



Morphology and structure of hydrogen–air turbulent premixed flames

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ABSTRACT

Direct numerical simulations of turbulent premixed planar flames in the corrugated flamelets and thin reaction zones regimes are analysed to investigate the effect of turbulence on the flame structure and morphology. A tool based on topological invariants called shapefinders, consisting of the planarity and filamentarity, is applied to assess the flame morphology. Several statistics show that the filamentarity, which represents lumped effects of the turbulence on the flame morphology, is closely correlated with the Damköhler number, but not with the Karlovitz number. To investigate which scale of turbulent fluctuations is responsible for the flame morphology evolution, the conditional averages of the Kolmogorov length scale and the Taylor microscale are studied. The conditional averages show strong correlation between the Taylor microscale and the filamentarity, while similar strong correlation is not observed for the Kolmogorov length scale. These results suggest that the turbulence–flame interaction relevant to the flame morphology occurs at the length scale greater than the Taylor microscale for relatively large Damköhler number conditions. The fractal dimension is computed for the DNS and filtered reaction progress variable fields with different filter sizes. The computed fractal dimensions between the resolved and the Taylor–microscale filtered fields are almost identical. Also, it was shown that 93–97% of flame surface area is recovered when the filter size of the Taylor microscale is used. However, this fraction rapidly decreases when the integral length scale is used for the filter size. A similar trend was observed for the flame wrinkling factor.

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1. Introduction

The influence of turbulence on the flame inner structure is an important topic for understanding and modelling of turbulent premixed combustion. Detailed studies on this question have been performed based on direct numerical simulations (DNS) [1–8] and highly-resolved laser diagnostics [9–11] for decades. These studies have shown that the flame structure, represented by conditional statistics for example, scatters around corresponding strained or unstrained flamelets. The deviation of these statistics from corresponding flamelets varies depending on the global flame–turbulence conditions such as Damköhler Da and Karlovitz Ka numbers. In particular, Ka identifies conditions at which small-scale turbulent eddies disturb the preheat zone and/or inner layers of reaction zones. For low Ka conditions (i.e. $Ka \lesssim 1$), it is believed that the turbulence modifies neither preheat nor reaction zones, while they disturb the preheat zone under moderate (i.e. $1 < Ka < 100$) Ka conditions. Recently, high- Ka turbulent combustion has been actively studied to further our understanding of turbulence–flame interaction phenomena to the limit of the

distributed reaction zones regime [7,11–15] either by using an intense turbulence or a highly diluted mixture conditions. However, many of key combustion devices are operated in the corrugated flamelets and thin reaction zones regimes as shown in Fig. 1 [16].

Morphology or shape of turbulent premixed flames is another characteristic which needs to be understood, especially for the combustion under the corrugated flamelets and thin reaction zones regimes, which were mentioned above. From a modelling point of view for large eddy simulations (LES) of turbulent premixed combustion, the flame morphology in sub-grid scale (SGS) is of great interest, and the prediction of such features is directly relevant to the accuracy of LES, when the turbulent burning velocity S_T is involved in the modelling framework such as G -equation and flame surface density. For example, the fractal properties, which represent the flame morphology characteristics, are used in modelling turbulent premixed combustion [17] with some limitations [18]. The flame morphology is influenced by many localised turbulent combustion phenomena such as turbulence–flame interaction (stretching and wrinkling of flames through turbulence), thermo-diffusive/hydrodynamic instabilities, flame–flame interaction, and localised flame extinction and reignition. For most practical combustion devices, the turbulence–flame and flame–flame interactions would be the major mechanisms by

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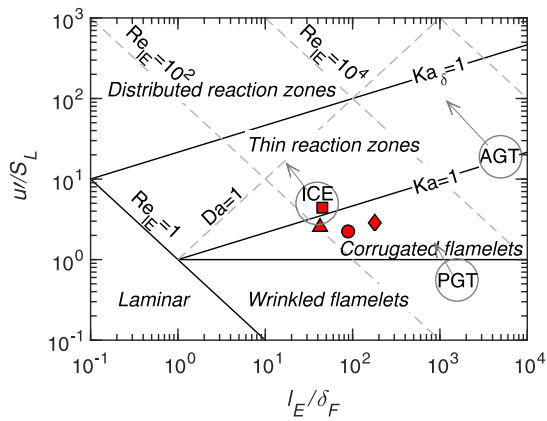


Fig. 1. Regime diagram of turbulent premixed combustion [35]. Circle, triangle and square symbols denote turbulent combustion conditions for R97CR (diamond symbol), R60CR (circle), R37CR (triangle) and R60TH (square), respectively. Typical conditions of three types of practical combustion devices are shown for ICE engine (ICE), power gas-turbine (PGT) and aero gas-turbine (AGT) engines, with the expected direction of general change due to lean-burn technologies suggested in [16].

which the flame morphology fluctuates in time and space. The Damköhler number Da would be a good indicator for degree of the flame convection, since this non-dimensional parameter considers the balance of characteristic time scales between large eddies and flame propagation. Typically, the premixed flame tends to be more convoluted for smaller Da , and the flame surface area per unit volume (or in SGS) increases with increasing turbulence level. The flame–flame interaction event, on the other hand, tends to decrease the flame surface area through the flame mutual annihilation [19–22]. Although it is difficult to predict individual flame–flame interaction events based on a global parameter such as Da , it is reasonable to say that flame–flame interaction events occur more frequently for smaller Da .

