Combustion and Flame 166 (2016) 229–242

Contents lists available at ScienceDirect

Combustion and Flame

journal homepage: www.elsevier.com/locate/combustflame

An investigation of turbulent premixed counterflow flames using large-eddy simulations and probability density function methods

Ranjith R. Tirunagari*, Stephen B. Pope

Sibley School of Mechanical and Aerospace Engineering, Cornell University, Ithaca, NY 14853, USA

ARTICLE INFO

Article history:
Received 10 November 2015
Revised 21 January 2016
Accepted 22 January 2016
Available online 11 February 2016

Keywords:
Large-eddy simulation
Probability density function methods
Turbulent premixed counterflow flames
Gas mixing layer interface
Conditional statistics
Direct numerical simulation limit

ABSTRACT

We report results from a coupled large-eddy simulation (LES)/probability density function (PDF) computational study of turbulent premixed flames in the Yale turbulent counterflow flame (TCF) burner. The Yale TCF burner in the premixed mode consists of two coaxial opposed nozzles: one emitting cold, fresh premixed reactants, $CH_4/O_2/N_2$, and the other hot stoichiometric combustion products. This results in a turbulent premixed flame close to the mean stagnation plane. Four critical parameters are identified in the experiments, namely, the bulk strain rate, the turbulent Reynolds number, the equivalence ratio of the reactants mixture and the temperature of the hot combustion products. These are varied independently. In the conditional statistics approach, the instantaneous centerline profiles of OH mass fraction and its gradient are used to identify (i) the interface between the two counterflowing streams referred to as the gas mixing layer interface (GMLI), and (ii) the turbulent flame front using a binary reaction progress variable, c. The conditional mean of the progress variable conditioned on distance Δ from the GMLI, $\langle c \,|\, \Delta \rangle$, and the PDF of the GMLI-to-flame-front distance, Δ_f, are used to quantify the effects of the critical parameters on the interactions of the turbulent premixed flame with the counterflowing hot combustion products, both in the experiments and in the simulations. The LES/PDF simulations are performed in a cylindrical domain between the two nozzle exit planes. A base case simulation involving reference values of the critical parameters is simulated, and the centerline profiles (both unconditional and conditional) of the velocity statistics and the mean progress variable are found to match well with the experimental data. Additionally, the LES/PDF simulations predict the experimentally-observed trends of the effects of the critical parameters on the turbulent premixed flame very well. More importantly, the probability of localized extinction at the GMLI (i.e., $1 - \langle c \,|\, \Delta = 0 \rangle$) and the PDF of the separation distance between the GMLI and flame front, Δ_f, compare well with the experiments for all the flow conditions explored in the parametric study. Three independent key quantities are computed from the LES/PDF simulations of the base case to examine if the simulations can be considered to be in the direct numerical simulation (DNS) limit. They are (i) the ratio of the resolved turbulent diffusivity to the resolved molecular diffusivity, $\widetilde{D}_T/\widetilde{D}$, (ii) the normalized mixing rate, $\Omega_R \tau_L$, and (iii) the normalized grid spacing, h/δ_L. The ratio of $\widetilde{D}_T/\widetilde{D}$ is sufficiently small (≤ 0.02) and the value of $\Omega_R \tau_L$ is sufficiently large (≈ 22) to be considered to be in the DNS limit. However, the ratio of h/δ_L is too large (≈ 0.6) and hence the LES/PDF cannot be considered to be in the DNS limit by this criterion. In spite of the poor spatial resolution, the particle-mesh method yields a flame speed close to the laminar flame speed and this likely explains the success of the present LES/PDF calculations of the TCF premixed flame over the full range of critical parameters.

1. Introduction

The understanding of the complex interactions between turbulence and chemical reactions is of fundamental importance to the design of efficient practical combustion devices. One way of understanding these turbulence–chemistry interactions is through modeling tools. However, for the modeling tools to be reliable and predictive, systematic validation of the underlying computational models with experiments is necessary.

Early experimental studies were performed on the turbulent opposed-jet configuration in isothermal, non-premixed and premixed modes to establish a framework for computational validation [1–4]. Following the initial work, turbulent counterflow flames (TCFs) have been considered as one of the benchmark

* Corresponding author.
E-mail address: rrt38@cornell.edu (R.R. Tirunagari).

http://dx.doi.org/10.1016/j.combustflame.2016.01.024
0010-2180/

configurations to study turbulence–chemistry interactions [5–9]. The TCF configuration has several features, which prove to be advantageous for experimentalists and modelers, such as: the stabilization of the flame and the achievement of high Reynolds number without pilot flames; the realization of a variety of combustion regimes from stable to local extinction/re-ignition; the compactness of the combustion region; and, the practical relevance of the configuration to industrial combustion devices, e.g., internal combustion engines and gas turbines [5]. Many collaborative works involving experimental and numerical investigations of turbulent counterflow flames have been performed (e.g., in Darmstadt, Imperial College and Yale burners) to test models for mixing, turbulence and chemical reactions [10–15]. High-fidelity large-eddy simulation (LES) coupled with mixture-fraction based formulations are commonly used for the computational studies [7,11,12,14].

Probability density function (PDF) methods have been successfully used in combination with the large-eddy simulation technique to treat both turbulent non-premixed [16–18] and premixed flames [19–21]. The computational work presented here aims to study the turbulence–chemistry interactions in the premixed mode of the turbulent counterflow flames (TCFs) using large-eddy simulation/probability density function (LES/PDF) methodology [22–24]. Of particular interest in this work are the turbulent premixed flames experimentally studied in the Yale turbulent counterflow flame (TCF) burner by research groups at Sandia National Laboratories and at Yale University [25]. A series of experiments are conducted on the Yale TCF burner in its premixed mode at different flame conditions, which are obtained by identifying four critical parameters and varying them independent of each other.

