the fine scales. In [19], the spatial resolution was not fine enough to study small-scale interactions quantitatively, and in [20], the DNS was performed with simple chemistry and at low Reynolds numbers. Hence, the coupling between mean strain, turbulent strain, and mixing and reaction is still not well understood.

Two cases are considered with different Damköhler numbers ($Da = \ l_T S_L / u'' \delta^*_{L,Lam}$: where l_T is the integral length scale; S_L the unperturbed planar laminar flame speed; u'' the r.m.s. of fluctuating velocity and $\delta^*_{L,Lam}$ the unperturbed planar laminar flame thickness), henceforth referred to as $Da-$ and $Da+$ for the smaller and larger Damköhler numbers, respectively, while the Reynolds number is held fixed. $Da+$ is greater than unity while $Da-$ is less than unity throughout the simulation as the turbulence–flame interaction develops in time. The turbulent jet Reynolds number is: $Re_{jet} = UH/\nu_0 \sim 10000$; where H is the slot jet height, U the peak mean jet velocity, and ν_0 the kinematic viscosity of the unburned reactants. The turbulence Reynolds number is: $Re_t = u'' l_T / \tilde{\nu} \sim 1000$; here $\tilde{\nu}$ is the Favre averaged kinematic viscosity. The number of grid points across $\delta^*_{L,Lam}$ is 14 for the $Da+$ case, while the $Da-$ case has nearly twice the resolution of the $Da+$ case. Other relevant simulation parameters are given in Table 1. The turbulent kinetic energy spectra exhibit Kolmogorov's $k^{-5/3}$ scaling over a decade of inertial range scales. In the temporal configuration, time-dependent statistics are obtained by averaging in the homogeneous streamwise and spanwise directions. In the present study, statistics are presented mostly at a normalized jet time, $t/t_j = 15$, corresponding to a time in the DNS with significant turbulence–flame interaction. Here the jet time is defined as $t_j = H/U$ at this particular instant in time; the flames at both $Da-$ and $Da+$ conditions are well developed (as can be verified from their near peak turbulent flame speeds, see Fig. 9 in [1]) and they have propagated into the strong shear region of the jet.

The evolution of the turbulence and flame conditions pertaining to the $Da-$ and $Da+$ cases are shown in the turbulent