In previous studies, these effects of turbulence on the flame morphology have been discussed based on the fractal properties or the flame wrinkling factor [23–28]. The focus has been on the smallest length scale of flame wrinkling and reflecting these information on combustion modelling. For example, it is well known that the inner cut-off scale of turbulent premixed flames is approximately $8–12\eta$ [25,27], where η is the Kolmogorov length scale. Thus, the smallest flame wrinkling scale is usually scaled using the Kolmogorov scale by a factor of ~ 10 . However, it is equally important to understand which smallest scale of the turbulent motion influences these morphological quantities—at which length scale the turbulence–flame interaction relevant to the flame morphology occurs.

In turbulent combustion, turbulent eddies at various scales could influence the flame morphology through turbulent strain and modification of the flame inner structure, thereby creating fluctuations of the local turbulent burning velocity. The dissipative (smallest) motions of turbulence scale with the Kolmogorov length scale with $k_{\max}\eta \approx 1$ (k_{\max} is the maximum wavenumber) [29]. In the present study, the question to ask is, whether these fine scale turbulent motions scaled by the Kolmogorov length scale η (note that they are not equal to η) [30–33] are still responsible for the flame morphology in the corrugated flamelets and thin reaction zones regime combustion? Such small-scale turbulent motion is believed to influence the microscopic flame structure at high Ka combustion mentioned above, but are they still important for the flame morphology? Or is it a turbulent fluctuation relevant to a larger length scale that is important to determine the flame morphology? Doan et al. [34] have made an interesting observation based on turbulent premixed planar flame DNS databases that tur-

bulent eddies smaller than $2\delta_{th}$ (δ_{th} : flame thermal thickness) contribute only less than 10% of total tangential strain rate a_t , suggesting that the majority of the turbulence–flame interaction relevant to the flame morphology occurs at the length scales greater than $2\delta_{th}$. However, the flame tangential strain rate already contains the flame morphology (wrinkling) information through the flame tangential direction vector, and focusing only on a_t may not Fig. 1 fully answer the question of which smallest scale of turbulence is responsible for the flame morphology. Also, normalising a relevant length scale using δ_{th} may not fully reflect turbulence–flame interaction, since different thermochemical conditions produce different flame thickness for similar turbulent velocity fields. Therefore, further investigation needs to be performed for turbulent premixed flames with a single thermochemical condition (same S_L and δ_{th}) parametrised by different turbulent velocity and/or length scales.

The present study investigates the effects of turbulence on both flame morphology and structure to answer the above question, and addresses the link between these two characteristics with some implication for LES of turbulent combustion. Hereafter, the microscale flame structure relevant to scalar dissipation rate, local flame thickness as well as reaction layers, is simply called (flame) structure, and the global flame structure such as flame shape and wrinkling is called (flame) morphology. The analysis is performed by using DNS of hydrogen–air turbulent premixed flames with a detailed kinetic mechanism, and an objective measure to investigate various morphological features called “shapefinders” is applied. The DNS methodology and the shapefinder analysis techniques are discussed in Section 2, which is followed by discussion on general statistics of the DNS results in Section 3.1. Then, the flame morphology and structure, and the effects of turbulence on these characteristics are discussed in Section 3.2. Finally, the results are summarised in the conclusions.

2. Simulation and analysis methods

2.1. Direct numerical simulations

The DNS data used in the present study have been already reported in previous studies [25,36–38], and the methodology is summarised in this section. The governing equations are for conservation of mass, momentum, energy and mass fractions of $N_s - 1$ species, where N_s is the number of species involved in the simulations. These equations are discretised on a uniform mesh using a fourth order central difference scheme in the x (streamwise) direction and the spectral method in y and z (periodic) directions, and are integrated in time using a third order Runge–Kutta scheme. Only the chemical source terms are integrated using a point implicit method to reduce stiffness [39]. The adiabatic combustion of a stoichiometric H_2 –air mixture at 0.1 MPa is simulated using a detailed kinetic mechanism [40] consisting of 27 elementary reactions and 12 species (H_2 , O_2 , H_2O , O , H , OH , HO_2 , H_2O_2 , N_2 , N , NO_2 and NO) including the effect of non-unity Lewis numbers. The temperature dependence of viscosity, thermal conductivity and diffusion coefficients are calculated using CHEMKIN-II packages [41,42], which are modified for vector/parallel computations. The effects of Soret, Dufour, pressure gradient and radiative heat transfer are neglected.

2.2. Configuration and numerical conditions

The DNS has been performed for freely-propagating statistically planar turbulent premixed flames in a cuboid domain, where the inflow and outflow boundaries are specified in x direction and periodic boundaries are specified in y and z directions. The inflowing turbulent velocity field has been obtained in a preliminary DNS of incompressible homogeneous isotropic turbulence

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