The premixed mode of the Yale TCF burner consists of two coaxial nozzles placed at some distance apart, and carrying counterflowing streams of cold, fresh premixed reactants ($CH_4/O_2/N_2$) against hot stoichiometric combustion products. The four critical parameters identified in the experiments are: (i) the bulk strain rate based on the bulk velocity of the fresh premixed reactants stream and the distance between the two nozzles, (ii) the equivalence ratio of the fresh premixed reactants, (iii) the turbulent Reynolds number of the premixed reactants stream, and (iv) the temperature of the hot stoichiometric products stream. It is interesting to note that different turbulent premixed flame behaviors are observed for different operating conditions of the premixed mode [25]. The rich experimental data available for this mode enable us to assess the validity and accuracy of the underlying models used in the LES/PDF computational methodology through detailed comparisons using the analysis of conditional statistics. By studying the effects of the above mentioned critical parameters on the turbulent premixed flame, we aim to elucidate the complex interactions between the flow and the chemistry.

Therefore, the main goal of this computational study is to demonstrate and characterize the performance of LES/PDF methodology for this experimentally-studied turbulent premixed flame that exhibits a variety of combustion regimes which (i) have practical relevance for devices such as gas turbines and combustion engines, and (ii) are known to be challenging to predict.

The remainder of the paper is organized as follows. In Section 2, we describe the experimental configuration of the Yale TCF burner in the premixed mode with base-case values of the critical parameters, followed by a description on the experimental methods employed to vary them. We then explain the procedures followed in the experiments to detect (i) the gas mixing layer interface (GMLI) between the two counterflowing streams, and (ii) the flame region, in which the binary progress variable c has a value of unity. This is followed by a description of the analysis of conditional statistics based on the GMLI. In Section 3, the coupled LES/PDF methodology is described along with a brief description of the velocity inflow boundary conditions. The key parameters used in the LES/PDF

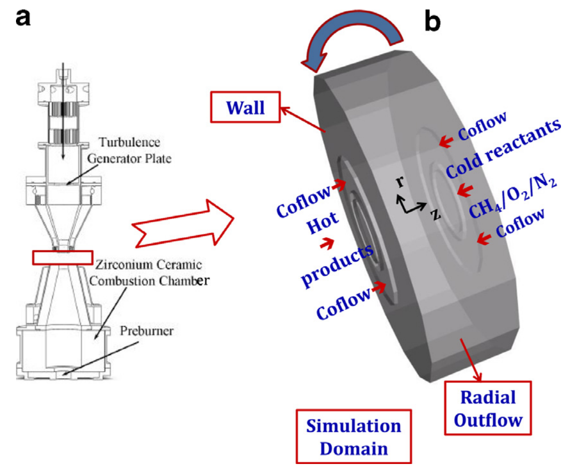

Fig. 1. (a) The experimental configuration of the Yale TCF burner in the premixed mode and (b) the simulation domain used in the LES/PDF simulations. The solution domain is taken as a cylindrical region between the two nozzle exit planes as highlighted by red box in (a). In the subsequent figures, the simulation results in the domain are shown such that the bottom stream (hot products) is on the left-hand side (LHS) and the top stream (cold reactants) is on the right-hand side (RHS). The computational domain aligns with the experimental configuration when it is rotated in the anti-clockwise direction as indicated by the arrow. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

code are also presented. In Section 4, the focus is on the parametric study of the critical parameters through the analysis of conditional statistics. Firstly, the simulation results on the centerline for the velocity and progress variable statistics are compared with the experimental data for the base case and subsequently, the parametric space is explored by quantifying the effects of the four critical parameters on the turbulent premixed flame through (i) the conditional mean of the progress variable conditioned on distance Δ from the GMLI as a function of Δ, $\langle c \,|\, \Delta \rangle$, and (ii) the PDF of the local separation between the GMLI and flame front, Δ_f. In Section 5, we examine the LES/PDF simulations of the base case in more detail by computing three independent key quantities to determine whether the LES/PDF simulations can be considered to be in the direct numerical simulation (DNS) limit. Finally, the conclusions from the study are summarized in Section 6.

2. Yale turbulent counterflow flame (TCF) burner in the premixed mode

2.1. Experimental configuration

The experimental study on the Yale turbulent counterflow flame (TCF) burner in the premixed mode is conducted at Sandia National Laboratories and at Yale University [25]. The influence of strain, reactants equivalence ratio, turbulence level, and mixing with counterflowing hot combustion products on the turbulent premixed flame is systematically investigated. In this sub-section, we describe the experimental configuration for the base-case values of the critical parameters.

Figure 1 (a) shows the experimental configuration of the counterflow burner in the premixed mode in which two coaxial opposed nozzles of diameter d_{jet} = 12.7 mm are placed at a distance d = 16 mm apart. The computational domain used in the LES/PDF simulations is shown in Fig. 1(b). The computational domain has axial inflows and a radial outflow. The two opposed streams are surrounded by coflow streams of pure N_2 at 294 K. The top stream is a highly-turbulent reactants stream of a premixed $CH_4/O_2/N_2$ mixture at a turbulent Reynolds number of Re_t = 1050 with an equivalence ratio of ϕ_u = 0.85 at unburnt temperature T_u = 294 K