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Direct numerical simulation of a high Ka CH_4/air stratified premixed jet flame

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ABSTRACT

Direct numerical simulation (DNS) of a high Karlovitz number (Ka) CH_4/air stratified premixed jet flame was performed and used to provide insights into fundamentals of turbulent stratified premixed flames and their modelling implications. The flame exhibits significant stratification where the central jet has an equivalence ratio of 0.4, which is surrounded by a pilot flame with an equivalence ratio of 0.9. A reduced chemical mechanism for CH_4/air combustion based on GRI-Mech3.0 was used, including 268 elementary reactions and 28 transported species. Over five billion grid points were employed to adequately resolve the turbulence and flame scales. The maximum Ka of the flame in the domain approaches 1400, while the jet Damköhler number (Da_{jet}) is as low as 0.0027. The flame shows early stages of CH_4/air combustion in the near field and later stages in the far field; the separation of combustion stages can be largely attributed to the small jet flow timescale and the low Da_{jet}. The gradient of equivalence ratio in the flame normal direction, $d\phi/dn$, is predominantly negative, and small-scale stratification was found to play an important role in determining the local flame structure. Notably, the flame is thinner, the burning is more intense, and the levels of the radical pools, including OH, O and H, are higher in regions with stronger mixture stratification. The local flame structure is more strained and less curved in these regions. The mean flame structure is considerably influenced by the strong shear, which can be reasonably predicted by unity Lewis number stratified premixed flamelets when the thermochemical conditions of the reactant and product are taken locally from the DNS and the strain rates close to those induced by the mean flow are used in the flamelet calculation. An enhanced secondary reaction zone behind the primary reaction zone was observed in the downstream region, where the temperature is high and the fuel concentration is negligible, consistent with the observed separation of combustion stages. The main reactions involved in the secondary reaction zone, including $CO + OH \Leftrightarrow CO_2 + H$ (R94), $H + O_2 + M \Leftrightarrow HO_2 + M$ (R31), $HO_2 + OH \Leftrightarrow H_2O + O_2$ (R82) and $H_2 + OH \Leftrightarrow H_2O + H$ (R79), are related to accumulated intermediate species including CO, H_2, H, and OH. The detailed mechanism of intermediate species accumulation was explored and its effect on chemical pathways and heat release rate was highlighted.

1. Introduction

In order to improve efficiency and reduce pollutant emission, many combustion applications, including gas turbines, furnaces and lean-burn internal combustion engines, operate in a lean premixed mode [1]. However, lean premixed combustion is difficult to achieve in highly turbulent environment due to operational issues including combustion instability and extinction, and emissions of CO and unburned hydrocarbons. Stratified premixed combustion has been shown to extend the flammability limits and improve the overall-lean combustion stability [2–6]. Better understanding of stratified premixed combustion is therefore desirable to enable improved design of efficient and clean combustion devices.

Earlier studies on stratified premixed combustion focused on laminar flame configurations. Pires da Cruz et al. [7] reported the flame speed of freely propagating laminar CH_4/air stratified premixed flames and showed that the laminar flame speed is strongly affected by the burnt gas temperature and composition. In particular, they found an increased flame speed in situations where the flames are supported by the higher temperature and/or concentration of H_2 in the burnt gas; these flames are denoted as

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back-supported flames. The laminar flame studies of Richardson et al. [8] and Zhou and Hochgreb [9] in counterflowing flame configurations also explored the thermal and chemical effects of the burnt gas on the stratified premixed flame structure and the results are consistent with Pires da Cruz et al. [7].

Recently, an increasing number of experiments have been performed to understand turbulent stratified premixed flames in various configurations, including slot burner flames [10], swirling flames [11,12], V-flames [13–15], spherical flames [16], and counterflowing flames [17]. Both large-scale stratification (mean gradient of mixture stoichiometry) and small-scale stratification (local inhomogeneity) have been found to influence the stratified premixed flame structure. The effects of mixture stratification on local flame speed were investigated in [16], flame curvature in [12,14–16] and flame surface density in [12,14,15]. It was shown that, in general, mixture stratification in back-supported regions increases the local flame speed and the flame surface density, and broadens the curvature distribution. The effects of product stoichiometry in counterflowing flames was explored in [17], and it was concluded that the flame ignitability and stability are improved in lean combustion products due to an excess of oxidising species in the combustion product stream.

Direct numerical simulation (DNS) is a promising approach for studying turbulent combustion, which resolves all of the relevant turbulence and chemical scales both in space and time. It provides access to full three-dimensional, time-varying scalars and velocity that are transported, and represents a unique tool to provide insights into the underlying physics governing turbulent stratified premixed flames. Surprisingly, only few DNS of turbulent stratified premixed flames have been reported so far, and most of them featured simple configurations such as freely propagating flames in isotropic turbulence. Poinsot et al. [18] were among the first to use DNS to study turbulent stratified premixed flames. They concluded that the increase of the total reaction rate is mainly due to the increase of flame surface area (or flame stretch). Two mechanisms were suggested to be responsible for the production of flame stretch. The first mechanism is due to interactions of turbulence and the flame surface, consistent with flame stretch production in turbulent homogeneous premixed flames, and the second one is due to mixture stratification, resulting in differential propagation leading to an increase of flame surface area. It was concluded that in highly turbulent flames, the contribution of the former is dominant. Later, the role of mixture stratification on flame propagation was also explored in [19,20]. Jiménez et al. [21] studied turbulent stratified premixed flames in a 2D isotropic pseudo-turbulence configuration. A secondary reaction zone behind the primary reaction zone was revealed. The modelling of the secondary reaction zone was also discussed in the context of flamelet and conditional moment closure (CMC) models, with the focus on a non-premixed type secondary reaction zone. More recently, DNS of spatially developing stratified premixed jet flames in the thin reaction zones regime was reported by Richardson and Chen [22]. The effects of stratification on flame surface area and burning intensity were examined. It was shown that the burning intensity is enhanced when the product is closer to stoichiometric conditions.

The above-mentioned DNS studies feature low-to-moderate Karlovitz numbers (Ka), which is defined as the ratio of flame characteristic time to Kolmogorov timescale. In many lean combustion applications, high Ka (Ka $>$ 100) is observed due to the strong interactions of small-scale turbulence and flame. A few DNS studies of high Ka homogenous premixed flames have been carried out [23–25], most of which have been limited to the canonical configuration of freely propagating flames in isotropic turbulence. However, no DNS of high Ka premixed jet flames with considerable mixture stratification have been reported before.

There have also been some Reynolds-averaged Navier–Stokes (RANS) and large-eddy simulation (LES) studies of stratified premixed flames in the literature, where flamelet-based tabulation methods were commonly used due to their simplicity and reasonable computational cost [26–29]. In these studies, the flamelet table was mainly generated based on unstrained freely propagating premixed flames at different equivalence ratios [10,26–28], which considers neither the species flux in the mixture-fraction space nor the strain rate effects. While stratified laminar premixed flames have been studied before [8,9], tabulation methods based on stratified premixed flamelets have not been applied to the modelling of turbulent stratified premixed flames so far. In an *a priori* sense, DNS data can be employed to verify the stratified premixed flamelets which consider the variation of mixture stoichiometry and enthalpy across the flame and the effect of strain rate, and provide insights into flamelet modelling of turbulent stratified premixed flames.

In this paper, we perform DNS of a high Ka stratified premixed jet flame. The jet has a small diameter of 1.5 mm and a large bulk velocity of 165 m/s, resulting in a small jet flow timescale τ_{jet}. As a consequence, the jet Damköhler number (i.e. $\mathrm{Da_{jet}} = \tau_{jet}/\tau_L$, where τ_L is the laminar flame timescale) is low ($\mathrm{Da_{jet}} = 0.0027$). Note that at the Reynolds numbers that are currently computationally feasible with DNS, high Ka flames can only be achieved at low $\mathrm{Da_{jet}}$. Although $\mathrm{Da_{jet}}$ can be higher in practical combustors, in the current DNS it is comparable to that reported in several experimental burners [30,31]. In these experiments, streamwise evolution of the flame structure was observed; however, no detailed analysis of chemical pathway evolution was provided [30,31].

Based on the above discussion, the objective of the paper is to improve our understanding of highly turbulent stratified premixed jet flames and their modelling. Using the DNS data, the consequence of the low $\mathrm{Da_{jet}}$ and the spatial evolution of the flame structure are discussed. The influence of mixture stratification on the flame structure is characterised and the statistics conditioned on the local equivalence ratio and its gradient along the flame normal are presented. The turbulent flame and laminar flames are compared and the modelling of turbulent stratified premixed flames using tabulated chemistry is discussed. Species accumulation in the downstream region is shown and its influence on the flame structure evolution is discussed in light of chemical pathway analyses. The paper is organised as follows. Section 2 describes the DNS configuration and numerical methods employed in the present study. The DNS results are presented and discussed in Section 3. Finally, conclusions are made in Section 4.

2. DNS configuration and numerical methods

2.1. DNS configuration

Recently, DNS of a high Ka experimental premixed flame [32–34] was carried out. The jet diameter was $D = 1.5$ mm, the jet bulk velocity, U_b, was 110 m/s, and the jet Reynolds number, Re, based on D and U_b was 10,500. The jet operated at atmospheric pressure and a temperature of 300 K. The case featured weak stratification since the jet equivalence ratio was $\phi_j = 0.7$ while a pilot flame of CH_4/air mixture at $\phi_c = 0.9$ was established surrounding the burner to provide a hot co-flow to assist with flame stabilisation. The pilot temperature, T_c, was 1,800 K and velocity, U_c, was 1.8 m/s. The pilot temperature was lower than its adiabatic one (2,135 K), which was primarily due to heat loss from the flame [33]. The DNS results were compared to experimental measurements [30] with good agreement [32,33]. In the present work, the same configuration is considered, where a schematic is shown in Fig. 1. However, the jet bulk velocity is increased to $U_b = 165$ m/s, and the jet Reynolds number attained is Re = 15,764. The present